Timeless Quantum Mechanics and the Early Universe

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Abstract

We discuss the construction and interpretation of observables in quantum theories with worldline diffeomorphism invariance, in which a preferred or absolute time parameter is absent. These theories are also called time-reparametrization invariant, and they can be seen as mechanical toy models of quantum gravity. The interest in these models stems from the necessity of understanding the so-called problem of time in a theory of quantum gravitation: how can the dynamics of quantum states of matter and geometry be defined in a diffeomorphism-invariant way? What is the relevant space of physical states and which operators act on it? How are the quantum states related to probabilities in the absence of a preferred time? The restriction to the mechanical case allows us to focus on this problem without further issues that accompany field-theoretical treatments.

We first analyze the consequences of diffeomorphism invariance in the classical theory, and we emphasize that it warrants a relational ontology of spacetime. Observers record the evolution of physical fields in generalized reference frames that are defined from the readings of generalized clocks and rods, which are themselves physical fields. As the only physical information that is available in an experiment are the values of the fields and not the spacetime points, one concludes that observables are relational: the outcomes of experiments can be described or predicted by determining the values of the fields relative to (or conditioned on) the values of the generalized clocks and rods (the reference fields that define a generalized reference frame).

The description of the dynamics in terms of relational observables is diffeomorphism invariant, as it does not refer to the underlying abstract spacetime but rather solely to the physical fields. Technically, relational observables can be seen as diffeomorphism-invariant extensions of geometrical objects in analogy to gauge-invariant extensions of noninvariant quantities in the usual gauge (Yang-Mills) theories. We take this analogy seriously and use it as a basis of a method of construction of invariant operators in the quantum theory. These operators act solely in the space of solutions to the quantum constraints (i.e., on the space of physical states) and, as such, they are defined solely in terms of the physical states. Furthermore, we discuss how the notion of a physical propagator may be used to define a unitary evolution in the quantum theory, which is to be understood in terms of a generalized clock, as is the classical theory. We then put forth a set of tentative postulates that dictate how an observer is to make use of probabilities in the description of the quantum dynamics in a quantum generalized reference frame. In this way, we emphasize that the dynamics is relational also in the quantum theory, and we define a notion of relative initial data, which determine the quantum evolution of the relational observables.

We also discuss under which circumstances the above mentioned formalism can be related to the use of conditional probabilities in the quantum theory. These probabilities are defined from the physical states, and we argue that our formalism can be regarded as a generalization of the well-known Page-Wootters approach. On this subject, we show that the quantum averages of relational observables can be related to conditional expectation values of worldline tensor fields. We discuss how our formalism is related to the earlier literature.

We also illustrate the method presented here with conceptually useful examples, such as the free quantum relativistic particle, the Kasner model, and a closed, recollapsing Friedmann-Lamaître-Robertson-Walker model. We construct the quantum relational observables for these models and discuss their quantum evolution. In the context of cosmology, we also mention how the notion of relative initial data may be used to establish a criterion for quantum singularity avoidance, which we refer to as the conditional DeWitt criterion.

In the interest of making contact with observations, we also examine how our formalism can be adapted to calculations of quantum-gravitational effects in the early Universe. To this end, we show that the usual weak-coupling expansion used in the Born-Oppenheimer approach to quantum gravity leads to a perturbative definition of the inner product on the space of physical states, with respect to which the dynamics is unitary. This is important because the issue of unitarity in the Born-Oppenheimer approach has been controversial. Interestingly, we also show how this perturbatively defined physical inner product corresponds to a quantization of the classical Faddeev-Popov determinant associated with the choice of background clock that is used in the weak-coupling expansion. In this way, the usual results of the Born-Oppenheimer approach coincide with a 'choice of gauge', and they can be extended beyond the semiclassical level of the gravitational field. Time is to be understood relationally in the exact quantum theory. We apply these results to the calculation of quantum-gravitational corrections to the primordial power spectra in (quasi-)de Sitter space, comparing the results to the ones previously obtained in the literature, and discussing the physical interpretation of such corrections.

Lastly, we conclude with some remarks about the relevance and usefulness of the approach presented here, as well as its limitations. In particular, we mention how the approach may be useful for the definition and interpretation of observables as diffeomorphism invariants in a full quantum theory of gravitation, and we offer some comments on possible future directions of research.

Zusammenfassung

Wir untersuchen die Konstruktion und Interpretation von Observablen in Quantentheorien mit Weltlinien-Diffeomorphismus-Invarianz, bei der ein bevorzugter oder absoluter Zeitparameter fehlt. Diese Theorien werden auch als invariant unter Zeitreparametrisierung bezeichnet und können als mechanische Spielzeugmodelle der Quantengravitation angesehen werden. Das Interesse an diesen Modellen ergibt sich aus der Notwendigkeit, das sogenannte Problem der Zeit in einer Theorie der Quantengravitation zu verstehen: Wie kann die Dynamik von Quantenzuständen von Materie und Geometrie auf diffeomorphismusinvariante Weise definiert werden? Was ist der relevante Raum physikalischer Zustände und welche Operatoren wirken darauf? Wie hängen die Quantenzustände mit Wahrscheinlichkeiten zusammen, wenn keine bevorzugte Zeit vorliegt? Die Beschränkung auf den mechanischen Fall ermöglicht es uns, uns auf dieses Problem zu konzentrieren, ohne die zusätzlichen Schwierigkeiten einer feldtheoretischen Behandlung.

Wir analysieren zunächst die Konsequenzen der Diffeomorphismusinvarianz in der klassischen Theorie und betonen, dass dadurch eine relationale Ontologie der Raumzeit gerechtfertigt ist. Beobachter zeichnen die Entwicklung physikalischer Felder in generalisierten Referenzrahmen auf, die durch die Messwerte generalisierter Uhren und Stäbe definiert werden, welche selbst physikalische Felder sind. Da die einzigen physikalischen Informationen, die in einem Experiment verfügbar sind, die Werte der Felder und nicht die Raumzeitpunkte sind, kommt man zu dem Schluss, dass Observablen relational sind: Die Ergebnisse von Experimenten können durch die Werte der Felder relativ zu den Werten (oder bedingt durch die Werte) der generalisierten Uhren und Stäbe (die Referenzfelder, die einen generalisierten Referenzrahmen definieren) beschrieben oder vorhergesagt werden.

Die Beschreibung der Dynamik in Bezug auf relationale Observablen ist diffeomorphismusinvariant, da sie sich nicht auf die zugrunde liegende abstrakte Raumzeit bezieht, sondern ausschließlich auf die physikalischen Felder. Technisch gesehen können relationale Observablen als diffeomorphismusinvariante Erweiterungen geometrischer Objekte angesehen werden, in Analogie zu eichinvarianten Erweiterungen von nicht-invarianten Feldern in den üblichen Eichtheorien (Yang-Mills Theorien). Wir nehmen diese Analogie ernst und verwenden sie als Grundlage für eine Methode zur Konstruktion invarianter Operatoren in der Quantentheorie. Diese Operatoren wirken ausschließlich auf den Raum der Lösungen der Quanten-Zwangsbedingungen (d.h. im Raum der physikalischen Zustände) und sind als solche ausschließlich im Bezug auf die physikalischen Zustände definiert. Darüber hinaus diskutieren wir, wie der Begriff eines physikalischen Propagators verwendet werden kann, um eine unitäre Entwicklung in der Quantentheorie zu definieren, die wie die klassische Theorie im Sinne einer generalisierten Uhr zu verstehen ist. Dann stellen wir eine Reihe vorläufiger Postulate auf, die vorschreiben, wie ein Beobachter Wahrscheinlichkeiten bei der Beschreibung der Quantendynamik in einem quantengeneralisierten Referenzrahmen verwenden soll. Auf diese Weise betonen wir, dass die Dynamik auch in der Quantentheorie relational ist, und definieren einen Begriff relativer Anfangsdaten, die die Quantenentwicklung der relationalen Observablen bestimmen.

Wir diskutieren auch, unter welchen Umständen der oben erwähnte Formalismus mit der Verwendung konditionaler Wahrscheinlichkeiten in der Quantentheorie zusammenhängen kann. Diese Wahrscheinlichkeiten werden aus den physikalischen Zuständen definiert, und wir argumentieren, dass unser Formalismus als Verallgemeinerung des bekannten Page-Wootters-Ansatzes angesehen werden kann. Zu diesem Thema zeigen wir, dass die Quantenerwartungswerte relationaler Observablen mit bedingten Erwartungswerten von (Weltlinien-) tensorfeldern in

Beziehung gesetzt werden können. Wir diskutieren, wie unser Formalismus mit der früheren Literatur zusammenhängt.

Wir veranschaulichen die hier vorgestellte Methode auch mit konzeptionell nützlichen Beispielen wie dem freien quantenrelativistischen Teilchen, dem Kasner-Modell und einem geschlossenen, rekollabierenden Friedmann-Lamaître-Robertson-Walker-Modell. Wir konstruieren die quantenrelationalen Observablen für diese Modelle und diskutieren ihre Quantenentwicklung. Im Zusammenhang mit der Kosmologie erwähnen wir auch, wie der Begriff der relativen Anfangsdaten verwendet werden kann, um ein Kriterium für die Vermeidung von Quantensingularitäten festzulegen, das wir als konditionales DeWitt-Kriterium bezeichnen.

Um Kontakt mit Beobachtungen aufzunehmen, untersuchen wir auch, wie unser Formalismus an Berechnungen von Quantengravitationseffekten im frühen Universum angepasst werden kann. Zu diesem Zweck zeigen wir, dass die im Born-Oppenheimer-Ansatz zur Quantengravitation übliche schwache Kopplungsentwicklung zu einer störungstheoretischen Definition des inneren Produkts im Raum physikalischer Zustände führt, für die die Dynamik unitär ist. Dies ist wichtig, da die Frage der unitäre Entwicklung im Born-Oppenheimer-Ansatz kontrovers ist. Interessanterweise zeigen wir auch, wie dieses störungstheoretisch definierte physikalische innere Produkt einer Quantisierung der klassischen Faddeev-Popov-Determinante entspricht, die mit der Wahl der Hintergrunduhr verbunden ist, die für die schwache Kopplungsentwicklung verwendet wird. Auf diese Weise fallen die üblichen Ergebnisse des Born-Oppenheimer-Ansatzes mit einer 'Eichwahl' zusammen, und sie können über das semiklassische Niveau des Gravitationsfeldes hinaus erweitert werden. Die Zeit ist in der exakten Quantentheorie relational zu verstehen. Wir wenden diese Ergebnisse auf die Berechnung von quantengravitativer Korrekturen der Leistungsspektren der kosmischen Hintergrundstrahlung im (quasi) de Sitter-Raum an, und wir vergleichen die Ergebnisse mit der Literatur. Wir diskutieren auch die physikalische Interpretation solcher Korrekturen.

Mit einigen Bemerkungen zur Relevanz und Nützlichkeit des hier vorgestellten Formalismus sowie zu seinen Einschränkungen schließen wir diese Arbeit ab. Insbesondere erwähnen wir, wie der Ansatz für die Definition und Interpretation von Observablen als invariant unter Diffeomorphismen in einer vollständigen Quantentheorie der Gravitation nützlich sein kann, und schlagen Ansätze für zukünftige Untersuchungen in diesem Feld vor.

Erklärung

Hiermit versichere ich an Eides statt, dass ich die vorliegende Dissertation selbstständig und ohne die Benutzung anderer als der angegebenen Hilfsmittel und Literatur angefertigt habe. Alle Stellen, die wörtlich oder sinngemäßaus veröffentlichten und nicht veröffentlichten Werken dem Wortlaut oder dem Sinn nach entnommen wurden, sind als solche kenntlich gemacht. Ich versichere an Eides statt, dass diese Dissertation noch keiner anderen Fakultät oder Universität zur Prüfung vorgelegen hat; dass sie - abgesehen von unten angegebenen Teilpublikationen und eingebundenen Artikeln und Manuskripten - noch nicht veröffentlicht worden ist sowie, dass ich eine Veröffentlichung der Dissertation vor Abschluss der Promotion nicht ohne Genehmigung des Promotionsausschusses vornehmen werde. Die Bestimmungen dieser Ordnung sind mir bekannt. Darüber hinaus erkläre ich hiermit, dass ich die Ordnung zur Sicherung guter wissenschaftlicher Praxis und zum Umgang mit wissenschaftlichem Fehlverhalten der Universität zu Köln gelesen und sie bei der Durchführung der Dissertation zugrundeliegenden Arbeiten und der schriftlich verfassten Dissertation beachtet habe und verpflichte mich hiermit, die dort genannten Vorgaben bei allen wissenschaftlichen Tätigkeiten zu beachten und umzusetzen. Ich versichere, dass die eingereichte elektronische Fassung der eingereichten Druckfassung vollständig entspricht.

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Teilpublikationen

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To my mother
and in memory of my father

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Notation, Conventions and Terminology

- **Mathematical symbols:**

$\emptyset$	denotes the empty set.
$\mathbb{R}$	denotes the set of real numbers.
$\mathbb{C}$	denotes the set of complex numbers.
$\in$	denotes set membership.
$\forall$	denotes universal quantification, i.e., "given any" or "for all".
$=$	denotes equality.
$\simeq$	denotes an approximate equality.
$\propto$	denotes proportionality.
e	denotes Euler's number.
i	denotes the imaginary unit.
$(\cdot)^*$	denotes complex conjugation – the parenthesis may be omitted. For example, given $a, b \in \mathbb{R}$, $(a + \mathrm{i}b)^* = a - \mathrm{i}b$.
$:=$	denotes definition. For example, given $q \in \mathbb{R}$, $f(q) := q^3$ or $q^3 =: f(q)$ defines the function $f : \mathbb{R} \to \mathbb{R}\ ,\ q \mapsto q^3$.
$\circ$	denotes composition of functions, e.g., $f \circ g(q) = f(g(q))$.
$\equiv$	denotes identities, e.g., $f(q) \equiv g(q)$ if $f(q) = g(q)\ \forall\ q$; also denotes equivalence between different notations, see **Conventions** below.
$\approx$	denotes Dirac's weak equalities or on-shell identities, see **Terminology** below.
$\otimes$	denotes a tensor product.
d	denotes an exterior derivative.
C^∞	denotes the class of infinitely differentiable objects (e.g., functions, manifolds).
$\{\cdot, \cdot\}$	denotes a Poisson bracket.
$[\cdot, \cdot]$	denotes a commutator.

- **Conventions:**

— The metric signature for Lorentzian manifolds is $(-,+,\ldots,+)$.
— Summation over repeated indices is implied; e.g., $A^i B_i \equiv \sum_i A^i B_i$.
— Local coordinates q^i on a C^∞-manifold are collectively denoted as q. For example, if $f : \mathbb{R}^d \to \mathbb{R}$, then $f(q) \equiv f(q^1, \ldots, q^d)$.
— The letter $\mathcal{O}$ is used to denote classical and quantum observables, but also signifies the error of an approximation; e.g., $\cos x = 1 - x^2/2 + \mathcal{O}(x^4)$.
— Linear operators that act on a Hilbert space are denoted with a circumflex, e.g., $\hat{\mathcal{O}}$.
— Unless specified otherwise, a dot denotes differentiation with respect to the worldline time coordinate; i.e., $\cdot \equiv \mathrm{d}/\mathrm{d}\tau$.
— The pullback by a diffeomorphism ϕ is denoted by ϕ^* and is not to be confused with complex conjugation.

- **Terminology:**

— Given two phase-space functions $A(q,p)$ and $B(q,p)$, if $\{A, B\} = 0$, we say that: A Poisson-commutes with B; B Poisson-commutes with A; A and B Poisson-commute.
— Given two operators $\hat{A}$ and $\hat{B}$, if $[\hat{A}, \hat{B}] = 0$ we say that: $\hat{A}$ commutes with $\hat{B}$; $\hat{B}$ commutes with $\hat{A}$; $\hat{A}$ and $\hat{B}$ commute.
— Identities that hold on the hypersurface defined by the constraints of a constrained Hamiltonian system are referred to as weak equalities or on-shell identities. For instance, if $C(q,p) = p$ is a constraint on a two-dimensional phase space, then the constraint hypersurface is defined by $p = 0$. In this case, $p \approx 0$, $q + p \approx q$ are examples of on-shell identities.

- **Abbreviations:**

BO	*Born-Oppenheimer*
BRST	*Becchi-Rouet-Stora-Tyutin*
CMB	*Cosmic Microwave Background*
FLRW	*Friedmann-Lamaître-Robertson-Walker*
GR	*General Relativity*
HJ	*Hamilton-Jacobi*
QFT	*Quantum Field Theory*
TDSE	*Time-Dependent Schrödinger Equation*
TISE	*Time-Independent Schrödinger Equation*
WDW	*Wheeler-DeWitt*
WKB	*Wentzel-Kramers-Brillouin*

Contents

Introduction

Caminante, son tus huellas
el camino, y nada más;
caminante, no hay camino:
se hace camino al andar.

— Antonio Machado, *"Proverbios y cantares XXIX"*
in *Campos de Castilla, 1912*

General relativity (GR) and quantum field theory (QFT) are two extremely successful theories that form the basis of our current understanding of the Universe. Completed by Albert Einstein over a hundred years ago, GR has withstood all experimental tests at the time of writing and it remains our best description of spacetime, gravitation and cosmology. Similarly, QFT is the theoretical framework which underlies the standard model of particle physics. Both theories have led to various exciting developments, such as the somewhat recent examples of the discovery of the Higgs boson, the detection of gravitational waves and the first image of a black hole. Nevertheless, both are currently applied and tested in fairly disjoint domains of validity. Whereas GR is well-understood at scales ranging from our Solar System to astrophysics and cosmology, the precise understanding of the gravitational interaction of particles and fields in the quantum realm is still lacking.

How can we describe gravitation at the quantum level? It could be the case that gravity is not a quantum phenomenon and, therefore, that the gravitational interaction of quantum fields must be understood by a different type of theory yet to be fully developed. Moreover, quantum theory itself may need to be modified at scales where the gravitational interaction of fundamental fields becomes important. However, as we currently know of no limitation to the linearity of quantum theory, we shall assume throughout this thesis that the superposition principle holds at all scales and that quantum theory is universal. Within this universal framework, it is reasonable to consider that gravitation is a quantum phenomenon, as all other known interactions admit a quantum-field-theoretical explanation. Thus, we assume that gravity can (and should) be quantized.

What should a quantum (field) theory of gravitation achieve? Or, in other words, what is the question that quantum gravity ought to answer? To paraphrase John

Archibald Wheeler [1], this may be the most difficult question related to quantum gravity. Ideally, quantizing gravitation should resolve or clarify long-standing problems that provide compelling reasons to search for extensions of GR and of the standard model. For example, due to the Hawking-Penrose singularity theorems [2], we know that singularities in GR appear under reasonably general assumptions. The initial Big Bang singularity found in the Friedmann-Lamaître-Robertson-Walker (FLRW) cosmological models and the singularity featured in the Schwarzschild solution are well-known particular examples. Thus, one expects that singularities would be absent in a more fundamental account of gravitation, which could be a quantum theory of GR (or of its classical modifications). Likewise, the standard model of particle physics does not account for gravity, dark matter or dark energy. The presence of a Landau pole in the running of the Higgs self-coupling motivates the search for an ultraviolet completion of the model, which may well be related to the inclusion of quantum gravity.

In this way, there is the expectation that we might improve our understanding of the origin of the Universe, of the evolution of black holes and of the fundamental interactions of quantum fields if we properly understand the singularity-resolving quantum nature of spacetime. Clearly, in order to determine whether these prospects are well grounded, we must first understand the fundamentals of quantum gravity. What is the theory about? What does it describe?

I.1 What is general relativity about?

To find clear answers, it is advisable to first ask the corresponding classical questions. What it GR about? What does it describe? The theory portrays gravitation as geometry and it arguably defines the dynamics of geometry ('geometrodynamics' [3]) and of matter fields in a (partly) relational manner [4]. This assertion is, in fact, a synthesis of several delicate features of GR, most notably the notions of 'background independence', 'general covariance' and 'diffeomorphism invariance'. In order to understand these concepts and what role they might play in the corresponding quantum theory, we first give a conceptual overview of the classical theory.

I.1.1 Background independence and diffeomorphism invariance

We consider a D-dimensional manifold $\mathcal{M}$, which we refer to as the 'abstract' spacetime, and a set of fields Φ defined on $\mathcal{M}$ (which we assume to be tensor fields for simplicity). We then impose a set of laws that determine the histories of physically allowed configurations of the fields, i.e., the trajectories. The laws are expressed as differential equations called the field equations. If certain features of $\mathcal{M}$, collectively denoted as $\mathcal{B}$, are not determined by the physical laws, we consider that they are part of the definition of the theory and that they serve as a background with respect to which the dynamics of fields is described [4,5]. In the absence of singularities or closed time-like curves [6], the background $\mathcal{B}$ in GR includes the dimension D and topology of $\mathcal{M}$, as well as its differential structure and metric signature [4]. The field equations, $\mathcal{F}[\Phi|\mathcal{B}] = 0$, then take the form of relations among the fields Φ given the input of the background structure $\mathcal{B}$ [5].

As the set Φ includes the metric field, one finds that the geometry of the abstract spacetime $\mathcal{M}$ is not fixed by the definition of the theory. Rather, it is a part of the solution of the field equations. For this reason (and despite the fact that certain features of $\mathcal{M}$ are fixed, i.e., $\mathcal{B} \neq \emptyset$), one says that GR is a 'background-independent' theory, as its definition does not rely on a geometry that is given *a priori*. Nevertheless, it must be stressed that background independence is a rather subtle notion, one that has been the source of physical and philosophical debates in the literature [4, 5].

Since one assumes that all dynamical objects Φ are geometric, one may cast the field equations in a form that is also well-defined geometrically and that has well-defined transformation properties (e.g., tensorial) under a general coordinate transformation on $\mathcal{M}$. This form of the equations is called 'generally covariant'. General covariance is simply a consequence of formulating the theory in terms of geometric entities such as tensor fields [7]. However, the field equations of GR satisfy a stronger condition of invariance. Namely, they have the same form (up to variable relabelings) regardless of the choice of coordinate system in the abstract spacetime [8]. This is perhaps most clearly seen if one adopts an 'active' point of view, i.e., if one considers diffeomorphisms instead of (passive) coordinate transformations. In this way, if Φ are solutions to the field equations, $\mathcal{F}[\Phi|\mathcal{B}] = 0$, and $\phi : \mathcal{M} \to \mathcal{M}$ is a diffeomorphism, then its action on tensor fields, $\phi \cdot \Phi$, also leads to solutions to the same field equations, i.e., $\mathcal{F}[\phi \cdot \Phi|\mathcal{B}] = 0$ [5, 8]. Thus, diffeomorphisms are a symmetry of the field equations and one says that GR is a 'diffeomorphism-invariant' theory.

It is important to note that, by using composition as a binary operation, diffeomorphisms form a group, which is denoted by $\mathrm{Diff}(\mathcal{M})$ [5]. The symmetry group of the field equations in GR is, in fact, larger than $\mathrm{Diff}(\mathcal{M})$. This is due to the fact that one may generate solutions to the equations by iterating infinitesimal diffeomorphisms that depend not only on points in $\mathcal{M}$ but also on the fields Φ [9, 10]. We refer to such maps as field-dependent diffeomorphisms. They constitute a local symmetry of the field equations because they generally vary in spacetime and they lead to a transformation of the trajectories that maps solutions of the field equations into solutions. We denote the group of field-dependent diffeomorphisms by $\mathrm{Diff}(\mathcal{M}, \Phi)$.

What is the physical significance of diffeomorphism [or $\mathrm{Diff}(\mathcal{M}, \Phi)$] invariance? This question is related to the meaning of coordinate choices in the abstract spacetime $\mathcal{M}$ and, in fact, to the physical interpretation of $\mathcal{M}$ itself. Let us first briefly discuss the meaning of coordinates in §I.1.2 and the construction of associated quantities known as relational observables in §I.1.3. Subsequently, we analyze the role of diffeomorphism invariance in the interpretation of $\mathcal{M}$ in §I.1.4.

I.1.2 Intrinsic coordinates

One might expect that coordinates could be interpreted as values to be read from a set of measuring instruments ('clocks' and 'rods'), which are used to locate events in a certain region of space and time. If such measuring instruments are themselves part of the dynamical degrees of freedom, the coordinate system determined by their readings is called 'intrinsic' [11]. More precisely, one could attempt to build an intrinsic coordinate system from certain combinations χ of the dynamical fields Φ, i.e., one could seek to unambiguously identify points in $\mathcal{M}$ by the values of some 'reference fields' χ. To achieve this, one would need to construct a coordinate chart $(\mathcal{U}, \chi)$ for an open subset $\mathcal{U} \subset \mathcal{M}$ and choose the reference fields such that χ is a homeomorphism from $\mathcal{U}$ to an open subset of $\mathbb{R}^D$. For consistency, the reference fields should then be invertible spacetime scalars [12], such that the numerical values of the coordinates χ would be independent of any arbitrary initial coordinatization, i.e., χ should be invariant under (passive) coordinate transformations. The χ fields would then play the role of 'generalized clocks and rods' that would define 'generalized reference frames'. We refer to $(\mathcal{U}, \chi)$ as an 'intrinsic chart' on $\mathcal{M}$. Likewise, an 'intrinsic atlas' is a family of intrinsic charts, the domains of which cover the abstract spacetime.

The construction of generalized reference frames would give an operational definition of coordinates, as events would be described in relation to the values of the reference fields. Alas, for generic situations in GR, it is not possible to find D scalar fields χ that are invertible everywhere in $\mathcal{M}$ such that the generalized reference frames could be defined globally [8,13]. This means that: (1) there is no preferred coordinate system in GR; (2) an operational interpretation of coordinates is necessarily an approximate one and, in general, coordinates are mere arbitrary labels (which, nevertheless, may aid in the description of the dynamics).

Moreover, it is, in principle, possible to cast any theory in a diffeomorphism-invariant form [5, 7, 8]. This procedure is sometimes called 'parametrization' [6] and it involves the promotion of a system of coordinate labels to new physical fields, i.e., one includes new degrees of freedom, which then define a preferred intrinsic coordinate system in the diffeomorphism-invariant version of the theory. Likewise, in the inverse procedure of 'deparametrization', a diffeormorphism-invariant theory is redefined in a non-invariant way. This is achieved by choosing an intrinsic coordinate system that is set as an 'absolute' (fixed) standard of space and time.

Due to the possibility of (de)parametrizing a theory, one might question the significance of diffeomorphism invariance in GR. Nevertheless, the above considerations imply that, as there is no preferred coordinate system or generalized reference frame, GR cannot be (globally) deparametrized [13] and, thus, diffeomorphism invariance is a necessary feature. In this way, no global and absolute standard of space and time can be fixed, which is another aspect of background independence. Although we focus on GR, similar conclusions can be reached in modified theories of gravity that classically extend GR and that do not violate background independence nor diffeomorphism invariance.

I.1.3 Relational observables

What is observable in a diffeomorphism-invariant theory? Which measurable quantities can be predicted in GR? One might expect that the tensor fields Φ, understood as solutions to the field equations, are observable quantities because one could measure field strengths in certain experiments. In particular, one could conceivably measure distances and time intervals, which are related to the metric field. Although this expectation is not entirely incorrect, one needs to take into account what are the consequences of the diffeomorphism symmetry of the field equations to the interpretation of its solutions.

There is a is a well-known analogy between diffeomorphism invariance and usual gauge symmetries, one that will also be of importance in the quantum theory. Indeed, as it is a local symmetry, one may treat diffeomorphism invariance analogously to the gauge symmetries of Yang-Mills theories featured in the standard model of particle physics. In fact, purely as a matter of terminology, we refer to local symmetry transformations as 'gauge transformations'. Likewise, a system that is invariant under gauge transformations is called a 'gauge system'. In this broad sense, both Yang-Mills theories and GR are gauge theories.[1]

Due to the fact that the field equations of a gauge theory are not deterministic for all degrees of freedom, it is necessary to construct gauge invariants in order to obtain a deterministic evolution from a given set of initial data (cf. Chapter 1 and Appendix A). In this way, physical observables must be invariant under gauge transformations and, more generally, one may consider equivalence classes of dynamical degrees of freedom under actions of the gauge group. The case of GR is similar and the 'gauge group' is $\text{Diff}(\mathcal{M}, \Phi)$ [9].

That there is some form of indeterminism in the dynamics of GR was already noticed by Einstein in the 'hole argument' [8, 15]. For example, this can be seen if the field equations can be formulated as an initial-value problem. In this case, one notes that Φ and $\phi \cdot \Phi$ may be solutions to the same initial-value problem if ϕ is a nontrivial diffeomorphism that reduces to the identity in a neighborhood of the Cauchy hypersurface on which the initial data are given [8] (see also the discussion in Chapter 1). To obtain a unique solution from a given set of initial data, one can follow the example of usual gauge theories and consider equivalence classes of the solutions Φ under the actions of diffeomorphisms. Thus, one is led to the view that only $\text{Diff}(\mathcal{M}, \Phi)$-invariant quantities are observable.

[1] Nevertheless, there are marked differences between them. A great deal of research is devoted to the construction of a theory of gravity that resembles the usual Yang-Mills type of gauge theories, such as Poincaré gauge theory [14]. We do not discuss this here.

It is worthwhile to mention how the active and passive views of the symmetry of the field equations affect the definition of observables. While tensor fields are invariant under general coordinate transformations (passive view), they are not invariant under general diffeomorphisms (active view).[2] In this way, it would seem that the definition of observables as $\mathrm{Diff}(\mathcal{M}, \Phi)$ invariants precludes the notion of observable tensor fields and that it is more restrictive than simply requiring invariance under general coordinate transformations. Nevertheless, if we consider that one does not measure tensor fields in any experiment, but rather their components, we should inquire whether either the passive or active views classify the general components of tensor fields as observable. The answer is no. As the components of tensor fields depend on a choice of coordinates or local basis, we conclude that they are generally not observable (invariant) in both the passive and active views.[3]

Should we then discard this definition of observables? No. Although seemingly exotic, $\mathrm{Diff}(\mathcal{M}, \Phi)$ invariants include a more familiar notion of observable quantities, which is that of the components of the dynamical fields Φ evaluated in a local intrinsic coordinate system. This partially satisfies the expectation that tensor fields could be observable, but what one discovers is that the components of tensor fields are only observable in a relational sense, i.e., if evaluated with respect to a certain choice of reference fields. This is reasonable because arbitrary coordinate labels do not have, in general, a physical interpretation. Only intrinsic coordinate choices can be given an operational meaning. Indeed, by using physical fields as a generalized reference frame, one intuitively sees that diffeomorphism invariance is guaranteed because one does not introduce into the theory any arbitrary extraneous parameters, and one works solely with the dynamical degrees of freedom. In other words, fields that can be measured in relation to a set of generalized clocks and rods (the reference fields χ) count as observables, at least in principle.

To see how the relational description of Φ relative to χ is captured by diffeomorphism-invariant quantities, we first note that, given an intrinsic chart $(\mathcal{U}, \chi)$, the reference fields χ can be used to identify a point $p \in \mathcal{U}$, which is determined by fixing the coordinate values $\chi = s$. The quantity $s \in \chi(\mathcal{U})$ denotes a fixed collection of numbers (the intrinsic coordinate representation of the point p), which is clearly invariant under diffeomorphisms. More precisely, we can define a collection of constant functions in $\mathcal{M}$, $f_p : \mathcal{M} \to \chi(\mathcal{U}) \subset \mathbb{R}^D$, where $f_p(p') := s$ $(\forall p' \in \mathcal{M})$. The functions f_p are invariant under diffeomorphisms and are defined to be trivial (or tautological) relational observables, which correspond to the values of χ relative to $\chi = s$.[4] Instead of f_p, we shall

[2]For example, vectors in an Euclidean plane are invariant under passive rotations but not under active ones.

[3]The images of scalars (functions on $\mathcal{M}$) and the integrals of top differential forms are, however, invariant in both views, albeit their physical interpretation (e.g., as measurable quantities) may not be immediately clear. In the rest of this section, in Sec. I.1.4 and, in fact, throughout this thesis, we will see that, in some circumstances, these objects may be interpreted as 'relational observables'.

[4]Incidentally, these tautological values can be measured but not predicted. For this reason, they

denote these observables by $\mathcal{O}[\chi|\chi = s] := s$.

More generally, let us schematically denote by $\Phi|_\chi$ the values of the components of Φ relative to the intrinsic coordinates defined by χ and let us assume that, for each fixed value of $\chi = s$, there are $d \geq D$ (not necessarily independent) $\Phi|_{\chi=s}$ quantities. Note that, as χ are included among the dynamical fields Φ, the set of values given by $\Phi|_{\chi=s}$ includes the trivial relational observables s. The quantities $\Phi|_{\chi=s}$ depend only on the dynamics, i.e., they are functions solely of the dynamical fields Φ, and they do not depend on any arbitrary choice of coordinate labels in $\mathcal{M}$. For this reason, $\Phi|_\chi$ may be seen as constant scalars in the abstract spacetime. As before, this is made precise if one defines the functions $\mathcal{O}[\Phi|\chi = s] : \mathcal{M} \to \mathbb{R}^d$, $\mathcal{O}[\Phi|\chi = s](p) := \Phi|_{\chi=s}$ $(\forall p \in \mathcal{M})$.

For each fixed value of s, the constant scalars $\mathcal{O}[\Phi|\chi = s]$ are the relational observables of the theory (of which the trivial observables $\mathcal{O}[\chi|\chi = s]$ are a particular case). They are diffeomorphism invariants that correspond to the values of the components of Φ relative to $\chi = s$. Moreover, the relational observables for different values of s form a D-parameter family of constant scalars, $\mathcal{O}[\Phi|\chi] := \{\mathcal{O}[\Phi|\chi = s], \forall s \in \chi(\mathcal{U})\}$, which may be used to define functions over the image of the reference fields, i.e., $f_{\Phi|\chi} : \chi(\mathcal{U}) \to \mathbb{R}^d, f_{\Phi|\chi}(s) := \Phi|_{\chi=s}$. With no risk of confusion, we will also denote $f_{\Phi|\chi}(s)$ by $\mathcal{O}[\Phi|\chi = s]$, and the interpretation of relational observables as constant scalars in $\mathcal{M}$ or as functions over the image of χ should be clear from context.[5]

As is well-known, this construction of relational observables has its parallel in usual gauge theories. Indeed, if one treats diffeomorphisms as a gauge symmetry, then a local choice of intrinsic coordinate system (a choice of reference fields) is a 'gauge choice'.[6] In this way, the components of the fields Φ are 'gauge-fixed' if evaluated in an intrinsic coordinate system, i.e., in relation to the values of reference fields χ. But, for general gauge theories, gauge-fixed quantities may be seen as a particular type of gauge invariants.[7] The same is true in GR, i.e., the gauge-fixed (relational) observables are $\mathrm{Diff}(\mathcal{M}, \Phi)$ invariants.

If we consider that every measurement involves a comparison between the values of some quantities to be measured Φ and some set of generalized clocks and rods χ, then relational observables $\mathcal{O}[\Phi|\chi]$ provide a representation of the measurement outcomes. An experiment is completely specified by a pair $(\chi = s, \mathcal{O}[\Phi|\chi = s])$ comprised of the values of the chosen generalized clocks and rods and the measurement outcomes.

correspond to quantities that are sometime called 'partial observables' [16]. However, this terminology is more frequently used to simply denote the (noninvariant) fields Φ.

[5]As we will argue that the abstract spacetime is only of an ancillary character, the fact that $\mathcal{O}[\Phi|\chi]$ is a constant on $\mathcal{M}$ is of little relevance and it does not erase the dynamics, which is encoded by the intrinsic time defined by one of the χ fields. This is the reason why relational observables are sometimes called 'evolving constants of motion' [17].

[6]The impossibility to globally deparametrize GR is then analogous to the 'Gribov obstruction' in usual gauge theories (cf. Appendix A).

[7]This holds due to the concept of invariant extensions (cf. Chapter 1 and Appendix A). See, in particular, equation (A.75).

In this way, results of local experiments, if expressed relationally, i.e., solely in terms of the relations between the values of the dynamical fields Φ and the readings of the generalized clocks and rods, are observable (as expected). For this reason, the gauge-theoretical definition of observables as invariants is justified, as it not only satisfies the requirement of a well-posed initial-value problem, but also can, in theory, describe what is observed empirically.

While it is, in principle, possible to construct more general diffeomorphism invariants, the relational observables have a direct physical interpretation. Nevertheless, as intrinsic coordinates cannot be constructed globally in $\mathcal{M}$ in the most general case, one also concludes that the relational description necessarily only captures local aspects of the dynamics (i.e., in the domain of an intrinsic chart or, as we shall see, only in a region of the physical spacetime).

I.1.4 Physical events

As mentioned above, the diffeomorphism invariance of GR may also have implications for the interpretation of the abstract spacetime manifold $\mathcal{M}$. The issue is whether $\mathcal{M}$ is considered to be a relevant physical entity in its own right or if it is only of an auxiliary character, i.e., an ancillary construct used in the description of the dynamics of fields. Similarly to the concept of background independence, this is a delicate and much debated topic [4], and one may adopt a variety of views regarding the ontology of $\mathcal{M}$. We consider $\mathcal{M}$ to be a subsidiary object, a choice that motivates the terminology 'abstract spacetime'. The reason for this is the well-known analogy between diffeomorphism invariance and usual gauge symmetries analyzed in the previous section.

As points are not invariant under general diffeomorphisms, the abstract spacetime $\mathcal{M}$ is not observable (according to the gauge-theoretical definition) and, thus, it does not correspond to the 'physical spacetime' $\mathcal{M}_{\text{phys}}$. This can be understood as follows. If the only observable physical quantities are diffeomorphism invariants and, in particular, the relations among the dynamical fields Φ (e.g., as captured by the relational observables), then the variations and dynamics (evolution) of Φ should be defined solely in terms of the fields themselves and their relations. There is no other physically meaningful object. This means that the field equations, $\mathcal{F}[\Phi|\mathcal{B}] = 0$, and the notion of events should be expressible only in terms of the fields. For instance, this is the description one obtains by using reference fields to define generalized reference frames, as was discussed in the previous sections.

As there is no preferred generalized reference frame, and in order to describe all possible relations among fields and their evolution, one can choose to use an abstract description in which all fields are treated on equal footing, and instead of describing the variations of Φ relative to χ, one describes the variations of all fields with respect to a certain number of arbitrary parameters or labels. The number of labels should be the same as the maximum number of independent reference fields used in a generalized reference frame. The field equations are then written as differential equations in terms of D independent arbitrary parameters, which can be regarded as local coordinates in a manifold. We identify this manifold with the abstract spacetime. Thus, the abstract spacetime $\mathcal{M}$ is only a 'parameter manifold' that facilitates the description of the dynamics [8]. The notion of a point $p \in \mathcal{M}$ is then an abstract one (an "abstract event"). Its purpose (e.g., via its local coordinate representations) is to describe the variations of the fields Φ. In this view, the background structure of GR (such as dimension and differential structure) should be (indirectly) extracted from the relations among the fields or, equivalently, from the field equations, and expressed as properties of $\mathcal{M}$ as an abstraction [8].

One could contest this view by arguing that an operationally meaningful definition of a point is, in fact, obtained with the use of intrinsic coordinates. In other words, one might argue that dynamical reference fields "individuate" the points in $\mathcal{M}$ through their role as homeomorphisms that define intrinsic coordinates. This is true, but is it enough to guarantee that points in $\mathcal{M}$ are physical entities in their own right? Could this be sufficient to grant $\mathcal{M}$ the status of a relevant physical object? In principle, the answer is no. As was argued in the previous section and in the preceding paragraph, the outcomes of measurements can be represented by relational observables, which are physical quantities that obey a well-defined, deterministic evolution and that describe the variations of Φ only with respect to the values of reference fields. The dynamics (and any discernible physical information) is described entirely by the relations among the fields, whereas arbitrary coordinate labels or, in fact, the notion of points in $\mathcal{M}$ are not required as a matter of principle, but can be used for convenience.

Can one then relinquish the abstract spacetime from the theory? The answer is a tentative yes. It is tentative because one must take into account the caveats: (1) in practical applications, it may be complicated to construct the relational observables and to dispense with $\mathcal{M}$; (2) if the notion of 'physical events' is to be expressed only in terms of the relations between the fields Φ and other diffeomorphism invariants, one must devise a way to distinguish physical events solely in terms of the values of fields, without recourse to domains of (intrinsic) charts in $\mathcal{M}$. This might be challenging if the fields assume the same values in several different domains.

In what follows, we will see how one can deal with both caveats (to some extent) by defining physical events and the physical spacetime $\mathcal{M}_{\text{phys}}$, which is the set of all physical events, in a suitable way. We will argue that: (1) the physical spacetime can be identified with a notion of 'physical trajectory' defined from the solutions of the field equations; (2) more generally, the relevant object is the equivalence class $[\mathcal{M}, \Phi]$ obtained from $(\mathcal{M}, \Phi)$ under actions of $\text{Diff}(\mathcal{M}, \Phi)$ [4]; (3) this equivalence class may be interpreted as the pair comprised of the physical spacetime and maps defined on $\mathcal{M}_{\text{phys}}$.

First, we discuss the notion of the physical trajectory. Let $\mathcal{A} := \{(\mathcal{U}_i, \chi_i), i \in \mathcal{I}\}$ be a smooth intrinsic atlas in $\mathcal{M}$. For every chart $(\mathcal{U}_i, \chi_i)$, the reference fields χ_i can be used to identify a point $p \in \mathcal{U}_i$, which is determined by fixing the values $\chi_i = s_i$. As before, we assume that there are $d \geq D$ quantities $\Phi|_{\chi_i = s_i}$ from which the relational observables $\mathcal{O}[\Phi|\chi_i = s_i](p) := \Phi|_{\chi_i = s_i}$ $(\forall p \in \mathcal{M})$ are constructed (cf. Sec. I.1.3). Note that, if Φ are solutions to the field equations $\mathcal{F}[\Phi|\mathcal{B}] = 0$, then $\mathcal{O}[\Phi|\chi_i = s_i]$ $(\forall s_i \in \chi_i(\mathcal{U}_i))$ represent the solutions written in the intrinsic chart $(\mathcal{U}_i, \chi_i)$. Thus, for each fixed value of $\chi_i = s_i$, the relational observables $\mathcal{O}[\Phi|\chi_i = s_i]$ may take different values for different solutions (e.g., due to different choices of initial conditions[8]). Let us assume that the set of all possible values of the observables is an d-dimensional manifold. More precisely, we assume that the possible independent[9] values of $\Phi|_{\chi_i = s_i}$ $(\forall s_i \in \chi_i(\mathcal{U}_i))$ serve as local coordinates in a region of a manifold $\mathcal{Q}$, which we refer to as the 'configuration space of independent scalar combinations of the dynamical fields' or, simply, the 'configuration space'.

We can then represent a solution to the field equations written in the chart $(\mathcal{U}_i, \chi_i)$ as a map $\tilde{\gamma}_i : \chi_i(\mathcal{U}_i) \to \mathcal{Q}$, $\tilde{\gamma}_i(s_i) = \mathcal{O}[\Phi|\chi_i = s_i]$. As $\tilde{\gamma}_i(s_i)$ includes the trivial observables $\mathcal{O}[\chi_i|\chi_i = s_i] = s_i$, we see that $\tilde{\gamma}_i(s_i') \neq \tilde{\gamma}_i(s_i)$ if $s_i' \neq s_i$ and, therefore, $\tilde{\gamma}_i$ is injective. The image of $\tilde{\gamma}_i$ represents a subset of the physical trajectory, i.e., a subset of the configuration space defined by all the values $\Phi|_{\chi_i = s_i}$ that are realized in a solution. If this image is a submanifold in $\mathcal{Q}$, we note that the map $\tilde{\gamma}_i$ corresponds to a parametrized description of this submanifold; i.e., the choice of χ_i as intrinsic coordinates in $\mathcal{M}$ corresponds to a parametrization of a subset of the physical trajectory. As χ_i is invertible on $\mathcal{U}_i$, we may forgo the intrinsic coordinates and consider the composition $\gamma_i := \tilde{\gamma}_i \circ \chi_i : \mathcal{U}_i \to \mathcal{Q}$, which is also injective and maps a region of $\mathcal{M}$ to a region of the configuration space. Let us denote $\mathcal{V}_i := \gamma_i(\mathcal{U}_i) = \tilde{\gamma}_i(\chi_i(\mathcal{U}_i))$. We define the union of images $\mathcal{M}_{\text{phys}} := \cup_i \mathcal{V}_i$ to be the physical trajectory and we assume that it is a smooth embedded submanifold in $\mathcal{Q}$. As γ_i is an injection (and a bijection onto its image), we see that there is a correspondence between the abstract spacetime $\mathcal{M}$ and the physical trajectory $\mathcal{M}_{\text{phys}}$. For this reason, we define the physical trajectory to be the physical spacetime, and one may forgo $\mathcal{M}$.

Physical events are then defined to be the elements (points) of the physical spacetime. As $\mathcal{M}_{\text{phys}}$ is a subset of $\mathcal{Q}$, physical events are also points $q \in \mathcal{Q}$, which can be specified by d-tuples of scalar combinations of the dynamical fields. These d-tuples represent 'coincidences' among the values of scalars and are sometimes referred to as 'point-coincidences' [8]. Is this a reasonable definition of physical events? If we understand a physical event to be an observable occurrence in the Universe, it should correspond to the result of an experiment in the sense defined in the previous sec-

[8] As discussed previously, the indeterminism of the field equations is eliminated by fixing the gauge, which is equivalent to working with a class of Diff$(\mathcal{M}, \Phi)$ invariants.

[9] Note that the values of $\Phi|_{\chi_i = s_i}$ $(\forall s_i \in \chi_i(\mathcal{U}_i))$ need not be independent for a given (fixed) solution. However, we assume that the set of all possible solutions is in one-to-one correspondence with the set of all possible independent values of $\Phi|_{\chi_i = s_i}$ $(\forall s_i \in \chi_i(\mathcal{U}_i))$.

tion, i.e., it should be specified by a complete set of relational observables $\mathcal{O}[\Phi|\chi = s]$ (qua measurement outcomes). As a complete set of $\mathcal{O}[\Phi|\chi = s]$ (including the trivial observables $\mathcal{O}[\chi|\chi = s]$) is by construction a point in $\mathcal{M}_{\text{phys}}$, we conclude that this definition of physical events is indeed sensible because it can, in theory, describe observable occurrences.

This definition obviates any reference to the abstract spacetime as a physical object in its own right. Rather than working with points $p \in \mathcal{M}$ and intrinsic charts $(\mathcal{U}_i, \chi_i)$, one describes the dynamics in terms of physical events $q \in \mathcal{M}_{\text{phys}}$. As we have discussed above, the choice of χ_i as reference fields is equivalent to a choice of parametrization of a subset $\mathcal{V}_i$ of $\mathcal{M}_{\text{phys}}$ via the map $\tilde{\gamma}_i$.

Physical events are, therefore, identified by the concomitant values of certain scalar combinations of the dynamical fields (the reference fields χ_i are equal to s_i and the components of Φ are equal to $\mathcal{O}[\Phi|\chi_i = s_i]$). In other words, "when and where" something occurs is defined by the coincidence of values of the reference fields χ_i, and "what" occurs is given by the components of Φ relative to χ_i. This description clearly distinguishes the set of independent variables (the values s_i) from the set of dependent variables (the relational observables, understood as functions of s_i) on the physical trajectory. Nevertheless, this distinction is not necessary.

The pair $\mathcal{O}[(\chi_i, \Phi)|\chi_i = s_i] := (s_i, \mathcal{O}[\Phi|\chi_i = s_i])$ specifies an experiment according to the above discussion, and it is an intrinsic coordinate representation of $(p, \Phi(p))$, which is a representative of the equivalence class obtained from $(p, \Phi(p))$ under actions of $\text{Diff}(\mathcal{M}, \Phi)$. Thus, the set $\mathcal{O}[(\chi_i, \Phi)|\chi_i(\mathcal{U}_i)] := \{(s_i, \mathcal{O}[\Phi|\chi_i = s_i]), \forall s_i \in \chi_i(\mathcal{U}_i)\}$ encodes the dynamics of the equivalence class of pairs $(\mathcal{U}_i, \Phi|_{\mathcal{U}_i})$ under diffeomorphisms $\phi : \mathcal{U}_i \to \mathcal{U}_i$. Note that the set $\mathcal{O}[(\chi_i, \Phi)|\chi_i(\mathcal{U}_i)]$ is invariant under arbitrary diffeomorphisms $\phi : \mathcal{M} \to \mathcal{M}$ because the relational observables are constant scalars on $\mathcal{M}$.

Moreover, since any pair of intrinsic charts $(\mathcal{U}_i, \chi_i)$ and $(\mathcal{U}_j, \chi_j)$ is smoothly compatible by hypothesis, then the transition map $\chi_i \circ \chi_j^{-1} : \chi_j(\mathcal{U}_i \cap \mathcal{U}_j) \to \chi_i(\mathcal{U}_i \cap \mathcal{U}_j)$ is a diffeomorphism. The map from one set of relational observables to the other may be obtained from the usual transformation properties of the tensor fields Φ under a (passive) change of coordinates on $\mathcal{U}_i \cap \mathcal{U}_j$. Indeed, $\mathcal{O}[\Phi|\chi_i]$ and $\mathcal{O}[\Phi|\chi_j]$ are simply the values of the components of Φ relative to intrinsic coordinate systems defined by χ_i and χ_j, respectively, and the map $\mathcal{O}[\Phi|\chi_i] \mapsto \mathcal{O}[\Phi|\chi_j]$ is a bijection that takes one diffeomorphism invariant to another. For this reason, the sets $\mathcal{O}[(\chi_i, \Phi)|\chi_i(\mathcal{U}_i \cap \mathcal{U}_j)]$ and $\mathcal{O}[(\chi_j, \Phi)|\chi_j(\mathcal{U}_i \cap \mathcal{U}_j)]$ yield equivalent descriptions of the dynamics of the equivalence class of pairs $(\mathcal{U}_i \cap \mathcal{U}_j, \Phi|_{\mathcal{U}_i \cap \mathcal{U}_j})$ under diffeomorphisms $\phi : \mathcal{U}_i \cap \mathcal{U}_j \to \mathcal{U}_i \cap \mathcal{U}_j$. In this way, the dynamics of the equivalence class $[\mathcal{M}, \Phi]$ is captured by relational observables, but there is no preferred set $\mathcal{O}[(\chi_i, \Phi)|\chi_i(\mathcal{U}_i \cap \mathcal{U}_j)]$. This corresponds to the fact that there is no preferred intrinsic coordinate system, which, in turn, corresponds to the freedom to choose different parametrizations of the physical trajectory, as was discussed above.

For this reason, we may regard all the field values in a point-coincidence on equal footing.

Does this notion of physical events avoid the above mentioned caveats? To some extent, the answer is affirmative. Although the construction of relational observables may indeed be complicated, the physical trajectory $\mathcal{M}_{\text{phys}}$, as manifold, is independent of any particular choice of its parametrization or, what is the same, insensitive to the separation of fields into generalized clocks and rods and nontrivial relational observables. The physical spacetime only depends on the point-coincidences; i.e., all the field values considered democratically. Observers, in order to record their experiments, may choose to work with a set of reference fields, but this is, in principle, a matter of convenience and convention. The selection of generalized reference frames simply assists the description of physical events [8]. As any given choice of parametrization of the physical trajectory may be applicable only to certain portions of $\mathcal{M}_{\text{phys}}$, local observers in generalized reference frames can only describe a portion of the physical spacetime.

Thus, one may take the view that it is the set of events, identified by the coincidences and relations among the Φ fields, that constitutes the physical spacetime, which encodes the dynamics of geometry (gravitation) and of matter fields in a diffeomorphism-invariant fashion. This is why GR is a relational theory (but only partly so, as some features of $\mathcal{M}$ are fixed; i.e., some background elements $\mathcal{B}$ are present [4]).

Motivated by the above discussion, and inspired by the words of the poet Antonio Machado, one could allow oneself an ever so momentary license to proclaim:

Wayfarer, only the physical trajectory
is the spacetime, and nothing more;
Wayfarer, there is no spacetime:
spacetime is made by coincidences.

Evidently, this view is not uncontroversial, and fruitful debates about the ontology of spacetime, e.g., regarding the notions of 'relationalism', 'spacetime substantivalism' and 'structuralism', can be found in the literature [18].

It may seem that this discussion regarding the nature and definition of the physical spacetime is not very useful for practical calculations and that it provides only an interpretational framework. This may be the case in the classical theory. However, some authors [4,16] are in favor of a relational description of the physical spacetime because, among other reasons, it seems to provide a suitable interpretation for the observables and dynamics in quantum gravity, one that guides the concrete calculations. This is a view that we share and it will be adopted throughout this thesis.

I.2 What quantum gravity ought to be about?

We may now return to the questions asked previously. What is quantum gravity about? What does it describe? Although the exact answer remains elusive, any candidate theory of quantum gravitation must establish what is the fate of diffeomorphism invariance and background independence at the quantum level. It may be the case that these features emerge semiclassically and that the fundamental quantum structure of spacetime possesses other symmetries or must be described in a different way. Assuming that diffeomorphism invariance and background independence should be central features of quantum gravity is, nonetheless, a conservative and instructive option. In any case, a proper understanding of the (emergence of the) diffeomorphism symmetry and background independence in the quantum theory is needed for the computation of quantum corrections to the classical dynamics of tensor fields interacting with the gravitational field or, more precisely, to the classical dynamics encoded in the physical spacetime $[\mathcal{M}, \Phi]$.

Let us consider the classical pair $(\mathcal{M}, \Phi)$ of an abstract spacetime (parameter manifold) and a set of tensor fields, which includes the metric field in $\mathcal{M}$. The classical dynamics is governed by the action $S[\Phi(x)]$, which is the sum of the Einstein-Hilbert action with the action for matter fields. In analogy to the path-integral quantization of field theories, a first attempt at quantizing gravity would be to define the formal transition amplitude ('propagator') [19]

$$\mathcal{Z} := \int \mathcal{D}\Phi \; \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S[\Phi(x)]} \; . \tag{I.1}$$

Heuristically, and in analogy to the usual gauge theories of the Yang-Mills type [20,21], the diffeomorphism invariance of the classical field equations derived from $S[\Phi(x)]$ seems to imply that one should functionally integrate only over Diff$(\mathcal{M}, \Phi)$ equivalence classes to avoid 'overcounting' possible observable configurations of the fields. However, aside from the obvious technical challenge of defining the functional integral in a rigorous way, the physical interpretation of the amplitude (I.1) is rather obscure. The following questions may be asked: (1) Does the amplitude (I.1) lead to a probability? If so, of which event? (2) If (I.1) is a transition amplitude (propagator) analogous to the usual transition amplitude in quantum mechanics or QFT, what are the *in* and *out* states? (3) With respect to which time variable (if any) are the *in* and *out* states defined? (4) Is the quantum evolution implied by the transition amplitude (propagator) unitary with respect to some time variable? If not, do probabilities make sense in quantum gravity?

In general, due to the absence of a preferred coordinate system in GR and the approximate nature of an operational interpretation of coordinates, there seems to be no global preferred time standard with respect to which the quantum dynamics encoded by the propagator (I.1) could be defined. This is an aspect of the well-known 'problem of time' in quantum gravity [22–24]. This problem stands in stark contrast to usual QFT and quantum theory, where a classical metric field (and, therefore, a time standard) is part of the definition of the theory, i.e., it constitutes a background. Thus, insisting on background independence and diffeomorphism invariance in the quantum theory seems to make the notion of unitary time evolution an approximate one, at best. Consequently, the conservation of probabilities or, in fact, their very definition, would seem to be challenged in quantum gravity [6]. One sees that the problem of time is inevitably intertwined with the measurement problem: not only the origin of probabilities and the Born rule must be explained, but one must now explain how quantum events are defined and with respect to which time variable (if any) the Born rule should be applied.

If $\mathcal{Z}$ could be defined rigorously, it would define the inner product between a pair of diffeomorphism-invariant states, $\mathcal{Z} = (out\,|in\,)$. The invariance under diffeomorphisms implies that $\mathcal{Z}$ cannot depend on any arbitrary choice of coordinates in $\mathcal{M}$ (just as the classical relational observables) and, in particular, it cannot depend on an arbitrary time coordinate. This implies that, if $\hat{H}$ is the quantum generator of time translations, then $(out\,|\hat{H}|in\,) = 0$. This can, in fact, be enforced by the stronger condition $\hat{H}\,|in\,\rangle = 0$, which is an example of a quantum constraint equation (cf. Chapter 2). In the context of quantum gravity, this constraint is called the Wheeler-DeWitt (WDW) equation, which is a stationary Schrödinger equation, and it is another aspect of the problem of time. If one attempts to construct a Hilbert space associated with the inner product $\mathcal{Z} = (out\,|in\,)$, the arduous task of constructing and interpreting quantum diffeomorphism-invariant observables arises. In this way, one could say that quantum gravity is about (overcoming) the problems of time, measurement and observables.

The lack of a global preferred time parameter has led to the view that quantum gravity is a 'timeless' theory and that time, as the orderer of dynamics, and probability should both be approximate or emergent concepts. DeWitt has suggested that both could be phenomenological [25]. That this is a viable option becomes clear in the so-called 'Born-Oppenheimer' (BO) approach to quantum gravity (cf. Chapters 5, 6 and Appendix B), where a 'semiclassical' time variable emerges in the limit where some of the fields Φ, denoted by Φ_{heavy}, exhibit a semiclassical dynamics, which is encoded in appropriate Wentzel-Kramers-Brillouin (WKB) factors in the amplitudes (wave functions). In this particular case, the semiclassical time can be defined as a parameter that: (1) labels the (approximately) classical trajectories of Φ_{heavy}; (2) orders the dynamics of the rest of the fields Φ. In the reasoning of the BO approach, conserved probabilities can only be (approximately) defined if the semiclassical time emerges. In its absence, the theory is generally considered to be strictly timeless and amplitudes (wave functions) are not directly tied to probabilities.

While the BO approach addresses the problem of time, one could argue that it does not offer a complete solution or, if the solution is complete, it is not the only possible one. Indeed, if the origin of the problem is the insistence on background independence and diffeomorphism invariance in the quantum realm, it is reasonable to expect that its solution will make prominent use of these concepts. As we have seen, one encounters a kind of problem of time in the classical theory as a form of indeterminism (related to the hole argument), which is analogous to the indeterminism found in usual gauge theories for quantities that are not gauge invariant. In principle, the solution to this issue is to construct the classical physical spacetime $[\mathcal{M}, \Phi]$, which captures the dynamics in a diffeomorphism-invariant way. As was discussed in §I.1.4, the physical spacetime is the physical trajectory, which encodes all the point-coincidences that occur in a solution to the field equations. However, there are no trajectories in the quantum theory[10]. For this reason, both the abstract and the physical spacetimes would then seem to disappear. The best one can hope for is to define a set of relational Heisenberg-picture operators, which would be the counterparts of the classical relational observables, and would describe the measurements performed by local observers. If this can be done, a notion of quantum relational dynamics becomes available. In particular, the *in* and *out* states should be understood in relational terms. This is the main idea to be pursued in this thesis (cf. Chapter 2). We will see that states used in the BO approach are a particular case of states for which a unitarity, relational time evolution is well-defined.

Although it is not obvious whether the traditional Hilbert space formulation of quantum theory is applicable to a theory constrained by the WDW equation, we will argue that a straightforward analogy between the classical and quantum theories shows that one can define a physical Hilbert space (as opposed to a physical spacetime) on which a notion of quantum relational evolution is available. The ambiguity of unitary evolution may be seen as an aspect of indeterminacy in gauge theories, and is simply related to ambiguity in the choice generalized reference frames with which observers record the evolution of the physical fields.

As there is no external, preferred time parameter, we refer to quantum theories governed by a WDW constraint as 'timeless'. However, this timelessness is not strict (i.e., dynamics is not abolished), but rather a symptom of the underlying relationalism of the theory. A strict timelessness may be overly restrictive. Although our usual experience of time is undeniably linked to a classical spacetime, we believe it is worthwhile to consider what the possible phenomenological consequences of a quantum relational evolution are.

I.3 What is this thesis about?

Efforts to build and understand quantum gravitation have been ongoing for nearly a century. From the early insights of Einstein [28] in the days of old quantum theory to the current sophisticated and elegant approaches [6, 29], we presently have a multitude of theories, each with its distinct advantages and shortcomings. Different approaches

[10] Unless one considers, for example, the de Broglie-Bohm theory [26, 27].

also rest on different sets of assumptions regarding how quantum gravity is to be built and which quantities should be quantized: the metric or some related geometric object; strings; or even some other entity. Nevertheless, the problems of time, measurement and observables seem to cloud the proper implementation and interpretation of all the known approaches.

In this thesis, we set out to present a (provisional) formalism for the construction and interpretation of quantum relational observables and their dynamics. We restrict ourselves to mechanical models in order to avoid the additional field-theoretical difficulties of regularization and the possibility of anomalies. Although these are important issues, we consider that they obscure the essence of the problem of time and diffeomorphism invariance and their interplay with quantum theory. Our interest is not to develop the ultimate, most realistic formalism, but rather to work with a framework which is as simple as possible and yet rich enough to capture the essence of the problem of time and a possible solution based on relationalism. Thus, we study "timeless quantum mechanics" in its own right, as a toy model that captures essential features of gravity (relationalism, diffeomorphism invariance) and quantum mechanics (probabilities, operators, Hilbert space).

I.3.1 Outline of the thesis

In Chapter 1, we discuss the classical theory of mechanics with worldline diffeomorphism symmetry, which is the analogue of the four-dimensional diffeomorphism symmetry in GR. We extensively discuss the implications of this symmetry for the notion of observables and their dynamics. Chapter 2 deals with the quantization of the results of the previous Chapter. Our focus is on proposing a consistent formalism of construction and interpretation of quantum relational observables. We believe that the framework we present is useful to a wide variety of models, and may help us sharpen the appropriate questions that we can ask in quantum gravity. We also compare our results with other proposals in the literature. Chapter 3 deals with the simple example of the free relativistic particle, which clearly illustrates the results of Chapters 1 and 2. In Chapter 4, we apply our formalism to cosmological toy models and discuss how the notion of relational quantum dynamics presented in Chapter 2 can be used to discuss the quantum evolution of model universes and, in particular, to establish a criterion of avoidance of the classical singularity in the quantum theory. Chapters 5 and 6 deal with a weak-coupling expansion that can be used to extract quantum-gravitational corrections to the relational dynamics in the early Universe. The general formalism is established in Chapter 5 and, in particular, we show how the dynamics obtained via the weak-coupling expansion procedure corresponds to the quantization of a classical relational system. Finally, in Chapter 6, we discuss the interpretation and observability of quantum-gravitational effects, which are embedded in a relational formalism, to a simple model of cosmological perturbations over a (quasi-)de Sitter universe.

Chapter 1

Classical Diffeomorphism Invariance on the Worldline

In this Chapter, we present a general framework for the analysis of mechanical systems with worldline diffeomorphism symmetry. The formalism presented here can be seen as a (partly) relational account of classical mechanics, and it is based on a direct application or extension of methods commonly used in constrained Hamiltonian systems or, in particular, in gauge theories, which are reviewed in Appendix A.[1]

1.1 The abstract worldline

As discussed in the **Introduction**, we start with a pair $(\mathcal{M}, \Phi)$ comprised of the abstract spacetime $\mathcal{M}$ and of tensor fields Φ defined on $\mathcal{M}$. The restriction to a mechanical model is obtained by considering that $\mathcal{M}$ is a one-dimensional topological manifold ($D = 0 + 1$), in which case it is referred to as the 'abstract worldline' or simply the 'worldline'. We assume that $\mathcal{M}$ is equipped with a smooth structure (a maximal smooth atlas $\mathcal{A}$). An arbitrary choice of local coordinate on $\mathcal{M}$ is denoted by τ. More precisely, we consider an arbitrary chart $(\mathcal{U} \subset \mathcal{M}, \zeta)$ in $\mathcal{A}$ such that $\zeta : \mathcal{U} \to \zeta(\mathcal{U}) \subset \mathbb{R}$, $\zeta(p) = \tau$, where $\zeta(\mathcal{U}) \subset \mathbb{R}$ is an open interval. The corresponding coordinate basis is given by $\mathrm{d}/\mathrm{d}\tau$. Given two charts $(\mathcal{U}_1, \zeta_1), (\mathcal{U}_2, \zeta_2) \in \mathcal{A}$, the local coordinate representation of a map $F : \mathcal{M} \to \mathcal{M}$ is $F_{\zeta_2\zeta_1} := \zeta_2 \circ F \circ \zeta_1^{-1} : \zeta_1(\mathcal{U}_1 \cap F^{-1}(\mathcal{U}_2)) \to \zeta_2(\mathcal{U}_2)$. If the two coordinate maps are the same, $\zeta_2 = \zeta_1 = \zeta$, we write $F_{\zeta_2\zeta_1} = F_\zeta$. Without risk of confusion, we will identify F with $F_{\zeta_2\zeta_1}$ or we will write "F in the local coordinate τ" instead of F_ζ. Analogously, the local coordinate representation of a function $f : \mathcal{M} \to \mathbb{R}$ in a chart $(\mathcal{U}, \zeta)$ is $f_\zeta := f \circ \zeta^{-1} : \zeta(\mathcal{U}) \to \mathbb{R}$. We will identify f with f_ζ or write "f in the local coordinate τ" instead of f_ζ.

Let $e(\tau)$ be a nonvanishing and continuous worldline scalar density; i.e., one with a constant sign on $\zeta(\mathcal{U})$. Then $\omega_e := e(\tau)\mathrm{d}\tau$ defines an orientation and it can be seen as

[1] Part of this Chapter is based on [30, 31].

a 'volume form' on $\mathcal{M}$. The quantity

$$\eta(\mathcal{U}) := \int_{\mathcal{U}} \omega_e = \int_{\zeta(\mathcal{U})} \mathrm{d}\tau \; e(\tau) \tag{1.1}$$

is the (signed) volume, more commonly referred to as the 'proper time', that corresponds to the region $\mathcal{U} \subset \mathcal{M}$. We may also define the proper time as the antiderivative of $e(\tau)$,

$$\eta := \int \mathrm{d}\tau \; e(\tau) \; , \; \frac{\mathrm{d}\eta}{\mathrm{d}\tau}(\tau) = e(\tau) \; . \tag{1.2}$$

Furthermore, $e(\tau)$ can be used to define a notion of distance on the worldline. For an arbitrary pair of worldline vector fields, $V_{(1,2)} = \epsilon_{(1,2)}(\tau)\mathrm{d}/\mathrm{d}\tau$, one can define the worldline metric as $g(V_{(1)}, V_{(2)}) = e^2(\tau)\epsilon_{(1)}(\tau)\epsilon_{(2)}(\tau)$.[2] For this reason, we refer to $e(\tau)$ as the 'einbein'. The transformation

$$e(\tau) = \tilde{e}(\tau)\Omega(\tau) \; , \tag{1.3}$$

where $\Omega(\tau)$ is a nonvanishing worldline scalar (with constant sign), corresponds to a 'change of einbein frame'.[3]

In principle, a general tensor field on the worldline is defined as $T := T(\tau)\,(\otimes_{i=1}^{\alpha}\mathrm{d}\tau)\otimes\left(\otimes_{i=1}^{\beta}\mathrm{d}/\mathrm{d}\tau\right)$. Under a general coordinate transformation, $\tau \mapsto \tau'$, its component transforms as $T(\tau) \mapsto T'(\tau') = T(\tau)\,(\mathrm{d}\tau/\mathrm{d}\tau')^{\alpha-\beta}$. For arbitrary values of $\alpha - \beta$, this also coincides with the general transformation of an arbitrary tensor density in the worldline. Without loss of generality, we may use the einbein to write the tensor component in terms of a worldline scalar $f(\tau)$,

$$T(\tau) := f(\tau)\,(e(\tau))^{\alpha-\beta} \; , \tag{1.4}$$

because $e(\tau)$ is nonvanishing.

1.2 Dynamics and gauge symmetry

A concrete choice of the fields Φ and of the dynamics defines the ontology of the $(0+1)$-dimensional universe modeled by $(\mathcal{M}, \Phi)$. For simplicity, let us consider a family of d scalars denoted by $q^i(\tau)$ $(i = 1, \ldots, d)$, the dynamics of which is obtained by imposing

[2] This is to be compared to the vielbein formula $g_{\mu\nu} = e^a_\mu e^b_\nu \eta_{ab}$ for a general (pseudo-)Riemannian manifold.

[3] This is the counterpart of the transformation $e^a_\mu = \Omega^a_b \tilde{e}^b_\mu$, $g_{\mu\nu} = \tilde{e}^a_\mu \tilde{e}^b_\nu \tilde{\eta}_{ab}$.

a set of field equations that may be derived by extremizing the action functional

$$S := \int_{\mathcal{U}} \omega_{\mathcal{L}} = \int_a^b \mathrm{d}\tau \ \mathcal{L} \ , \tag{1.5}$$

where we have defined the interval $\zeta(\mathcal{U}) := (a, b) \subset \mathbb{R}$. We have also defined $\omega_{\mathcal{L}} := \mathcal{L}\mathrm{d}\tau$; i.e., the Lagrangian is a worldline scalar density. How can we construct $\mathcal{L}$? First, we make the simplifying assumption that the dynamics of the scalar fields is described by differential equations which are, at most, of second order in τ. In this way, we consider that $\mathcal{L}$ depends on $q(\tau)$ and, at most, on $\dot{q}(\tau)$, where $\cdot \equiv \mathrm{d}/\mathrm{d}\tau$. Second, we define a reparametrization to be a change of worldline coordinate, $\tau \mapsto \tau'(\tau)$. A field-dependent reparametrization is one in which τ' has a functional dependence on a solution to the field equations. This means that it depends on τ and on the boundary conditions, and we adopt the condensed notation

$$\tau \mapsto \tau'(\tau) \equiv \tau'(\tau; q(\tau), \dot{q}(\tau)) \equiv f(\tau; q(a), q(b)) \ , \tag{1.6}$$

where f is an arbitrary function. We will often omit the field dependence and simply write $\tau \mapsto \tau'(\tau)$. We note that (possibly field-dependent) reparametrizations constitute a symmetry if the functional form of the action (1.5) remains the same (up to a boundary term) under the transformations (1.6) [see also (A.6)]. This means that these transformations amount to relabeling the arguments of the Lagrangian, whereas the structure of the action remains the same. What can be said of the functional form of $\mathcal{L}$ in this case?

If $\mathcal{L} \equiv \mathcal{L}(q, \dot{q}; \tau)$ has an explicit time dependence, a reparametrization (1.6) would not only correspond to a relabeling of the arguments of the Lagrangian, but also to a change in the structure of the action, as the explicit dependence on τ would generally acquire a different functional form, $\tau \mapsto \tau'(\tau)$.[4] For this reason, in order to guarantee the form invariance of the action, we discard the possibility of an explicit dependence on τ in the Lagrangian; i.e., $\mathcal{L} \equiv \mathcal{L}(q, \dot{q})$. Furthermore, we note that a scalar-density potential term, which only depends on $q(\tau)$, cannot be constructed solely from worldline scalars.[5] All terms in $\mathcal{L}$ must then depend on the velocities, such that the Lagrangian $\mathcal{L}$ must be a 'generalized kinetic term', which we denote by $\mathcal{L} \equiv \mathcal{K}(q, \dot{q})$. The requirement

[4] For example, the worldline scalar density $\mathcal{K}(\dot{q}; \tau) = \tau\dot{q}$, which is the identity function times a velocity, is mapped to $(\tau' + 1)\mathrm{d}q'/\mathrm{d}\tau' =: \mathcal{K}'(\mathrm{d}q'/\mathrm{d}\tau'; \tau')$ [with $q'(\tau') = q(\tau(\tau'))$] under the reparametrization $\tau'(\tau) = \tau - 1$. In this way, the form of the coefficient of the velocity is changed and the transformation does not amount to a relabeling of τ by τ' and of $q(\tau)$ by $q'(\tau')$.

[5] Evidently, one can define the worldline one-form $V(q(\tau))\mathrm{d}\tau$. However, if this one-form is used to define a scalar-density potential term, then the functional form of the action (1.5) will not be invariant under (1.6) because the potential term acquires a Jacobian factor $\mathrm{d}\tau/\mathrm{d}\tau'$ under reparametrizations, which alters the structure of (1.5). In this way, reparametrizations would not correspond to a mere relabeling of the physical fields. See also the discussion after (1.9).

of form invariance of the action then implies that $\mathcal{K}$ must satisfy

$$\mathcal{K}\left(q'(\tau'),\frac{\mathrm{d}q'}{\mathrm{d}\tau'}(\tau')\right)=\mathcal{K}\left(q(\tau),\frac{\mathrm{d}\tau}{\mathrm{d}\tau'}\frac{\mathrm{d}q}{\mathrm{d}\tau}(\tau)\right)=\frac{\mathrm{d}\tau}{\mathrm{d}\tau'}\mathcal{K}\left(q(\tau),\frac{\mathrm{d}q}{\mathrm{d}\tau}(\tau)\right) \tag{1.7}$$

under the reparametrization (1.6). This corresponds to the conditions that: (1) $\mathcal{K}$ is a homogeneous function of the velocities; (2) the scalar-density character of $\mathcal{K}$ is derived solely from its field constituents and not from an ad hoc definition (such as in footnote 5). For every fixed value of τ, we find from (1.7) the relation

$$\mathcal{K}(q(\tau),\dot{q}(\tau))=\frac{\partial\mathcal{K}}{\partial\dot{q}^i}\dot{q}^i(\tau)\ , \tag{1.8}$$

where $i=1,\ldots,d$ and a summation over repeated indices is implied. From (1.8), we also conclude that the quantities $\partial\mathcal{K}/\partial\dot{q}^i$ are worldline scalars.[6] Due to (1.7), it is straightfoward to verify that the functional form of the action (1.5) is indeed invariant under the reparametrizations (1.6), without an additional boundary term, if $\tau'(a)=a,\tau'(b)=b$. One then says that the action is invariant under (possibly field-dependent) time reparametrizations that preserve the endpoints.

To construct a potential term $\mathcal{V}$ for the scalars, we allow the introduction of the einbein as an extra degree of freedom, such that

$$\mathcal{V}(q(\tau);e(\tau)):=e(\tau)V(q(\tau))\ , \tag{1.9}$$

where $V(q(\tau))$ is a scalar. In this way, we may define $\mathcal{L}:=\mathcal{K}-\mathcal{V}$. Note that the functional form of the action (1.5) is only invariant under reparametrizations (1.6) [with $\tau'(a)=a,\tau'(b)=b$] if $e(\tau)$ is considered as a dynamical variable (with its own field equation). Otherwise, if $e(\tau)$ is taken as a 'background' element (an entity that is not subject to dynamical law), the functional form of (1.5) may change under reparametrizations, as the transformations would amount not only to relabeling the arguments of the Lagrangian [in this case, $q(\tau)$ and $\dot{q}(\tau)$], but also to changing its structure [e.g., the form of the background pre-factor of $V(q(\tau))$; see also footnote 5]. Thus, although $e(\tau)$ serves as an auxiliary quantity in the description of the dynamics of the scalars, it must be considered as an additional physical field. Then, our choice of fields is $\Phi(\zeta^{-1}(\tau))=(q(\tau),\omega_e=e(\tau)\mathrm{d}\tau)$.

More generally, we can also allow a dependence on $e(\tau)$ in the kinetic term[7] and

[6] In addition to $q(\tau)$, the functions $\partial\mathcal{K}/\partial\dot{q}^i$ may depend on scalar combinations of the velocities, such as $\dot{q}^i/\dot{q}^j$ or $\dot{q}^i\dot{q}^j/(\dot{q}^k)^2$ $(i,j,k=1,\ldots,d)$.

[7] Note that, if the only dependence of the Lagrangian on $e(\tau)$ is in the potential term, the field equation for the einbein is the constraint $V(q(\tau))=0$. If the kinetic term also depends on $e(\tau)$, the

in the reparametrizations (1.6), $\tau'(\tau) \equiv \tau'(\tau; q(\tau), \dot{q}(\tau); e(\tau))$. Then, the Lagrangian could have a general functional form $\mathcal{L} \equiv \mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau))$. Similarly to (1.8), we find

$$\mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau)) = \frac{\partial \mathcal{L}}{\partial \dot{q}^i} \dot{q}^i(\tau) + \frac{\partial \mathcal{L}}{\partial e} e(\tau) \tag{1.10}$$

as a consequence of the requirement of form invariance. Thus, $\mathcal{L}$ it is a homogeneous function of $\dot{q}(\tau)$ and $e(\tau)$. From (1.10), the quantities $\partial\mathcal{L}/\partial\dot{q}^i$ and $\partial\mathcal{L}/\partial e$ are are seen to be scalars.[8] Although one might attempt to include other types of fields or different kinds of dynamics [such as higher derivatives of $q(\tau)$ or, perhaps, of $e(\tau)$], this will not be done here, and (1.10) will be sufficient for our purposes [see discussion preceding (1.19)].

As already mentioned, the action (1.5) with Lagrangian (1.10) and with $e(\tau)$ as a physical field is invariant under the (passive) reparametrizations (1.6) with $\tau'(a) = a$ and $\tau'(b) = b$. The action is also invariant under (active) worldline diffeomorphisms that preserve $\mathcal{U}$. As before, this is a consequence of the fact that the scalar-density character of $\mathcal{L}$ is derived solely from its field constituents. Indeed, let $\phi : \mathcal{M} \to \mathcal{M}$ be a diffeomorphism, then the action (1.5) can be rewritten as

$$S = \int_{\mathcal{U}} \omega_{\mathcal{L}} = \int_{\phi^{-1}(\mathcal{U})} \phi^* \omega_{\mathcal{L}} \ , \tag{1.11}$$

where ϕ^* is the pullback by ϕ. Moreover, in the local coordinate τ, we obtain

$$\mathcal{L}(\phi^* q(\tau), \phi^* \dot{q}(\tau); \phi^* e(\tau)) = \phi^* \mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau)) \ , \tag{1.12}$$

in a similar fashion to (1.7). Thus, if $\phi(\mathcal{U}) = \mathcal{U}$, then (1.11) leads to

$$S = \int_a^b \mathrm{d}\tau \ \mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau)) = \int_a^b \mathrm{d}\tau \ \mathcal{L}(\phi^* q(\tau), \phi^* \dot{q}(\tau); \phi^* e(\tau)) \ ; \tag{1.13}$$

i.e., the functional form of the action is invariant under ϕ, and the diffeomorphism amounts to a relabeling of the arguments of the Lagrangian. Thus, the field-dependent (passive) reparametrizations and (active) diffeomorphisms constitute the gauge (local symmetry) transformations of the theory [9,10], which can then be seen as a toy model of GR [32,33].

Let $\mathcal{S}(\tau) := (q(\tau), e(\tau))$ be a solution to the field equations derived from (1.5). Then,

constraint will involve the velocities and, in the canonical theory, the momenta (cf. §1.3.1).

[8] As in the case of $\mathcal{K}$, the functions $\partial\mathcal{L}/\partial\dot{q}^i$ and $\partial\mathcal{L}/\partial e$ may depend on scalar combinations of the velocities and the einbein, such as $\dot{q}^i/e$ or $\dot{q}^i\dot{q}^j/(\dot{q}^k e)$ $(i, j, k = 1, \ldots, d)$.

due to (1.13), we note that $\mathcal{S}'(\tau) = \phi^*\mathcal{S}(\tau) = (\phi^* q(\tau), \phi^* e(\tau))$ is another solution. We refer to the equivalence classes of solutions under diffeomorphisms as 'gauge orbits'. In this way, we denote the gauge orbit of $\mathcal{S}(\tau)$ as $[\mathcal{S}(\tau)]$, and any solution on $[\mathcal{S}(\tau)]$ can be written as $\mathcal{S}'(\tau) = \phi^*\mathcal{S}(\tau)$ for $\phi \in \mathrm{Diff}(\mathcal{M}, \Phi)$. We can regard $\mathcal{S}(\tau)$ as a choice of 'origin' in the gauge orbit. Clearly, this choice is arbitrary, since $\mathcal{S}(\tau) = \phi_0^*\mathcal{S}_0(\tau)$ implies that $\mathcal{S}'(\tau) = \phi^*\mathcal{S}(\tau) = (\phi_0 \circ \phi)^*\mathcal{S}_0(\tau) =: \phi_0'^*\mathcal{S}_0(\tau)$. We assume that it suffices to consider diffeomorphisms that are connected with the identity, which amounts to the hypothesis that gauge orbits have a trivial topology. In this way, it is useful to consider the one-parameter family of diffeomorphisms $\phi_l : \mathcal{M} \to \mathcal{M}$ generated by a vector field $V = v(\tau)\mathrm{d}/\mathrm{d}\tau$, where $v(\tau) \equiv \tilde{v}(\tau; q(\tau), \dot{q}(\tau), e(\tau))$. In the local coordinate τ, we have $\phi_l(\tau) = \tau(l)$, where $\tau(l)$ is an integral curve of V; i.e., it is a solution to $\mathrm{d}\tau(l)/\mathrm{d}l = v(\tau(l))$ with $\tau(0) = \tau$, and thus ϕ_0 is the identity. The transformed scalars and scalar densities are, respectively, given by

$$\begin{aligned} q_l'^i(\tau) &:= \phi_l^* q^i(\tau) = q^i(\tau(l)) \ , \\ \omega_l'(\tau) &:= \phi_l^*\omega(\tau) = \frac{\mathrm{d}\tau(l)}{\mathrm{d}\tau}\omega(\tau(l)) \ , \end{aligned} \tag{1.14}$$

and, in particular, the transformed Lagrangian reads [cf. (1.12)]

$$\mathcal{L}(q_l'(\tau), \dot{q}_l'(\tau); e'(\tau)) = \frac{\mathrm{d}\tau(l)}{\mathrm{d}\tau}\mathcal{L}(q(\tau(l)), \dot{q}(\tau(l)); e(\tau(l))) \ . \tag{1.15}$$

Infinitesimal displacements along the integral curves of V can be seen as local time translations,

$$\tau' := \tau(\delta l) = \tau + v(\tau)\delta l =: \tau + \epsilon(\tau) \ , \tag{1.16}$$

and the infinitesimal change of worldline scalars and scalar densities is found from (1.14) to be

$$\begin{aligned} \delta_{\epsilon(\tau)} q(\tau) &:= \delta l \pounds_V q(\tau) = \epsilon(\tau)\frac{\mathrm{d}q(\tau)}{\mathrm{d}\tau} \ , \\ \delta_{\epsilon(\tau)}\omega(\tau) &:= \delta l \pounds_V \omega(\tau) = \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\epsilon(\tau)\omega(\tau)\right) \ , \end{aligned} \tag{1.17}$$

where $\pounds_V$ is the Lie derivative along V.[9] In particular, the change in $\mathcal{L}$ is found to be [cf. (1.10), (1.15) and (1.17)]

$$\delta_{\epsilon(\tau)}\mathcal{L} = \frac{\mathrm{d}}{\mathrm{d}\tau}(\epsilon(\tau)\mathcal{L}) \ . \tag{1.18}$$

[9] Note that (1.16) and (1.17) are, respectively, particular cases of the general transformations (A.3) and (A.4) considered in Appendix A. In this case, there are $N = 1$ arbitrary functions $\varepsilon_i(\tau) \equiv \varepsilon(\tau)$, and $\epsilon(\tau) = \varepsilon(\tau)$.

Due to (1.18), the action (1.5) is seen to be invariant up to a boundary term, and the field equations remain of the same form.[10]

Incidentally, if one introduces more general worldline tensors as fundamental degrees of freedom, it is possible to construct potential terms solely from the scalars. For example, let $K(\tau)$ be a field that transforms inhomogeneously as $\delta_{\epsilon(\tau)}K(\tau) = \epsilon\dot{K} + \epsilon$. The Lagrangian $\mathcal{L}_K := -V(q)\dot{K} + \alpha_i(q)\dot{q}^i - V(q)$, where $V(q)$ and $\alpha_i(q)$ are scalars, then transforms as in (1.18); i.e., its scalar-density character follows solely from its field constituents [cf. discussion after (1.7)]. In [33], a similar example was considered in section 4.3.3, where it was noted that $\mathcal{L}_K$ can be obtained from a Lagrangian of the form $-V(q)\dot{q}^1 + \alpha_{i\neq 1}(q)\dot{q}^{i\neq 1}$ [cf. (1.10)] via the field redefinition $q^1(\tau) = K(\tau) + \tau$. Notice, however, that this redefinition is not to be interpreted as expressing $q^1(\tau)$ as the sum of an object $K(\tau)$ with the identity function $f(\tau) = \tau$, since $K(\tau)$ would otherwise be a scalar; i.e., $K(\tau) = q^1(\tau) - \tau$ would imply $K'(\tau) = q^{1\prime}(\tau) + \tau'(\tau)$ [cf. (1.16) and (1.14)]. Rather, the redefinition is to be seen as definition of $K(\tau)$ at all points of the gauge orbit; i.e., $K(\tau) = q^1(\tau) - \tau$ implies $K'(\tau) = q^{1\prime}(\tau) - \tau$. This then leads to the inhomogeneous transformation

$$\delta_{\epsilon(\tau)}K(\tau) = K'(\tau) - K(\tau) = \epsilon(\tau)\dot{q}(\tau) = \epsilon(\tau)(K(\tau) + 1) \ . \tag{1.19}$$

As already mentioned, our choice of fields is comprised of the scalars $q(\tau)$ and the einbein $e(\tau)$, and we will not consider degrees of freedom such as $K(\tau)$.

1.3 The total Hamiltonian

The local symmetry (1.17) implies that the canonical theory is constrained. This is a general feature of canonical gauge systems (cf. Appendix A).[11] The constraints follow from the fact that the Lagrangian is 'singular'; i.e., the determinant of its Hessian matrix with respect to the velocities vanishes [34]. Indeed, we find from (1.10) the identity $\partial^2\mathcal{L}/\partial\dot{e}^2 = 0$. In this case, some of the field equations do not involve accelerations, and they constrain the possible values of the fields and velocities. In the corresponding canonical theory, the possible values of the fields and conjugate momenta are constrained, and this signals that not all points of phase space correspond to physically allowed motions.

[10]The action (1.5) is, in general, only invariant if $\epsilon(a) = \epsilon(b) = 0$; i.e., if the diffeomorphisms ϕ_l reduces to the identity at the endpoints. This can be obtained if $v(\tau) = 0$ for $\tau \notin \zeta(\mathcal{U}) = (a, b)$. If this is not the case, the action can be made invariant if one adds appropriate boundary terms in the right-hand side of (1.5), but this will not be done here (see [35] for details).

[11]However, not all constrained Hamiltonian theories correspond to gauge systems due to the presence of second-class constraints (cf. §A.2.4).

1.3.1 General case and gauge indeterminism

To construct the constrained canonical theory, we first define canonical momenta via the usual Legendre map,

$$p_e := \frac{\partial \mathcal{L}}{\partial \dot{e}} = 0 \ , \ p_i := \frac{\partial \mathcal{L}}{\partial \dot{q}^i} \ (i = 1, \ldots, d) \ . \tag{1.20}$$

We note that the momenta $p_i(\tau)$ conjugate to $q^i(\tau)$ are also worldline scalars because they are equal to $\partial\mathcal{L}/\partial\dot{q}^i$ $(i = 1, \ldots, d)$. The momentum conjugate to the einbein is constrained to vanish, and thus $p_e = 0$ is a primary constraint of the theory (according to the terminology used in the Rosenfeld-Dirac-Bergmann algorithm [36–39]; cf. §A.2.3). We assume this is the only primary constraint.[12] It determines a hypersurface in Γ, the unconstrained phase space of the theory (also called the auxiliary phase space; cf. §A.2.1). We refer to this hypersurface as the 'primary constraint hypersurface' and we denote it by $\Sigma_{(1)}$.

The primary constraint implies that one cannot invert $p_e = \partial\mathcal{L}/\partial\dot{e}$ to find $\dot{e}(\tau)$ in terms of $e(\tau), p_e(\tau)$ and $q(\tau), p(\tau)$, and $\dot{e}(\tau)$ remains undetermined. In contrast, it is possible to invert $p_i = \partial\mathcal{L}/\partial\dot{q}^i$ to express the velocities $\dot{q}^i(\tau)$ in terms of $q^i(\tau), p_i(\tau)$ and $e(\tau)$ because no other primary constraints are present. Due to the arbitrariness of $\dot{e}(\tau)$, the Legendre transform that defines the canonical Hamiltonian is only well defined on the primary constraint hypersurface. In this way, the canonical Hamiltonian reads

$$H_c(q(\tau), p(\tau); e(\tau)) := p_i(\tau)\dot{q}^i(\tau) - \mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau)) = -\frac{\partial \mathcal{L}}{\partial e} e(\tau) \ , \tag{1.21}$$

where a summation over repeated indices is implied. We used (1.10) and (1.20) to obtain the last equality in (1.21). Thus, the canonical Hamiltonian is a worldline scalar density (as it should be).

Furthermore, the primary constraint must be conserved by the time evolution if the dynamics defined by (1.5) is consistent. Using the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial e} = \frac{\mathrm{d}p_e}{\mathrm{d}\tau} = 0 \ , \tag{1.22}$$

we find that the conservation of $p_e = 0$ leads to a new (secondary) constraint,

$$C(q(\tau), p(\tau)) := -\frac{\partial \mathcal{L}}{\partial e} = 0 \ . \tag{1.23}$$

[12] See the comment on footnote 13.

As $\partial\mathcal{L}/\partial e$ is a scalar, the secondary constraint cannot depend on $e(\tau)$; i.e., it is a function solely of $q(\tau)$ and $p(\tau)$. For simplicity, we assume that the Rosenfeld-Dirac-Bergmann algorithm (cf. §A.2.3) terminates at this stage. This means that demanding conservation of the secondary constraint does not lead to new constraints. In this way, the theory only has one primary and one secondary constraint.[13] We will see how these two constraints are related to the gauge symmetry in §1.6. From (1.21) and (1.23), we note that the canonical Hamiltonian is proportional to the secondary constraint, $H_c(q(\tau), p(\tau); e(\tau)) = e(\tau)C$.

The dynamics dictated by the canonical Hamiltonian, which is only well-defined on the primary constraint hypersurface $\Sigma_{(1)}$, can be determined by considering variations of $q(\tau), p(\tau), e(\tau)$ and $p_e(\tau)$ that are tangent to $\Sigma_{(1)}$ but otherwise arbitrary [33]. Since $\Sigma_{(1)}$ is defined by $p_e = 0$, we may take $\delta q(\tau), \delta p(\tau)$ and $\delta e(\tau)$ to be arbitrary, and $\delta p_e = 0$. From (1.21) and (1.23), we find

$$\left(\frac{\partial H_c}{\partial q}^i + \frac{\partial \mathcal{L}}{\partial q^i}\right)\delta q^i + \left(\frac{\partial H_c}{\partial p_i} - \dot{q}^i\right)\delta p_i + C\delta e = 0 \ , \tag{1.24}$$

which leads to the equations

$$\begin{aligned} &\dot{q}^i = \frac{\partial H_c}{\partial p_i} \ , \ \dot{p}_i = \frac{\partial L}{\partial q^i} = -\frac{\partial H_c}{\partial q^i} \ , \\ &C(q(\tau), p(\tau)) = 0 \ . \end{aligned} \tag{1.25}$$

We note that (1.25) are valid on $\Sigma_{(1)}$; i.e., they hold if $p_e = 0$. Let Σ be the hypersurface defined by the constraints $p_e = 0$ and $C = 0$. From (1.25), we can then define the evolution of any function $f(q, p; e, p_e; \tau)$ on the auxiliary phase space as follows:

$$\dot{f} \equiv \frac{\mathrm{d}f}{\mathrm{d}\tau} = \left(\frac{\partial f}{\partial \tau} + \frac{\partial f}{\partial q^i}\dot{q}^i + \frac{\partial f}{\partial p_i}\dot{p}_i + \frac{\partial f}{\partial e}\dot{e} + \frac{\partial f}{\partial p_e}\dot{p}_e\right)_\Sigma \ . \tag{1.26}$$

The restriction to Σ implies, in particular, that $\dot{p}_e = -C = 0$ [cf. (1.22) and (1.23)]. Moreover, as $\dot{e}$ is undetermined, we may define it to be an arbitrary function in the auxiliary phase space Γ; i.e., $\dot{e} = \lambda(q, p; e, p_e; \tau)$. Finally, we may recast (1.26) in terms of the Poisson brackets defined in Γ [cf. (A.24)],

$$\{f, g\} := \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} + \frac{\partial f}{\partial e}\frac{\partial g}{\partial p_e} - \frac{\partial f}{\partial p_e}\frac{\partial g}{\partial e} \ . \tag{1.27}$$

[13] Following the comment on footnote 7, if the Lagrangian is of the form $\mathcal{K}(q, \dot{q}) - eV(q)$, then a secondary constraint is $V(q) = 0$. In this case, further constraints will be present due to the structure of the kinetic term (cf. §1.3.2). For simplicity, we assume that this is not the case here.

We find

$$\dot{f} \equiv \frac{\mathrm{d}f}{\mathrm{d}\tau} = \left(\frac{\partial f}{\partial \tau} + \{f, H_c\} + \lambda\{f, p_e\}\right)_\Sigma \tag{1.28}$$

from (1.25). In what follows, identities that are only valid on Σ will be denoted by Dirac's weak equality sign $\approx$ [40] (cf. **Notations, Conventions and Terminology** and Appendix A). For example, if f, g, α and β are auxiliary phase-space functions such that $\{f, g\} = \alpha C + \beta p_e$, then we write $\{f, g\} \approx 0$. Similarly, for $\lambda \equiv \lambda(q, p; e, p_e; \tau)$, we obtain $\lambda\{\cdot, p_e\} \approx \{\cdot, \lambda p_e\}$. Note that we set the constraint functions to zero only after the Poisson brackets are evaluated. In this way, we can rewrite (1.28) as [see also (A.41)]

$$\dot{f} \equiv \frac{\mathrm{d}f}{\mathrm{d}\tau} \approx \frac{\partial f}{\partial \tau} + e\{f, C\} + \lambda\{f, p_e\} \approx \frac{\partial f}{\partial \tau} + \{f, H_T\} \ , \tag{1.29}$$

where we defined

$$H_T(q, p; e, p_e; \tau) := eC(q, p) + \lambda(q, p; e, p_e; \tau) p_e \ . \tag{1.30}$$

We refer to this function as the total Hamiltonian (cf. §A.2.2), and we note that it is a combination of the primary and secondary constraints of the theory. Thus, $H_T \approx 0$; i.e., H_T vanishes on the constraint hypersurface (one also says that it vanishes 'on shell'). The total Hamiltonian is a worldline tensor of the same type as H_c and $\mathcal{L}$; i.e., it is a scalar density.

In the particular case in which $f(q, p; e, p_e; \tau) = e(\tau)$, we find from (1.29) the condition $\dot{e} = \lambda$, as expected.[14] Due to the arbitrariness of λ, the total Hamiltonian H_T can be seen as an arbitrary extension of the canonical Hamiltonian H_c off the primary constraint hypersurface.[15] A choice of λ corresponds to a choice of this extension and to a choice of gauge, as we will see in §1.6.

Is the evolution determined by $H_T(q, p; e, p_e; \tau)$ well defined? From (1.27), it is straightforward to verify that the constraint functions Poisson-commute, $\{p_e, C\} = 0$, which means that: (1) the constraint algebra is Abelian; (2) the constraint functions are first class (cf. §A.2.4). The first property is a special feature of $0 + 1$ dimensions, and the algebra of constraints in higher dimensions (e.g., in GR) is more complicated (more constraints are present, and they are associated with a non-trivial algebra) [6]. As reviewed in Appendix A, property (2) is related to the gauge symmetry, a topic we

[14] This result, together with (1.21), (1.23) and (1.30), implies that we can write the total Hamiltonian in the suggestive form $H_T = p_e \dot{e} + p_i \dot{q}^i - \mathcal{L}$. Nevertheless, this is not a proper Legendre transform because $\dot{e} = \lambda$ is arbitrary.

[15] See Theorem 1.1 and Appendix 1.A of [33] and the derivation of (A.42) in Appendix A for a general procedure to extend functions off the constraint hypersurface.

discuss in §1.6. Due to (1.30), the total Hamiltonian weakly Poisson-commutes with the constraint functions, and thus it is also first class.

In particular, we obtain from (1.29) the equations $\mathrm{d}C/\mathrm{d}\tau \approx 0$, $\mathrm{d}p_e/\mathrm{d}\tau \approx 0$ and $\mathrm{d}H_T/\mathrm{d}\tau \approx 0$; i.e., the constraint functions are weakly conserved by the time evolution or, equivalently, the constraint hypersurface is invariant under time translations because H_T is first class. We conclude from this that the constraints are satisfied at all times provided the initial data $(q(\tau_0), p(\tau_0), p_e(\tau_0))$ are chosen such that $C(q(\tau_0), p(\tau_0)) = 0$ and $p_e(\tau_0) = 0$ at an arbitrary instant of time τ_0. Thus, the constraints are seen to be restrictions on the initial values of the fields or, equivalently, on the allowed (physical) motions. This holds irrespective of the values of $e(\tau)$ and $\lambda(q, p; e, p_e; \tau)$, and it follows from the consistency of the theory ensured by the Rosenfeld-Dirac-Bergmann algorithm (cf. §A.2.3).

As λ is arbitrary, we conclude that the evolution of the einbein and, consequently, of the scalars $q(\tau)$ and $p(\tau)$ is also arbitrary [cf. (1.25) and (1.29)]. In this way, the specification of initial data at an arbitrary coordinate instant τ_0 is not sufficient to determine the physical trajectory, as different solutions associated with the same set of allowed initial values can be obtained if different choices of λ are made. Equivalently, one can state that the solutions of the field equations generally depend on arbitrary functions of time τ. We will see that this kind of indeterminism is related to the gauge symmetry of the theory (cf. §1.6 and §A.2.5) and that it warrants a discussion on the definition of observables, the evolution of which is well-defined (cf. §1.7, §1.8 and §A.2.7).

Finally, the evolution (1.29) determined by the total Hamiltonian on the constraint hypersurface Σ may be derived by extremizing an action [33] as follows: from (1.21), we can rewrite the action (1.5) as

$$S = \int_a^b \mathrm{d}\tau \ \left[p_i(\tau)\dot{q}^i(\tau) - e(\tau)C(q(\tau), p(\tau))\right] \ . \tag{1.31}$$

The field equation associated with $e(\tau)$ is the secondary constraint, and $e(\tau)$ is arbitrary. The primary constraint has been tacitly solved. However, we can include an additional field $\lambda(\tau)$ to obtain both the primary constraint and the equation $\dot{e} = \lambda$ from a variational principle. The modified action reads

$$\begin{aligned} S &= \int_a^b \mathrm{d}\tau \ \left[p_i(\tau)\dot{q}^i(\tau) + p_e(\tau)\dot{e}(\tau) - e(\tau)C(q(\tau), p(\tau)) - \lambda(\tau)p_e(\tau)\right] \\ &=: \int_a^b \mathrm{d}\tau \ \left[p_i(\tau)\dot{q}^i(\tau) + p_e(\tau)\dot{e}(\tau) - H_T(q, p; e, p_e; \lambda)\right] \ . \end{aligned} \tag{1.32}$$

In the variational principle associated with (1.32), the variations of the fields are only constrained to vanish at the endpoints, but the primary constraint is no longer imposed. Rather, it follows as the field equation associated with the arbitrary field $\lambda(\tau)$, which serves as a Lagrange multiplier. Note that, by considering $\lambda(\tau)$ as one of the dynamical fields (with its own field equation), the functional form of the action (1.32) is invariant under diffeomorphisms, which correspond to a relabeling of the arguments of the Lagrangian [including $\lambda(\tau)$; see footnote and 5 and the discussion after (1.9)]. Furthermore, as already mentioned, we will see in §1.6 that the fixation of a choice of $\lambda(\tau) \equiv \lambda(q, p; e, p_e; \tau)$ (i.e., of a particular extension $H_T(q, p; e, p_e; \tau)$ of the canonical Hamiltonian) corresponds to fixing the gauge freedom. Finally, in the variational principle associated to (1.32), $e(\tau)$ and $\lambda(\tau)$ are independent fields. The relation $\dot{e}(\tau) \approx \lambda(\tau)$ follows as a field equation, rather than a definition.

1.3.2 A particular case

Let us briefly consider the particular case in which $\mathcal{L}$ does not depend on $e(\tau)$; i.e., the Lagrangian is a function solely of $q(\tau)$ and $\dot{q}(\tau)$ [it is a generalized kinetic term; cf. (1.7)]. Then, we do not include the pair (e, p_e) in the auxiliary phase space of the theory. Using $\partial\mathcal{L}/\partial e \equiv 0$ in (1.21), we see that the canonical Hamiltonian H_c vanishes identically [32, 33].[16] Moreover, by taking derivatives of (1.21) and using $H_c \equiv 0$, we obtain the condition

$$\frac{\partial^2 \mathcal{L}}{\partial \dot{q}^i \partial \dot{q}^j} \dot{q}^j = 0 \; , \tag{1.33}$$

which implies that the Lagrangian is singular also in this case [34]. Due to (1.33), it is not possible to invert $p_i(\tau) = \partial\mathcal{L}/\partial\dot{q}^i$, and thus the velocities cannot all be expressed in terms of the configuration variables and momenta. Rather, the momenta $p_i(\tau)$ obey a set of primary constraints (cf. Appendix A). As before, we assume that there is only one primary constraint. Thus, instead of $p_e = 0$, one now finds a primary constraint on the values of the scalars, $C(q, p) = 0$. Although the canonical Hamiltonian is zero in this case, one can still extend it off the primary constraint hypersurface in analogy to (1.30) [see also (A.42)] if $C(q, p)$ obeys suitable regularity conditions (see §A.2.1 and [33, 34] for details). Here, these conditions correspond to requiring that the primary constraint function obeys

$$\frac{\partial C}{\partial q^i} \mathrm{d}q^i + \frac{\partial C}{\partial p_i} \mathrm{d}p_i \neq 0 \tag{1.34}$$

[16] In principle, it is possible to obtain a nonvanishing canonical Hamiltonian as a function of $q(\tau)$ and $p(\tau)$ if one includes a field that transforms inhomogeneously [cf. discussion preceding (1.19)], but this will not be done here. See, for example, section 4.3.3 of [33].

on a family of open regions that cover the primary constraint hypersurface [33].[17] Notice that there is, in principle, no preferred functional form of C. The constraint hypersurface can be described by $f(C) = 0$, where f is a function that obeys $f(0) = 0$ and $\mathrm{d}f/\mathrm{d}C|_{C=0} \neq 0$, because $f(C)$ locally obeys (1.34) on the primary constraint hypersurface provided C also obeys the regularity condition.[18]

By varying (1.21) with $H_c \equiv 0$, we obtain

$$0 = \dot{q}^i \delta p_i - \frac{\partial \mathcal{L}}{\partial q^i} \delta q^i = \dot{q}^i \delta p_i - \dot{p}_i \delta q^i \ , \tag{1.35}$$

where the Euler-Lagrange equations were used to reach the last equality. The variations δp_i and δq^i in (1.35) must be tangent to the primary constraint surface $\Sigma_{(1)}$ defined by $C = 0$, where the canonical Hamiltonian is well-defined. Since we assume there are d scalar fields $q(\tau)$, the tangent space $T_p\Sigma_{(1)}$ at a point p in the primary constraint surface is $(2d-1)$-dimensional. Due to (1.34), the vector gradient $(\partial C/\partial q^i, \partial C/\partial p_i)$ forms a basis for the orthogonal complement of $T_p\Sigma_{(1)}$. Together with (1.35), this implies that $(-\dot{p}_i, \dot{q}^i)$ must be proportional to $(\partial C/\partial q^i, \partial C/\partial p_i)$. In this way, the following equations must be satisfied:

$$\dot{q}^i = \omega \frac{\partial C}{\partial p_i} \ , \ -\dot{p}_i \ = \omega \frac{\partial C}{\partial q^i} \ , \tag{1.36}$$

where $\omega \equiv \omega(q, p; \tau)$ is an arbitrary function in the auxiliary phase space Γ. By using the Poisson brackets (1.27) [without the pair (e, p_e)] and (1.36), the evolution of a function $f(q, p; \tau)$ in Γ can then be written as

$$\begin{aligned} \dot{f} \equiv \frac{\mathrm{d}f}{\mathrm{d}\tau} &= \left(\frac{\partial f}{\partial \tau} + \omega \{f, C\} \right)_{\Sigma_{(1)}} \\ &\approx \frac{\partial f}{\partial \tau} + \{f, \omega C\} =: \frac{\partial f}{\partial \tau} + \{f, H_T\} \ , \end{aligned} \tag{1.37}$$

where the total Hamiltonian is now defined as

$$H_T(q, p; \tau) := \omega(q, p; \tau) C(q, p) \approx 0 \ . \tag{1.38}$$

[17] This ensures that one can locally perform a canonical transformation to bring the constraint to the form $C(q, p) = p_1$. Subsequently, one can repeat the construction given in (A.42) to define the total Hamiltonian (1.38). Once (1.38) has been constructed, it is not necessary to assume that the constraint coincides with one of the momenta, and one may invert the local canonical transformation such that the functional form of $C(q, p)$ is only restricted by regularity condition (1.34).

[18] It is also possible to describe the constraint hypersurface in a redundant manner [33]. For example, one can define the hypersurface by the pair of equations $C = 0$ and $C^2 = 0$. For simplicity, we do not consider such redundant constructions.

As only one constraint $C(q,p) = 0$ is present in this particular case, the constraint function is trivially first class and Abelian. As before, we conclude that the evolution generated by the total Hamiltonian (1.38) is indeterministic because ω is arbitrary. The variational principle in the canonical theory can be written as

$$S = \int_a^b \mathrm{d}\tau \; p_i(\tau)\dot{q}^i(\tau) \;, \tag{1.39}$$

where the primary constraint is tacitly solved. Alternatively, we introduce ω as an additional field that serves as a Lagrange multiplier. The primary constraint is not imposed, but it follows as the field equation associated with ω. The modified action reads

$$S = \int_a^b \mathrm{d}\tau \; \left[p_i(\tau)\dot{q}^i(\tau) - \omega(\tau)C(q(\tau),p(\tau))\right] \;. \tag{1.40}$$

Notice that field $\omega(\tau)$ must be a scalar density, such that the Lagrangian in (1.40) is well-defined. In this case, we may choose $\omega(\tau)\mathrm{d}\tau$ as the volume form and $\omega(\tau)$ as the einbein (cf. §1.1), such that (1.40) becomes identical to (1.31). Incidentally, a change of einbein frame [cf. (1.3)] induces a change in the functional form of the constraint function,

$$C = \frac{1}{\Omega(\tau)}\tilde{C} \;, \tag{1.41}$$

such that $\omega C = (\tilde{\omega}\Omega)(\Omega^{-1}\tilde{C}) = \tilde{\omega}\tilde{C}$ is invariant under changes of einbein frame. Eq. (1.41) is a particular case of the general representation of the constraint function $f(C)$ with $f(0) = 0$ and $\mathrm{d}f/\mathrm{d}C|_{C=0} \neq 0$ [cf. discussion after (1.34)].

As before, the functional form of the action (1.40) is invariant under diffeomorphisms because $\omega(\tau)$ is an additional dynamical field, and thus the symmetry transformations merely relabel the arguments of the Lagrangian. We will see in §1.6 that a choice of $\omega(\tau) \equiv \omega(q,p;\tau)$ corresponds to a fixation of the gauge freedom.[19] Moreover, we note that the total Hamiltonians (1.30) and (1.38) are similar. In fact, we will also see in §1.6 that (1.38) can be seen as a 'gauge-fixed' version of (1.30).

[19] As we will see in §1.6, the fixed function $\omega(q,p;\tau)$ is a worldline scalar. This does not contradict the fact that the multiplier $\omega(\tau)$ is a scalar density because the fixation of the gauge freedom corresponds to a definition of the (arbitrary) coordinate τ on the worldline (cf. §1.6). In this way, fixing $\omega(\tau) \equiv \omega(q,p;\tau)$ simply corresponds to defining the value of the scalar density for a particular choice of coordinate.

1.4 Parametrization of noninvariant models and Jacobi's principle

As mentioned in the **Introduction**, it is possible to elevate a theory that is not diffeomorphism invariant to one in which diffeomorphisms are a symmetry of the field equations through a procedure that is sometimes called parametrization [6]. This consists of promoting the spacetime coordinates to physical fields. In the case of mechanical theories, we start from a noninvariant action

$$S_{\text{non}} := \int_{\eta_a}^{\eta_b} \mathrm{d}\eta \; L\left(f(\eta), \frac{\mathrm{d}f}{\mathrm{d}\eta}(\eta); \eta\right) \;, \tag{1.42}$$

where $f(\eta)$ denotes a collection of $d-1$ worldline scalar fields. The Lagrangian L is not a scalar density by hypothesis, and thus the action (1.42) is not invariant under worldline diffeomorphisms. In particular, a reparametrization $\eta \mapsto \tau(\eta)$ [cf. (1.6)] not only corresponds to a relabeling of the arguments of L, but it also changes the functional form of the action (1.42) through the introduction of factors of $\mathrm{d}\eta/\mathrm{d}\tau \equiv \dot{\eta}$. For this reason, the time coordinate η, although arbitrary, acquires a preferred status (e.g., Newton's absolute time).

Let us denote derivatives with respect to the time coordinate η by a subscript; i.e., $f^i_\eta(\eta) \equiv \mathrm{d}f^i/\mathrm{d}\eta$ $(i = 1, \ldots, d-1)$. Furthermore, we assume that L is regular; i.e., that the determinant of its Hessian matrix with respect to f_η is not zero. The canonical momenta with respect to η are defined as $\pi_i := \partial L/\partial f^i_\eta$, and it is possible to invert this relation to find f_η in terms of f and π. The canonical Hamiltonian, $h(f(\eta), \pi(\eta); \eta)$, may then be defined via the Legendre transform. As L is not a scalar density, the canonical Hamiltonian will also not have the necessary transformation law to render the action invariant. Nevertheless, the theory can be redefined in an invariant way if we perform an arbitrary reparametrization, $\eta \mapsto \tau(\eta)$, and we promote $\eta(\tau)$ to a worldline scalar field [cf. (1.2)]. The result is

$$\begin{aligned} S_{\text{non}} \mapsto S_{\text{par}} &:= \int_a^b \mathrm{d}\tau \; \dot{\eta}(\tau) L\left(\tilde{f}(\tau), \frac{\dot{\tilde{f}}(\tau)}{\dot{\eta}(\tau)}; \eta(\tau)\right) \\ &=: \int_a^b \mathrm{d}\tau \; \mathcal{L}(\tilde{f}(\tau), \dot{\tilde{f}}(\tau), \eta(\tau), \dot{\eta}(\tau)) \;, \end{aligned} \tag{1.43}$$

where $\tilde{f}(\tau) := f(\eta(\tau))$ and $a = \tau(\eta_a)$, $b = \tau(\eta_b)$. The action (1.43) is invariant because $\mathcal{L}$ is a worldline scalar density. As $\eta(\tau)$ is now a physical entity (with its own field equation), the functional form of the action (1.43) does not change under reparametrizations that preserve the endpoints. We refer to (1.43) as the parametrization of the noninvariant model [6].

The canonical momenta with respect to τ are

$$\begin{aligned}\tilde{\pi}_i &:= \frac{\partial \mathcal{L}}{\partial \dot{\tilde{f}}^i} = \frac{\partial L}{\partial f^i_\eta} = \pi_i \ , \\ \pi_\eta &:= \frac{\partial \mathcal{L}}{\partial \dot{\eta}} = L(f, f_\eta; \eta) - \pi_i \frac{\dot{\tilde{f}}^i}{\dot{\eta}} = -h(f, \pi; \eta) \ ,\end{aligned} \tag{1.44}$$

where a summation over repeated indices is implied. In this way, the momentum conjugate to $\eta(\tau)$ is constrained to be equal to the Hamiltonian of the noninvariant model. As h only depends on $f(\eta)$ and $\pi(\eta)$, we cannot invert (1.44) to find $\dot{\eta}(\tau)$ as a function of the fields and their momenta. For this reason, $\pi_\eta = -h$ is the primary constraint of the parametrized theory. From the Euler-Lagrange equation $\dot{\pi}_\eta = \partial\mathcal{L}/\partial\eta$, we see that a secondary constraint is present if L and h have an explicit dependence on η. If this is not the case, then $\dot{\pi}_\eta = 0$, and the primary constraint implies that $h = \text{const.}$, which is consistent with the conservation of the Hamiltonian in the noninvariant model.

From (1.44) and the primary constraint, we also note that $\mathcal{L} = \dot{\eta}(\pi_i \dot{f}^i/\dot{\eta} - h) = \pi_i \dot{f}^i + p_\eta \dot{\eta}$. Thus, the Lagrangian $\mathcal{L}$ is a generalized kinetic term [cf. (1.8)], and the parametrized theory is an instance of the particular case analyzed in the previous section (cf. §1.3.2). The d scalar fields consist of $f^i(\tau)$ $(i = 1, \ldots, d-1)$ and $\eta(\tau)$; i.e., $q(\tau) = (f(\tau), \eta(\tau))$. The primary constraint, $C = \pi_\eta + h$, obeys the regularity condition (1.34), and the total Hamiltonian is $H_T = \omega(\pi_\eta + h)$. In particular, the field equation for $\eta(\tau)$ is $\dot{\eta} = \omega$. As ω is an arbitrary worldline scalar density, we may choose it as the einbein, in which case η is the proper time [cf. (1.2)]. Thus, the procedure of parametrization is equivalent to assuming the existence of a worldline scalar that varies monotonically along the worldline and serves as a global time coordinate. As was discussed in the **Introduction**, this corresponds to the assertion that the model can be globally deparametrized. This is true by construction because the model was built from a noninvariant action by parametrization. Nevertheless, this is a particular case of the formalism we present, both in the classical and quantum theories.

It is worthwhile to mention that there is another way to cast a noninvariant theory in invariant form. Instead of (1.42), let us consider the action

$$\tilde{S}_{\text{non}} := \int_{\eta_a}^{\eta_b} \mathrm{d}\eta \ L\left(\tilde{q}(\eta), \frac{\mathrm{d}\tilde{q}}{\mathrm{d}\eta}(\eta)\right) \ ; \tag{1.45}$$

i.e., we now consider a theory with d scalar fields $\tilde{q}^i(\eta)$ $(i = 1, \ldots, d)$ and a Lagrangian L that is not a scalar density and does not depend explicitly on the preferred time η. We assume that L is regular and, in addition, that the canonical Hamiltonian $h(\tilde{q}(\eta), \tilde{p}(\eta))$ may equal zero for certain nontrivial field configurations. If these conditions are met, we can redefine the theory in an invariant form if we perform an arbitrary reparametrization, $\eta \mapsto \tau(\eta)$, and we promote $e(\tau) := \dot{\eta}(\tau)$ to an auxiliary field that is a worldline scalar density. The result is

$$\begin{aligned} \tilde{S}_{\rm non} \mapsto \tilde{S}_{\rm par} &:= \int_a^b {\rm d}\tau \; e(\tau) L \left(q(\tau), \frac{\dot{q}(\tau)}{e(\tau)} \right) \\ &=: \int_a^b {\rm d}\tau \; \mathcal{L}(q(\tau), \dot{q}(\tau); e(\tau)) \;, \end{aligned} \tag{1.46}$$

where $q(\tau) := \tilde{q}(\eta(\tau))$ and $a = \tau(\eta_a)$, $b = \tau(\eta_b)$. In other words, instead of promoting $\eta(\tau)$ to a physical field, one introduces an arbitrary einbein into the theory. In this way, it is not necessary to assume the existence of an extra scalar degree of freedom that serves as a global time parameter, and the resulting Lagrangian $\mathcal{L}$ is of the type considered in §1.2 and §1.3.1. In particular, one finds the primary constraint $p_e = 0$ and the secondary constraint (cf. §1.3.1)

$$0 = C(q,p) := -\frac{\partial \mathcal{L}}{\partial e} = -L + \frac{\partial L}{\partial \tilde{q}^i_\eta} \frac{\dot{q}^i}{e} \equiv h(\tilde{q}(\eta), \tilde{p}(\eta)) \;; \tag{1.47}$$

i.e., the canonical Hamiltonian of the noninvariant theory becomes the secondary constraint associated with the invariant action. A well-known example of this kind of parametrization is given by Jacobi's variational principle, which can be constructed as follows: we consider that the configuration space of the scalars $\tilde{q}(\eta)$ has the line element ${\rm d}s^2 = G_{ij}(\tilde{q}){\rm d}\tilde{q}^i {\rm d}\tilde{q}^j$ and the action (1.45) reads

$$\tilde{S}_{\rm non} := \int_{\eta_a}^{\eta_b} {\rm d}\eta \; \left[\frac{1}{2} G_{ij}(\tilde{q}(\eta)) \frac{{\rm d}\tilde{q}^i}{{\rm d}\eta} \frac{{\rm d}\tilde{q}^j}{{\rm d}\eta} - V(\tilde{q}(\eta)) + \Lambda \right] \;, \tag{1.48}$$

where $V(\tilde{q}(\eta))$ is a potential term and Λ is a constant that plays the role of a "cosmological constant" in this model universe. Upon introduction of the einbein, the invariant action is [cf. (1.46)]

$$\tilde{S}_{\rm par} = \int_a^b {\rm d}\tau \; \left[\frac{1}{2e(\tau)} G_{ij}(q(\tau)) \frac{{\rm d}q^i}{{\rm d}\tau} \frac{{\rm d}q^j}{{\rm d}\tau} - e(\tau) V(q(\tau)) + e(\tau)\Lambda \right] \;. \tag{1.49}$$

The secondary constraint, which coincides with the Hamiltonian of the noninvariant theory, is $C(q,p) = 1/2 G^{ij}(q) p_i p_j + V(q) - \Lambda$, where $G^{ij}(q)$ are the components of the inverse configuration-space metric and $p_i(\tau)$ are the momenta conjugate to $q^i(\tau)$ $(i = 1, \ldots, d)$. Note that $C = 0$ corresponds to the conservation of $1/2 G^{ij}(q) p_i p_j + V(q)$ with value Λ. It is also possible to use the Euler-Lagrange equation for $e(\tau)$ to eliminate the einbein and rewrite the Lagrangian in (1.49) as a generalized kinetic term. Indeed, one finds the Euler-Lagrange equation

$$0=\frac{\partial\mathcal{L}}{\partial e}=-\frac{1}{2e^2(\tau)}G_{ij}(q(\tau))\frac{\mathrm{d}q^i}{\mathrm{d}\tau}\frac{\mathrm{d}q^j}{\mathrm{d}\tau}-V(q(\tau))+\Lambda\ , \tag{1.50}$$

the solution of which reads $e(\tau)=\pm\{G_{ij}\dot{q}^i\dot{q}^j/[2(\Lambda-V)]\}^{1/2}$. If we insert this solution back into (1.49), we obtain

$$\tilde{S}_{\mathrm{par}}=\pm\int_a^b\mathrm{d}\tau\ \sqrt{2[\Lambda-V(q(\tau))]G_{ij}(q(\tau))\dot{q}^i(\tau)\dot{q}^j(\tau)}\ , \tag{1.51}$$

which is the action considered in Jacobi's principle [41].[20] In particular, the action of a free relativistic particle with mass m is of the form (1.51) with $V(q(\tau))=0$ and $\Lambda=m^2/2$. In GR, a similar elimination of the einbein (which coincides with the lapse function) is possible in principle. The result is the so-called Baierlein-Sharp-Wheeler action [6, 42]. In string theory, the analogues of (1.49) and (1.51) are, respectively, the so-called Polyakov and Nambu-Goto actions [6].

Clearly, the two parametrization strategies above are related. Assuming the same form of the Lagrangian L and the same number of scalar fields, one can map (1.46) into (1.43) by replacing $e(\tau)=\dot{\eta}(\tau)$ and promoting $\eta(\tau)$ to a physical field. Conversely, the action (1.43) is taken to (1.46) if we replace $\dot{\eta}=e(\tau)$ and consider that $e(\tau)$ is an auxiliary field. In the particular case of Jacobi's principle, we also note that the total Hamiltonian associated with (1.49) is $H_T=e(1/2G^{ij}(q)p_ip_j+V(q)-\Lambda)+\lambda p_e$ [cf. (1.30)]. As was mentioned in the previous section (§1.3.2) and as will be shown in §1.6, the total Hamiltonian $H_T'=\omega(1/2G^{ij}(q)p_ip_j+V(q)-\Lambda)$ can be obtained from H_T by gauge fixing. Thus, if we treat Λ as a free (rather than fixed) parameter, then we may formally set it to $\Lambda=-p_\eta$; i.e., we may consider that the cosmological constant is the opposite of the conserved momentum conjugate to proper time. In this way, one recovers the form of the total hamiltonian associated with (1.43), $H_T'=\omega(p_\eta+1/2G^{ij}(q)p_ip_j+V(q))$. One can then globally deparametrize the theory to obtain a noninvariant model with canonical Hamiltonian equal to $1/2G^{ij}(q)p_ip_j+V(q)$. As will be discussed in §2.2, this is sometimes used as a point of departure for the quantization of theories based on Jacobi's principle [43–47], and it can be seen as a particular case of the general framework presented here.

[20] One can interpret (1.51) as the 'arc length' between two points in a curve (the physical trajectory) in the configuration space of the scalar fields, provided the metric is redefined as $\tilde{G}_{ij}:=2[\Lambda-V(q(\tau))]G_{ij}$. The coordinate τ is then simply a parametrization of this curve (cf. discussion in the **Introduction**).

1.5 The gauge generator

To understand the physical interpretation and dynamical consequences of the arbitrary auxiliary phase-space function λ in (1.30), we must analyze how the constraints are related to the gauge symmetry of theory, and what this implies for the notion of observables. In this section, we examine the connection between the constraint functions and the gauge transformations. In §1.6, we discuss how the gauge freedom can be interpreted in terms of a notion of 'generalized frames of reference'. Finally, we address the definition of observables in §1.7 and §1.8.

First, we note that the transformation laws (1.7) and (1.12) imply that the primary constraint $p_e = 0$ is invariant under diffeomorphisms,

$$0 = \frac{\partial}{\partial \dot{e}}\mathcal{L}(q,\dot{q};e) =: p_e \mapsto p'_e := \frac{\partial}{\partial \dot{e}'}\mathcal{L}(q',\dot{q}';e') = 0\ ; \tag{1.52}$$

i.e., $\delta_{\epsilon(\tau)} p_e = 0$. Notice that the pullback of the fields by a general diffeomorphism is denoted by a prime in (1.52) [cf. (1.14)]. In this way, the gauge transformation of an auxiliary phase-space function $f(q,p;e,p_e;\tau)$ reads

$$\begin{aligned}
\delta_{\epsilon(\tau)} f &= \delta^{\text{expl.}}_{\epsilon(\tau)} f + \frac{\partial f}{\partial q^i}\delta_{\epsilon(\tau)} q^i + \frac{\partial f}{\partial p_i}\delta_{\epsilon(\tau)} p_i + \frac{\partial f}{\partial e}\delta_{\epsilon(\tau)} e + \frac{\partial f}{\partial p_e}\delta_{\epsilon(\tau)} p_e \\
&= \delta^{\text{expl.}}_{\epsilon(\tau)} f + \frac{\partial f}{\partial q^i}\epsilon(\tau)\frac{\mathrm{d}q^i}{\mathrm{d}\tau} + \frac{\partial f}{\partial p_i}\epsilon(\tau)\frac{\mathrm{d}p_i}{\mathrm{d}\tau} + \frac{\partial f}{\partial e}\frac{\mathrm{d}}{\mathrm{d}\tau}(\epsilon(\tau)e) \\
&= \delta^{\text{expl.}}_{\epsilon(\tau)} f + \epsilon(\tau)\left(\frac{\partial f}{\partial q^i}\frac{\partial H_T}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H_T}{\partial q^i} + \frac{\partial f}{\partial e}\frac{\partial H_T}{\partial p_e}\right) + \dot{\epsilon}(\tau) e \frac{\partial f}{\partial e} \\
&\approx \delta^{\text{expl.}}_{\epsilon(\tau)} f + \epsilon(\tau)\{f, H_T\} + \dot{\epsilon}(\tau) e \{f, p_e\} \\
&\approx \delta^{\text{expl.}}_{\epsilon(\tau)} f + \{f, \epsilon(\tau) H_T + \dot{\epsilon}(\tau) e p_e\} \\
&=: \delta^{\text{expl.}}_{\epsilon(\tau)} f + \{f, G\}\ ,
\end{aligned} \tag{1.53}$$

where $\delta^{\text{expl.}}_{\epsilon(\tau)} f$ corresponds to the transformation of the explicit dependence of f on τ,[21] and we used (1.17) and (1.29) together with the fact that $\partial H_T/\partial e = C + p_e \partial\lambda/\partial e \approx 0$. The quantity $G := \epsilon(\tau) H_T + \dot{\epsilon}(\tau) e p_e$ is called the 'gauge generator' [9, 11, 12, 48]. From (1.53), we conclude that infinitesimal worldline diffeomorphisms can be represented as on-shell canonical transformations; i.e., they coincide with canonical trans-

[21] The explicit time dependence of $f(q,p;e,p_e;\tau)$ could conceivably involve a general worldline tensor. However, since any worldline tensor can be written in terms of a scalar and powers of the einbein [cf. (1.4)], there is no loss of generality in assuming that the explicit dependence on τ of a general auxiliary phase-space function is of scalar type; i.e., $\delta^{\text{expl.}}_{\epsilon(\tau)} f(q,p;e,p_e;\tau) = \epsilon(\tau)\partial f/\partial\tau$ [cf. (1.16) and (1.17)]. More precisely, given any solution $\mathcal{S}(\tau)$ to the field equations, in which $e(\tau)$ is equal to some function $\omega(\tau)$, we can use (1.4) to define an auxiliary phase-space function $T(\tau)(e/\omega)^{\alpha-\beta}$ that coincides with the tensor $T(\tau)$ in the solution $\mathcal{S}(\tau)$, and that has an explicit time-dependence given by the scalar $T(\tau)\omega(\tau)^{\beta-\alpha}$.

formations in the auxiliary phase space that are restricted to solutions to the field equations and, in particular, to the constraint hypersurface. For example, the transformation $\{e, G\} \approx \epsilon(\tau)\lambda + \dot{\epsilon}(\tau)e$ only coincides with the correct gauge transformation of the einbein if restricted to a solution, since then $\lambda(\tau) \approx \dot{e}(\tau)$ [cf. discussion after (1.32)], and we find $\{e, G\} \approx \mathrm{d}(\epsilon(\tau)e(\tau))/\mathrm{d}\tau = \delta_{\epsilon(\tau)}e(\tau)$ [cf. (1.17)].

As $\epsilon(\tau)$ can depend on the fields, we may alternatively define $\xi(\tau) := \epsilon(\tau)e(\tau)$ as an independent infinitesimal quantity, which is arbitrary but possibly dependent on $q(\tau)$ and $p(\tau)$. This amounts to considering diffeomorphisms generated by the vector field [cf. (1.16)]

$$V = \frac{\xi(\tau)}{e(\tau)\delta l}\frac{\mathrm{d}}{\mathrm{d}\tau} \equiv \frac{\xi(\tau)}{\delta l}\frac{\mathrm{d}}{\mathrm{d}\eta} \ , \tag{1.54}$$

where η is the proper time [cf. (1.2)]. In this case, we can rewrite the gauge generator as

$$G \equiv G(q(\tau), p(\tau), p_e(\tau); \xi(\tau)) := \xi(\tau)C(q(\tau), p(\tau)) + \dot{\xi}(\tau)p_e \ , \tag{1.55}$$

where we used (1.30) and the fact that $\lambda \approx \dot{e}(\tau)$ on solutions. The connection between the constraints and the gauge symmetry is thus clarified by (1.55), as we see that the generator of on-shell canonical transformations that correspond to gauge transformations is a combination of the (primary and secondary) first-class constraints of theory. Indeed, this derivation of the functional form of the gauge generator is a particular case of the one reviewed in §A.2.5, and (1.55) is an instance of (A.60). Our hypothesis that only one primary and one secondary first-class constraints are present then corresponds to the assumption that the only gauge (local) symmetry of the theory is given by worldline diffeomorphisms.

At first, the focus on diffeomorphisms generated by (1.54) may seem restrictive because $\xi(\tau)$ is taken to be an arbitrary function that possibly depends on $q(\tau)$ and $p(\tau)$ but not on $e(\tau)$. Nevertheless, there is no loss of generality in the description of gauge transformations of solutions to the field equations. As was emphasized in [9, 11, 12, 49], the change in a solution $q(\tau), e(\tau)$ under any infinitesimal diffeomorphism associated with an arbitrary $\epsilon(\tau)$ can be described by the gauge generator (1.55) with $\xi(\tau) = \epsilon(\tau)e(\tau)$, where $e(\tau)$ is understood as a specific (fixed) function given in the solution [49]. As before, we note that $\{e, G\} = \dot{\xi}(\tau)$ coincides with the correct transformation on a solution, $\{e, G\} = \dot{\xi}(\tau) = \mathrm{d}(\epsilon(\tau)e(\tau))/\mathrm{d}\tau = \delta_{\epsilon(\tau)}e(\tau)$.[22] As a scalar density of the form $\omega(q(\tau), p(\tau); e(\tau))$ can be written, without loss of generality, as the product of a scalar $f(q(\tau), p(\tau); e(\tau))$ with the einbein, $\omega = fe$, it follows that G generates the correct transformation of any scalar density (with no explicit time dependence) on shell. In

[22]The change from the arbitrary functions $\epsilon(\tau)$ to $\xi(\tau)$ is an instance of the redefinition (A.5). In this case, the arbitrary functions considered in (A.4) correspond to $\xi(\tau)$.

fact, due to (1.4) (see also footnote 21), one may verify that the correct transformation of any worldline tensor (with no explicit dependence on τ) is generated by G. Moreover, it is clear from (1.55) that gauge transformations preserve the constraints: $\{C, G\} \approx 0$ and $\{p_e, G\} \approx 0$.

The set of diffeomorphisms generated by vectors of the form (1.54) is a proper subgroup of Diff$(\mathcal{M}, \Phi)$ that is often referred to as the 'Bergmann-Komar group' [9]. Incidentally, one notes that global translations in τ, which are generated by the vectors $V = \epsilon \mathrm{d}/\mathrm{d}\tau$ with $\epsilon =$ const., are not of the form given in (1.54), and thus are not elements of the Bergmann-Komar group [49]. Nevertheless, as mentioned above, the pullback of solutions in phase space by any diffeomorphism can be recovered from the elements of the Bergmann-Komar group.[23] Moreover, it is important to note that, in contrast to the case of a general coordinate τ, global translations in proper time are of the form (1.54) (with $\xi =$ const.).

If G generates gauge transformations, then it must map a solution to the field equations to another solution. To see that this is the case, let $f(q, p; e, p_e; \tau)$ be an auxiliary phase-space function that solves (1.29) for a given choice of λ, and define $f' := f + \delta_{\epsilon(\tau)} f \approx f + \delta^{\text{expl.}}_{\epsilon(\tau)} f + \{f, G\}$. Note that, in general, G introduces an explicit dependence on τ through $\xi(\tau)$. In this way, f' generally has an explicit time dependence even if $\partial f/\partial \tau = 0$. The time derivative of f' reads

$$\begin{aligned} \dot{f}' &\approx \dot{f} + \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\delta^{\text{expl.}}_{\epsilon(\tau)} f + \{f, G\}\right) \\ &= \frac{\partial f}{\partial \tau} + \{f, H_T\} + \frac{\partial}{\partial \tau}\delta^{\text{expl.}}_{\epsilon(\tau)} f + \{\delta^{\text{expl.}}_{\epsilon(\tau)} f, H_T\} \\ &+ \left\{\frac{\partial f}{\partial \tau}, G\right\} + \left\{f, \frac{\partial G}{\partial \tau}\right\} + \{\{f, G\}, H_T\} \ . \end{aligned} \tag{1.56}$$

It is straightforward to show that (1.56) is equivalent to $\dot{f}' \approx \partial f'/\partial \tau + \{f', H_T\}$ (as it should be). However, we must show that f' is a solution to (1.29) in terms of the transformed variables $q' = q + \delta_{\epsilon(\tau)} q$, $p' = p + \delta_{\epsilon(\tau)} p$ and $e' = e + \delta_{\epsilon(\tau)} e$ [cf. (1.14)]. This means that the total Hamiltonian should also be written as a function of $q'(\tau), p'(\tau)$

[23] As explained in [9, 49, 50], one motivation to consider the Bergmann-Komar group is the requirement of 'Legendre projectability'. This means that one should consider gauge transformations in the Lagrangian formalism that are projectable under the Legendre map (1.20). A function $f(q, \dot{q}; e, \dot{e})$ is projectable if it is the pullback of an auxiliary phase space function $g(q, p; e, p_e)$ by the Legendre map; i.e., if $f(q, \dot{q}; e, \dot{e}) = g(q, p; e, p_e)|_{p=\partial\mathcal{L}/\partial\dot{q}, p_e=\partial\mathcal{L}/\partial\dot{e}}$. This implies that f cannot change in the direction of the null eigenvector(s) of the singular Lagrangian, since $\partial f/\partial \dot{e} = \partial^2\mathcal{L}/\partial\dot{e}^2 \partial g/\partial p_e|_{p_e=\partial\mathcal{L}/\partial\dot{e}} = 0$ (a similar conclusion holds for Lagrangians that are purely kinetic terms, as considered in §1.3.2). Thus, the infinitesimal transformations $\delta_{\epsilon(\tau)} e(\tau) = \dot{\epsilon}(\tau) e(\tau) + \epsilon(\tau)\dot{e}(\tau)$ are not projectable, whereas $\delta_{\xi(\tau)} e(\tau) = \dot{\xi}(\tau)$ are, since $\xi(\tau)$ is taken to be independent of $e(\tau)$.

and $e'(\tau)$; i.e., we must use the identity [cf. (1.30)]

$$\begin{aligned} H_T' &\approx H_T + \delta^{\text{expl.}}_{\epsilon(\tau)} H_T + \{H_T, G\} \\ &\approx H_T + \left(\delta^{\text{expl.}}_{\epsilon(\tau)} \lambda\right) p_e - \{G, H_T\} \ . \end{aligned} \tag{1.57}$$

Moreover, for consistency, we demand that $\partial f'/\partial\tau = 0$ if, and only if, $\partial f/\partial\tau = 0$. In other words, we will not include the explicit time dependence induced by G in f'. This amounts to the substitution $\partial f'/\partial\tau \mapsto \partial f'/\partial\tau + \{f', \partial G/\partial\tau\}$.[24] In this way, we can rewrite (1.56) as

$$\begin{aligned} \dot{f}' &\approx \frac{\partial f'}{\partial\tau} + \left\{f', \frac{\partial G}{\partial\tau}\right\} + \{f', H_T'\} + \left\{f', \{G, H_T\} - \left(\delta^{\text{expl.}}_{\epsilon(\tau)} \lambda\right) p_e\right\} \\ &\approx \frac{\partial f'}{\partial\tau} + \{f', e'C + \lambda p_e\} + \left\{f, \frac{\partial G}{\partial\tau} + \{G, H_T\} + \{\lambda, G\} p_e\right\} \ , \end{aligned} \tag{1.58}$$

where we used the definition of the transformed variables together with (1.57) and the fact that the pullback of the initial choice of λ leads to $\delta^{\text{expl.}}_{\epsilon(\tau)}\lambda + \{\lambda, G\}$. Subsequently, we compute

$$\begin{aligned} \frac{\partial G}{\partial\tau} &= \frac{\partial\xi}{\partial\tau} C + \frac{\partial}{\partial\tau}\frac{\mathrm{d}\xi}{\mathrm{d}\tau} p_e \ , \\ \{G, H_T\} &= \{G, \lambda\} p_e + \{\xi, H_T\} C - \dot{\xi} C + \{\dot{\xi}, H_T\} p_e \ , \end{aligned} \tag{1.59}$$

from which we find

$$\frac{\partial G}{\partial\tau} + \{G, H_T\} + \{\lambda, G\} p_e = \ddot{\xi} p_e + \mathcal{O}(2) \ , \tag{1.60}$$

where we used (1.29), and the symbol $\mathcal{O}(2)$ denotes terms that are quadratic in the constraints [49], which satisfy $\{\cdot, \mathcal{O}(2)\} \approx 0$. Equation (1.60) is an instance of the general case found in (A.52). Due to (1.60), we may rewrite (1.58) as

$$\dot{f}' \approx \frac{\partial f'}{\partial\tau} + \left\{f', e'C + \left(\lambda + \ddot{\xi}\right) p_e\right\} \ , \tag{1.61}$$

which motivates us to define the transformed multiplier as

$$\lambda' := \lambda + \ddot{\xi} \ , \tag{1.62}$$

[24] Notice that, up to first order in $\xi(\tau)$, we can replace f by f' in $\{f, \partial G/\partial\tau\}$.

and, instead of (1.57), we define the transformed total Hamiltonian as $H'_T := e'C + (\lambda + \ddot{\xi})p_e$, such that (1.61) becomes $\dot{f}' \approx \partial f'/\partial\tau + \{f', H'_T\}$. In particular, the multiplier $\lambda(\tau)$ is an independent field. It transforms according to (1.62), which is consistent with the fact that $\lambda \approx \dot{e}$ and $\lambda' \approx \dot{e}'$, since $e'(\tau) = e(\tau) + \xi(\tau)$ implies that $\dot{e}'(\tau) = \dot{e}(\tau) + \ddot{\xi}(\tau)$. We thus see that any solution f to (1.29) is mapped to another solution, written in terms of the transformed variables, and the field equations remain of the same form under the transformation. In this way, G indeed generates gauge transformations.

1.6 Gauge fixing, intrinsic coordinates, and generalized reference frames

The considerations in §1.5, particularly those following (1.62), lead us to the conclusion that the arbitrariness of the multiplier $\lambda(\tau)$ in the canonical theory corresponds to the arbitrariness in the choice of diffeomorphism ϕ in (1.13), which determines the functional form of the dynamical variables via the pullback. Notice that, in principle, the choice of coordinate τ in (1.13) [and (1.32)] is inessential. It is the functional form of fields, $\phi^*q(\tau), \phi^*p(\tau)$ and $\phi^*e(\tau)$, that is of relevance to the solutions to the field equations and to the definition of observables, as we will examine in §1.7 and §1.8. A particular choice of ϕ can be enforced by imposing extra constraints (in addition to C and p_e) on the dynamical variables that fix their functional form (i.e., their dependence on τ). These additional constraints are called 'gauge conditions' or simply 'gauges' (cf. §A.2.7). In particular, the gauge conditions should fix the multiplier and thus render the evolution determined by the total Hamiltonian (1.30) well-defined. The process of choosing a gauge condition and thereby fixing λ is referred to as 'gauge fixing' or 'gauge fixation'.

Let us consider a gauge condition of the form $\chi_1(q, p; e; \tau) = 0$. Due to (1.4), we may assume that any explicit dependence on τ is of scalar type (see comment on footnote 21). In this way, if we assume that $\chi_1(q, p; e; \tau) = 0$ can be solved in terms of the einbein, we may rewrite it as

$$\chi_1(q, p; e; \tau) := e(\tau) - \omega(q, p; \tau) \ , \tag{1.63}$$

where $\omega(q, p; \tau)$ is a fixed, nonvanishing auxiliary phase-space function with a constant sign, which is a worldline scalar because it only depends on $q(\tau), p(\tau)$ and τ [cf. (1.16) and (1.17)]. As $e(\tau)$ is a scalar density, we can only impose $\chi_1 = 0$ for a certain class of charts.[25] Below, we will see how this is achieved (see also the comment in footnote 19). If we impose that (1.63) is satisfied at all instants of time, we obtain another constraint

[25]Notice that (1.63) corresponds to a fixation of $e(\tau)$ irrespective of the chosen einbein frame [cf. (1.3)]. We tacitly choose $\Omega(\tau) \equiv 1$.

[cf. (1.29)]

$$0 = \dot{\chi}_1 \approx \lambda - \dot{\omega} \ , \tag{1.64}$$

which fixes λ. Let $\Sigma|_\chi$ be the subspace of the auxiliary phase space Γ determined by $C = p_e = \chi_1 = 0$ (for all instants of time). We can then rewrite the total Hamiltonian (1.30) as

$$H_T = \omega C + \dot{\omega} p_e + \chi_1 C + \dot{\chi}_1 p_e \equiv \omega C + \dot{\omega} p_e + \mathcal{O}(2) =: H_T^{\mathrm{gf}} + \mathcal{O}(2) \ , \tag{1.65}$$

where the symbol $\mathcal{O}(2)$ now denotes terms that are quadratic in all the constraint functions (including $\chi_1, \dot{\chi}_1$) [49], such that $\{\cdot, \mathcal{O}(2)\} \approx 0$ on $\Sigma|_\chi$. For this reason, the evolution determined by H_T is well-defined on $\Sigma|_\chi$, where it also coincides with the evolution determined by the function $H_T^{\mathrm{gf}} := \omega C + \dot{\omega} p_e$, which we call the 'gauge-fixed Hamiltonian'. Notice that, due to (1.29), $\dot{\omega} \approx \{\omega, \omega C\}$ on $\Sigma|_\chi$. In particular, as the scalars $q(\tau)$ and $p(\tau)$ Poisson-commute with p_e, we find that any function of the form $f(q(\tau), p(\tau); \tau)$ obeys

$$\left.\frac{\mathrm{d}f}{\mathrm{d}\tau}\right|_{\Sigma|_\chi} = \left.\frac{\partial f}{\partial \tau}\right|_{\Sigma|_\chi} + \{f, \omega C\}_{\Sigma|_\chi} \ , \tag{1.66}$$

which is precisely the evolution determined by (1.38). It is in this sense that the canonical theory presented in §1.3.2 can be seen as a gauge-fixed version of the one presented in §1.3.1. The gauge freedom associated with the total Hamiltonian (1.38) corresponds to the freedom in choosing the specific form of the function ω. More precisely, we note that the condition (1.63) does not completely fix the gauge freedom associated with the total Hamiltonian (1.30) and the gauge generator (1.55). In other words, it does not completely fix the functional form of the fields in terms of an arbitrary coordinate τ [in the chart $(\mathcal{U}, \zeta)$; cf. §1.1]. This is a consequence of the fact that there exist diffeomorphisms $\phi : \mathcal{U} \to \mathcal{U}$ that preserve the gauge condition (1.63), and thus a 'residual' gauge (local) symmetry remains in theory even after (1.63) is fixed [49]. To see that this is true, we need to show that there exists a one-parameter family of diffeomorphisms ϕ_l such that

$$\chi_1(\phi_l^* q, \phi_l^* p; \phi_l^* e; \tau) := \phi_l^* e(\tau) - \omega(\phi_l^* q, \phi_l^* p; \tau) = 0 \tag{1.67}$$

holds if $\chi_1(q, p; e; \tau) = 0$ is satisfied for a given solution $(q(\tau), p(\tau), e(\tau))$ to the field equations obtained from (1.32) [or from (1.13)]. Notice that the explicit time dependence in (1.67) is not transformed [in relation to $\chi_1(q, p; e; \tau) = 0$] because we are interested in the possibility that a different solution $(\phi_l^* q(\tau), \phi_l^* p(\tau), \phi_l^* e(\tau))$ to the field equations (a different functional form of the fields), written with respect to the same arbitrary coordinate τ, may still satisfy the gauge condition. This is line with the symmetry exhibited in (1.13). As before, we consider that ϕ_l are generated by the vector field (1.54). In this way, the residual symmetries are found as solutions to the equation [cf. (1.16), (1.17) and (1.53)]

$$0 \approx \chi_1(\phi^*_{\delta l}q, \phi^*_{\delta l}p; \phi^*_{\delta l}e; \tau) - \chi_1(q, p; e; \tau) \approx \{\chi_1, G\} \approx -\{\omega, C\}\xi(\tau) + \dot{\xi}(\tau) \ . \tag{1.68}$$

It is straightforward to verify that the solution to (1.68) is

$$\xi(\tau) = \xi(\tau_0) \exp\left[\int_{\tau_0}^{\tau} \mathrm{d}\tau' \ \left(\{\omega, C\}(\tau')\right)\right] \ , \tag{1.69}$$

and the initial value $\xi(\tau_0)$ is arbitrary. The residual gauge transformations are generated by $G = \xi(\tau)C + \dot{\xi}(\tau)p_e$ with $\xi(\tau)$ given by (1.69). In particular, due to the arbitrariness of $\xi(\tau_0)$ and the fact that the value of τ_0 may be freely chosen, the residual gauge transformations of scalars at τ_0, $\delta_{\epsilon(\tau_0)}f(q, p; \tau) \approx \delta^{\text{expl.}}_{\epsilon(\tau_0)}f + \xi(\tau_0)\{f, C\}$, encompass all the gauge freedom of the theory presented in §1.3.2. Indeed, for any value of τ_0, $\xi(\tau_0)C$ is the gauge generator associated with the total Hamiltonian (1.38). If one repeats the derivation of (1.61) for this particular case (with ω understood as a multiplier), one finds that the field equations with respect to τ_0 remain of the same form under the transformations generated by $\xi(\tau_0)C$, provided the multiplier is transformed as $\omega \mapsto \omega' = \omega + \mathrm{d}\xi/\mathrm{d}\tau_0$ [instead of (1.62)]. This is consistent with the fact that the multiplier $\omega(\tau)$ can be chosen as the einbein in this particular case [cf. (1.40)].

In order to eliminate the residual gauge symmetry, it is necessary to impose an additional gauge condition. As the einbein has been fixed by (1.63), we consider a condition on the scalars, $\chi_2(q, p; \tau) = 0$, which must be chosen so as to remove the residual diffeomorphisms and to be preserved by the evolution determined by (1.65) [49]. The residual gauge transformations that preserve $\chi_2(q, p; \tau)$ are solutions to the equation

$$0 \approx \chi_2(\phi^*_{\delta l}q, \phi^*_{\delta l}p; \tau) - \chi_2(q, p; \tau) \approx \{\chi_2, G\} \approx \xi(\tau)\{\chi_2, C\} \ , \tag{1.70}$$

where $\xi(\tau)$ is given by (1.69). If (1.70) only admits the trivial solution ($\xi(\tau) = 0$), then the residual symmetry has been eliminated. This corresponds to setting the arbitrary initial value in (1.69) to zero, $\xi(\tau_0) = 0$. We note that (1.70) only admits the trivial solution if $\{\chi_2, C\} \neq 0$. Furthermore, we now use the symbol $\Sigma|_\chi$ to denote the subspace of the auxiliary phase space determined by $C = p_e = \chi_1 = \chi_2 = 0$ (for all instants of time). The condition $\chi_2(q, p; \tau) = 0$ is preserved by the evolution in $\Sigma|_\chi$ if

$$0 \approx \frac{\partial \chi_2}{\partial \tau} + \{\chi_2, H^{\text{gf}}_T\} \approx \frac{\partial \chi_2}{\partial \tau} + \omega(q, p; \tau)\{\chi_2, C\} \ , \tag{1.71}$$

where we used (1.65) and the constraints are imposed only after the Poisson brackets are computed. If χ_2 satisfies (1.71) and $\{\chi_2, C\} \neq 0$, then the set of gauge conditions (χ_1, χ_2) completely fixes the gauge freedom of the theory presented in §1.3.1 (and χ_2 completely fixes the freedom of the particular case discussed in §1.3.2). In this case, there are no nontrivial diffeomorphisms that preserve the gauge conditions (χ_1, χ_2). Nevertheless, we must still ascertain if these conditions are accessible; i.e., if it is possible to start with a solution $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ to the field equations [written in an arbitrary chart $(\mathcal{U}, \zeta)$ in the worldline] for which $\chi_1 \neq 0$ and $\chi_2 \neq 0$, and subsequently perform a well-defined diffeomorphism to reach a solution $\mathcal{S}_0(\tau)$ for which the conditions are satisfied. In other words, the gauge conditions are accessible if there exists a diffeomorphism $\phi_{\mathcal{S}}$ that fulfills

$$\begin{aligned} 0 &= \chi_i(\phi_{\mathcal{S}}^* q, \phi_{\mathcal{S}}^* p; \phi_{\mathcal{S}}^* e; \tau) \ , \\ 0 &\neq \chi_i(q, p; e; \tau) \ , \end{aligned} \tag{1.72}$$

for $i = 1, 2$. If the pair (χ_1, χ_2) is chosen such that (1.72) has a solution for $\phi_{\mathcal{S}}$ without a residual gauge symmetry, then we say (χ_1, χ_2) forms a complete gauge fixing (cf. §A.2.7).[26] Notice, however, that the diffeomorphism $\phi_{\mathcal{S}}$ that solves (1.72) will generally depend on the arbitrary solution $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$. For this reason, the complete gauge fixing induces a map on the gauge orbit of $\mathcal{S}(\tau)$,

$$\begin{aligned} P_{(\chi_1,\chi_2)} : [\mathcal{S}(\tau)] &\to [\mathcal{S}(\tau)] \\ \mathcal{S}(\tau) &\mapsto \phi_{\mathcal{S}}^* \mathcal{S}(\tau) = \mathcal{S}_0(\tau) \end{aligned} \tag{1.73}$$

which projects any solution on the gauge orbit to the solution $\mathcal{S}_0(\tau)$ that satisfies the gauge conditions. This map is not injective, as different arbitrary solutions are mapped to the same $\mathcal{S}_0(\tau)$. In this way, we conclude that the transformation $(q(\tau), p(\tau), e(\tau)) \mapsto (\phi_{\mathcal{S}}^* q(\tau), \phi_{\mathcal{S}}^* p(\tau), \phi_{\mathcal{S}}^* e(\tau))$, where $\phi_{\mathcal{S}}$ solves (1.72), is not canonical because it is not invertible, and thus the fixation of the gauge freedom does not preserve the Poisson brackets.[27] This stands in contradistinction to (1.53), which is an on-shell canonical transformation. The crucial difference between (1.53) and (1.73) is that any worldline tensor is pulled back by the same diffeomorphism in (1.53). This induces an invertible map on the gauge orbit, $\mathcal{S}(\tau) \mapsto \phi^* \mathcal{S}(\tau)$; i.e., any solution on $[\mathcal{S}(\tau)]$ is pulled back by the same ϕ, and this simply corresponds to a "displacement" along the orbit. In contrast, different solutions are "displaced" differently (pulled back by a different $\phi_{\mathcal{S}}$)

[26] More precisely, the condition $\{\chi_2, C\} \neq 0$ may only be fulfilled in certain regions of the auxiliary phase space. The pair (χ_1, χ_2) only forms a complete gauge fixing when restricted to such regions. See the comments following (A.71).

[27] This observation was discussed and clarified in [11], where Pons *et al.* use a formalism that, although different from the one we present here, yields results that are equivalent to ours at the classical level. The quantum theory was not discussed. See also footnote 30.

in (1.73).

What is then the significance of (1.73)? It corresponds to a choice of origin in the gauge orbit, as was discussed in the paragraph preceding (1.14). Indeed, any solution on $[\mathcal{S}(\tau)] = [\mathcal{S}_0(\tau)]$ can be written as

$$\mathcal{S}(\tau) = \left(\phi_{\mathcal{S}}^{-1}\right)^* \mathcal{S}_0(\tau) \ , \tag{1.74}$$

and the fact that $\phi_{\mathcal{S}}$ differs from one solution to another simply means that it encodes the "displacement" along the gauge orbit from the origin $\mathcal{S}_0(\tau)$ to $\mathcal{S}(\tau)$. If $\mathcal{S}(\tau)$ coincides with $\mathcal{S}_0(\tau)$, then $\phi_{\mathcal{S}}$ is the identity. Moreover, if the choice of origin is changed, $\mathcal{S}_0(\tau) = \phi_0^* \tilde{\mathcal{S}}_0(\tau)$, then the "displacement" is also changed, $\tilde{\phi}_{\mathcal{S}} = \phi_{\mathcal{S}} \circ \phi_0^{-1}$, so as to keep $\mathcal{S}(\tau)$ invariant. Conversely, for a fixed choice of origin, the gauge transformation $\mathcal{S}(\tau) \mapsto \tilde{\mathcal{S}}(\tau) = \phi^* \mathcal{S}(\tau)$ implies that $\phi_{\mathcal{S}} \mapsto \tilde{\phi}_{\mathcal{S}} = \phi^{-1} \circ \phi_{\mathcal{S}}$, such that the origin is invariant

$$\tilde{\phi}_{\mathcal{S}}^* \tilde{\mathcal{S}}(\tau) = \phi_{\mathcal{S}}^* \mathcal{S}(\tau) = \mathcal{S}_0(\tau) \ . \tag{1.75}$$

This is merely a rewriting of (1.73), and it means that the map $P_{(\chi_1,\chi_2)}$ is constant along the gauge orbit (by definition). As the gauge transformations (1.53) are on-shell canonical transformations [expressed in terms of the Poisson brackets with respect to the $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ fields as well as p_e], one then expects that $P_{(\chi_1,\chi_2)}(\mathcal{S}(\tau))$ (understood as a function on the auxiliary phase space) weakly Poisson-commutes with the gauge generator. We will see that this is indeed the case in §1.8. Finally, we note that the choice of origin on each gauge orbit corresponds to a choice of section ℓ that selects a representative in each equivalence class, $\ell([\mathcal{S}(\tau)]) = \mathcal{S}_0(\tau)$.

Let us now analyze how a complete gauge fixing (χ_1, χ_2) can be seen as a definition of a chart $(\mathcal{U}_\chi, \zeta)$ in the worldline. Notice that (1.71) implies that the gauge condition χ_2 must have an explicit time dependence, $\partial\chi_2/\partial\tau \neq 0$, because $\{\chi_2, C\} \neq 0$ and $\omega \neq 0$. This well-known fact [49, 51] has important consequences for the definition of observables and the physical interpretation of the theory, as we will discuss in §1.7. Indeed, as it depends explicitly on time, we may interpret $\chi_2(q, p; \tau) = 0$ as a definition of the arbitrary worldline coordinate τ in terms of the canonical scalars $q(\tau), p(\tau)$ [49]. To see this, let us assume that one can solve $\chi_2(q, p; \tau) = 0$ for its explicit time dependence, such that we may rewrite this constraint as

$$\chi_2(q, p; \tau) := \chi(q(\tau), p(\tau)) - \tau \ , \tag{1.76}$$

where $\chi(q(\tau), p(\tau))$ is a worldline scalar with no explicit dependence on τ. Given a certain solution to the field equations (with fixed boundary conditions), we may interpret χ as a function solely of τ, $\chi(\tau) \equiv \chi(q(\tau), p(\tau))$. The condition $\{\chi_2, C\} \neq 0$

is then translated to

$$0 \neq \{\chi, C\} \approx \frac{1}{\omega(q,p;\tau)}\{\chi, H_T^{\mathrm{gf}}\} \approx \frac{1}{\omega(q,p;\tau)}\frac{\mathrm{d}\chi}{\mathrm{d}\tau} = \frac{\mathrm{d}\chi}{\mathrm{d}\eta}\ , \tag{1.77}$$

which is the condition that $\chi(\tau)$ is invertible ($\omega \neq 0$). Let us then assume that there exists an interval $\mathcal{I}_\chi = (\tau_0, \tau_1)$ in which $\chi(\tau)$ is a diffeomorphism; i.e., it is smooth with a smooth inverse. There may be several such intervals, and they may depend on the boundary conditions that define the solution to the field equations (cf. footnote 26). If $\chi_2 = 0$ is not fulfilled for the solution in question, we may use (1.72) to reach a functional form of the fields that enforces this gauge condition. It is straightforward to see that the solution to $0 = \chi(\phi_{\mathcal{S}}^* q, \phi_{\mathcal{S}}^* p) - \tau \equiv \phi_{\mathcal{S}}^* \chi(\tau) - \tau$ is simply $\phi_{\mathcal{S}} = \chi^{-1}$; i.e., the diffeomorphism corresponds to the function that is the inverse of $\chi(\tau)$.

The above considerations can be used to define a chart $(\mathcal{U}_\chi, \zeta)$ as follows: first, we let ζ be an arbitrary homeomorphism, and we define $\mathcal{U}_\chi := \zeta^{-1}(\mathcal{I}_\chi)$, where $\mathcal{I}_\chi$ is an interval in which (1.77) holds. Second, we define the composition $\tilde{\chi} := \chi \circ \zeta : \mathcal{U}_\chi \to \chi(\mathcal{I}_\chi)$, which is assumed to be a smooth function. Under an arbitrary diffeomorphism $\phi : \mathcal{U}_\chi \to \mathcal{U}_\chi$, we obtain $\tilde{\chi}' := \phi^* \tilde{\chi} = \tilde{\chi} \circ \phi$, such that $\tilde{\chi}'(\mathcal{U}_\chi) = \tilde{\chi}(\mathcal{U}_\chi)$; i.e., the image of $\tilde{\chi}$ is preserved. If the condition $\tilde{\chi} = \zeta$ is not satisfied for the given solution to the field equations, we consider the diffeomorphism $\phi_{\mathcal{S}} := \zeta^{-1} \circ \chi^{-1} \circ \zeta : \mathcal{U}_\chi \to \mathcal{U}_\chi$,[28] such that $\tilde{\chi}' = \tilde{\chi} \circ \phi_{\mathcal{S}} = \zeta$. Although this may be interpreted as the condition that enforces that $\tilde{\chi}'$ is equal to an arbitrarily chosen coordinate map, it may alternatively be seen as the definition of the coordinate map in terms of a combination of the dynamical fields. The possible values of the time coordinate τ are elements of the image of this combination, $\tilde{\chi}(\mathcal{U}_\chi)$, which is invariant under diffeomorphisms. In this way, a complete gauge fixing corresponds to a choice of chart in the worldline.

There may be more than one choice of $\chi_2(q,p;\tau)$ that is compatible with $\chi_1(q,p;e;\tau)$, in the sense of providing a complete gauge fixing. First, notice it is often more convenient to consider that (1.71) determines which function $\omega(q,p;\tau)$ can be used in (1.63) for a given choice of $\chi_2(q,p;\tau)$. For example, we find $\omega(q,p;\tau) \equiv \omega(q(\tau),p(\tau)) \approx 1/\{\chi, C\}$ from (1.71) for the choice (1.76). Furthermore, let us consider the choices $\chi_2^{(1)}(q,p;\tau) := \chi(q,p) - \tau$ and $\chi_2^{(2)}(q,p;\tau) := \chi(q,p) + \mathcal{O}(q,p) - \tau$ where $\mathcal{O}(q,p)$ weakly Poisson-commutes with C. Due to (1.77), both choices determine the same function $\omega(q,p;\tau) \equiv \omega(q(\tau),p(\tau)) \approx 1/\{\chi, C\}$ to be used in (1.63). Therefore, both $\chi_2^{(1)}(q,p;\tau)$ and $\chi_2^{(2)}(q,p;\tau)$ form a complete gauge fixing in conjunction with $\chi_1(q,p;e;\tau)$. Never-

[28] Recall that, as we are considering a smooth atlas on $\mathcal{M}$, for any two charts $(\mathcal{U}_1, \zeta_1)$ and $(\mathcal{U}_2, \zeta_2)$ with $\mathcal{U}_1 \cap \mathcal{U}_2 \neq \emptyset$, the transition map $\zeta_2 \circ \zeta_1^{-1}$ is a diffeomorphism. The local coordinate representation of ϕ is $\phi_{\zeta_2\zeta_1} = \zeta_2 \circ \zeta^{-1} \circ \chi^{-1} \circ \zeta \circ \zeta_1^{-1}$ (cf. §1.1), which is a composition of smooth maps, and is therefore smooth. Its inverse, $\phi_{\zeta_1\zeta_2}^{-1} = \zeta_1 \circ \zeta^{-1} \circ \chi \circ \zeta \circ \zeta_2^{-1}$, is also smooth. In particular, for the single chart $(\mathcal{U}_\chi, \zeta)$, we obtain $\phi_\zeta = \chi^{-1}$, which is itself assumed to be a diffeomorphism, as we discussed in the preceding paragraph.

theless, the coordinate maps that are determined by $\chi_2^{(1)}(q,p;\tau)$ and $\chi_2^{(2)}(q,p;\tau)$ may be different. It is in this sense that the gauge condition $\chi_1 = 0$ can only be imposed in a certain class of charts, as mentioned before. Likewise, the fixation of the multiplier $\lambda(\tau)$ through (1.64) corresponds to the definition of a class of charts in the worldline.

The above discussion leads us to the conclusion that a complete gauge fixing yields an intrinsic definition of the time coordinate, as explained in the **Introduction**. The level sets of $\chi(q(\tau), p(\tau))$ in (1.76) represent of instants of time in the regions of the auxiliary phase space where $\{\chi, C\} \neq 0$ [cf. footnote 26 and (1.77)]. In this way, instants are defined 'intrinsically' from the dynamics, and one does not invoke extrinsic absolute notions of time. The function $\chi(q(\tau), p(\tau))$ serves as a 'generalized clock' with respect to which the dynamics can be described, and $(\mathcal{U}_\chi, \tilde{\chi}' = \zeta)$ is an intrinsic chart (cf. the **Introduction**). In general, a function of the dynamical degrees of freedom that is continuous in $\mathcal{M}$ is a generalized clock if it serves as a local coordinate map on the worldline; i.e., if there exists an open region $\mathcal{U}_\chi \subset \mathcal{M}$ where χ is a homeomorphism (invertible with a continuous inverse). Thus, a complete gauge fixing entails a choice of generalized clock.

In the $(0+1)$-dimensional universe modeled by $(\mathcal{M}, \Phi)$, experiments consist of measurements of the dynamical fields at certain instants of time. Different instants are distinguished solely by the readings of generalized clocks defined from the dynamical degrees of freedom. Each observer (experimenter) uses a choice of generalized clock to record the experimental results. Therefore, observers employ complete gauge fixings in their description of the dynamics. For this reason, we consider that that a complete gauge fixing defines a 'generalized reference frame' with respect to which an experimenter makes observations. We will take the following terms as synonyms: complete gauge fixing; generalized clock; generalized reference frame; intrinsic chart. Moreover, even though the fixation of the multiplier $\lambda(\tau)$ corresponds to a class of charts (generalized clocks), we will also refer to a choice of $\lambda(\tau)$ as a choice of generalized reference frame (cf. §A.2.5). The fact that $\lambda(\tau)$ is undetermined signals that the theory does not depend on a preferred choice of frame. Due to (1.61) and (1.62), we see that G generates changes of reference frames.

Finally, we note that the number of gauge conditions in a complete gauge fixing (that are independent at each instant of time) is equal to the number of first-class constraints ($p_e = 0$ and $C = 0$). This is a general feature of canonical gauge systems (cf. §A.2.7). Although conditions of the form (1.63) and (1.76) are well motivated, it is possible consider more general gauge conditions, which may depend on λ and the canonical variables, as well as on their time derivatives. We will focus on the so-called 'canonical gauge conditions' (or 'canonical gauges'), which have the form $\chi(q,p;e;\tau) = 0$. From the above discussion (see also §A.2.7), we conclude that a set of independent canonical gauge conditions (χ_1, χ_2) is admissible or forms a complete gauge fixing if: (1) they are accessible, which means that any arbitrary set of canonical variables can be mapped to one that satisfies $\chi_{(1,2)} = 0$ by a finite gauge transformation associated with a definite choice of $\xi(\tau)$; (2) the conditions $\chi_{(1,2)} = 0$ are only preserved by the gauge transformations that correspond to on-shell identity transformations, which are the ones determined by $\xi(\tau) \approx 0$ for all instants of time. Clearly, this only holds if

$$\det \begin{pmatrix} \{\chi_1, p_e\} & \{\chi_1, C\} \\ \{\chi_2, p_e\} & \{\chi_2, C\} \end{pmatrix} \neq 0 \ . \tag{1.78}$$

The determinant (1.78) is an instance of (A.70), and it is called the 'Faddeev-Popov determinant' [20, 21]. In the particular case in which χ_1 and χ_2 are given by (1.63) and (1.76), respectively, we find that the determinant (1.78) coincides with $\{\chi, C\} \neq 0$, as we have previously discussed. As in the case of $\{\chi, C\} \neq 0$, the determinant (1.78) may be nonvanishing only in certain regions of the auxiliary phase space, and it may be impossible to define gauge conditions which globally satisfy (1.78). This impossibility is the well-known 'Gribov obstruction' (cf. §A.2.7), and it implies that complete gauge fixings (and thus generalized reference frames) are typically local constructions.

1.7 Observables and invariant extensions

We have seen in §1.5 and §1.6 that the arbitrariness of the multiplier $\lambda(\tau)$ is equivalent to the arbitrariness in the choice of diffeomorphism in (1.13), which in turn corresponds to a choice of generalized reference frame (complete gauge fixing; intrinsic chart). It is precisely the arbitrariness in the choice of reference frames that must be addressed by the definition of observables in gauge theories. Observable quantities must have a well-defined time evolution, in contrast to the indeterministic character of the evolution dictated by the total Hamiltonian (1.30) [or (1.38)].

In the usual gauge theories of internal symmetries (such as the Yang-Mills theories of the standard model of particle physics), in which the gauge freedom does not involve a definition of the time coordinate nor the functional form of the fields with respect to their time dependence, it is customary to define observables as gauge-invariant quantities. The reason for this is simple: in these theories, the total Hamiltonian involves a term that does not vanish on the constraint hypersurface, denoted by H_0, and a term δH which is a combination of constraints and involves the arbitrary multipliers [see (A.47) and (A.66)]. If an auxiliary phase-space function $\mathcal{O}$ is gauge invariant, it must weakly Poisson-commute with the constraints (cf. Definition A.1), and thus it weakly Poisson-commutes with δH. In this way, the evolution of a gauge-invariant function is well-defined because it is independent of the arbitrary multipliers, $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau + \{\mathcal{O}, H_T\} \approx \partial\mathcal{O}/\partial\tau + \{f, H_0\}$.

Is there an analogous result for the case of diffeomorphisms? The answer is yes, although a few preliminary comments are in order. First, diffeomorphisms constitute an 'external' symmetry, in the sense that they involve a definition of the time coordinate or the functional form of the fields with respect to their τ dependence, as we have seen in the preceding sections. Second, the total Hamiltonian is a combination of the (primary and secondary) constraints [cf. (1.30) or (1.38)], such that it vanishes on the constraint hypersurface and $H_0 \equiv 0$. In this way, if one requires that observables weakly Poisson-commute with all the constraints [and, therefore, with the gauge generator (1.55)], one reaches the apparently unsatisfactory conclusion that the evolution of an observable $\mathcal{O}$ is solely encoded in its explicit time dependence [9, 11, 12], $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau + \{\mathcal{O}, H_T\} \approx \partial\mathcal{O}/\partial\tau$. Although this evolutionary law is well-defined (as it does not depend on arbitrary multipliers), it hardly fits the canonical paradigm of orbits in phase space generated by a Hamiltonian vector field. Third, it is important to note that the requirement that $\mathcal{O}$ Poisson-commutes with the constraints does not render it gauge (diffeomorphism) invariant, in contrast to the case of internal symmetries, because of its explicit time dependence. Indeed, we find from (1.53) the transformation $\delta_{\epsilon(\tau)}\mathcal{O} = \delta^{\text{expl.}}_{\epsilon(\tau)}\mathcal{O}$. Then, if one further requires that $\mathcal{O}$ does not have an explicit dependence on τ, such that it is a diffeomorphism invariant, one reaches the seemingly paradoxical conclusion that only constants can be observed; i.e., one finds $\dot{\mathcal{O}} \approx 0$. These difficulties with the determination of a well-defined evolutionary law for observables in a diffeomorphism-invariant theory are collectively referred to as the 'problem of time' [22–24].

It is the opinion of the author of this thesis that the classical problem of time is nothing but a confusion (or, at best, a matter of semantics), although its quantum counterpart is more serious due to the measurement problem. Let us then analyze a solution to the classical "problem", which will inspire us to develop a method of construction and interpretation of dynamical observables in the quantum theory (cf. §2.5.1, §2.5.2). We will see that the aforementioned pictures of evolution, $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau$ or $\dot{\mathcal{O}} \approx 0$, can be reconciled with the usual picture of orbits generated by a Hamiltonian vector field (in principle), and that this also informs us on how the quantum theory can be built. The key is to primarily define observables as quantities that can be, in principle, measured in an experiment and that have a well-defined time evolution. Their diffeomorphism invariance (or lack thereof) follows as a secondary quality.

To begin with, let us note that diffeomorphism invariants can be obtained by integrating worldline one-forms $\omega(\tau)\mathrm{d}\tau$ over an interval $\mathcal{I} = (\tau_0, \tau_1) \subset \mathcal{M}$,

$$\mathcal{O}_\omega = \int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \omega(\tau)\ , \tag{1.79}$$

as was discussed in [52–56]. Note that the proper time (1.2) and the action (1.5) are particular examples of such objects. It is straightforward to verify that (1.79) is invariant under arbitrary diffeomorphisms if the integral converges and appropriate boundary conditions for $\omega(\tau)$ are adopted. Alternatively, as in the case of the action (cf. footnote 10), one could leave the boundary values $\omega(\tau_0)$ and $\omega(\tau_1)$ unspecified and add suitable boundary terms to the right-hand side of (1.79). It is also possible to restrict the (infinitesimal) diffeomorphisms considered by selecting boundary conditions for $\epsilon(\tau)$. For example, one notes from (1.17) that (1.79) remains invariant if $\epsilon(\tau)$ and $\omega(\tau)$ satisfy periodic boundary conditions, $\epsilon(\tau_0) = \epsilon(\tau_1), \omega(\tau_0) = \omega(\tau_1)$. Moreover, if $\mathcal{M}$ is isomorphic to $\mathbb{R}$ and $\omega(\tau)$ is integrable, one could take $\tau_0 \to -\infty$ and $\tau_1 \to +\infty$ and consider the condition $\lim_{|\tau|\to\infty} \omega(\tau)\epsilon(\tau) = 0$ such that (1.79) is invariant.

The physical relevance of (1.79) is, however, often elusive. As was argued in the **Introduction**, the diffeomorphism invariants that have a straightforward physical interpretation are relational observables, which encode the values of the dynamical fields relative to a choice of generalized clock. Following the arguments in the **Introduction** and §1.6, we conclude that one should consider complete gauge fixings, which correspond to the definition of generalized reference frames adopted by an observer in the description of an experiment. We will see how these gauge fixings lead to diffeomorphism invariants.

It is worthwhile to mention that, although the diffeomorphism and reparametrization invariance of the action (1.5) implies that any arbitrary choice of coordinate map is permissible, it is crucial that the complete gauge fixing be based on canonical gauge conditions; i.e., it is paramount that time be defined through a combination of the canonical fields of the theory. An arbitrary coordinate map has no direct physical interpretation, it is merely a choice of parametrization. In contrast, if time is defined by (the level sets of) a generalized clock χ, this corresponds to an experimental setup that can, in principle be realized: the dynamics is described with respect to the evolution of the clock. In this way, as was remarked in the **Introduction** and [33], the dynamics of a gauge theory admits a relational interpretation in the sense that the degrees of freedom can be understood with respect to (or relative to) a generalized reference frame (complete gauge fixing).[29]

Let us then consider an observer who describes experiments and measurements with respect to a generalized clock $\chi(q(\tau), p(\tau))$. The observer adopts a complete gauge fixing defined by the conditions (1.63) and (1.76), with $\omega(q, p; \tau) \equiv \omega(q(\tau), p(\tau)) := 1/\{\chi, C\} \approx 1/\{\chi + \mathcal{O}, C\}$, where $\mathcal{O}$ is any auxiliary phase-space function that weakly Poisson-commutes with C. Note that $\omega(q(\tau), p(\tau)) \neq 0$ has a constant sign due to the gauge condition (1.63). The dynamics recorded by the observer can be written in terms of a solution $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ to the field equations written in an arbitrary frame as $\mathcal{S}_0(\tau) = (q'(\tau) := \phi^*_{\mathcal{S}} q(\tau), p'(\tau) := \phi^*_{\mathcal{S}} p(\tau), e'(\tau) := \phi^*_{\mathcal{S}} e(\tau))$, where $\phi_{\mathcal{S}} = \chi^{-1}$ [cf. discussion after (1.77)]. Thus, the solution $\mathcal{S}_0(\tau) = (q'(\tau), p'(\tau), e'(\tau))$ satisfies the gauge conditions, and we say it is 'gauge-fixed'. In the generalized reference frame of the observer, any auxiliary phase-space function of the form $f' := f(q', p'; e'; \tau)$ evolves

[29] Notice that, in theory, the generalized reference frame or gauge conditions can be arbitrarily chosen at each instant. Nevertheless, in a feasible experimental arrangement, one expects that a generalized clock is used to record the dynamics throughout a certain succession of instants.

according to

$$\dot{f}' \approx \left.\frac{\partial f}{\partial \tau}\right|_{\Sigma|_\chi} + \omega(q', p')\{f, C\}_{\Sigma|_\chi} + \dot{\omega}(q', p')\{f, p_e\}_{\Sigma|_\chi} \,, \tag{1.80}$$

where we used (1.29) and (1.65) and, as before, all the constraints (including the gauge conditions or the pullback by $\phi_{\mathcal{S}}$) are imposed only after the partial time derivative and the Poisson brackets are evaluated. This is a well-defined evolution law because no arbitrary multipliers are present [$\omega(q', p')$ is fixed]. In this way, we assume that (1.80) is integrable and a choice of initial conditions uniquely determines the solution (see also the discussion in §1.9.2). As was mentioned in the end of §1.6, the gauge indeterminism of the evolution law (1.29) is then understood as the indetermination in the choice of reference frame (there is no preferred frame). This choice is left to the observer. Any observer who employs χ as a generalized clock will record the dynamics according to (1.80), and the observations will be cast in terms of the solution $\mathcal{S}_0(\tau) = (q'(\tau), p'(\tau), e'(\tau))$. In this way, it is reasonable to define any function $f' = f(q', p'; e'; \tau)$ as an observable. There is no "problem" of time for this definition, although there is the need to specify with respect to which clock χ (or, more precisely, which intrinsic chart) the dynamics is described. To be clear, we consider that the solution to the classical "problem" of time is to define observables as gauge-fixed quantities. But how is this definition related to diffeomorphism invariants? And how can the evolution (1.80) be connected with the laws $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau$ or $\dot{\mathcal{O}} \approx 0$? The answer depends on the concept of 'invariant extensions', which we now briefly discuss (see§A.2.6 for a general discussion on gauge orbits and §A.2.7 for further details on invariant extensions).

First, let us consider a function $f : \mathcal{M} \to \mathcal{M}$ that only has an explicit time dependence. As it is a scalar, this function is not invariant under diffeomorphisms, $\delta_{\epsilon(\tau)} f(\tau) = \epsilon(\tau)\mathrm{d}f/\mathrm{d}\tau$ [cf. (1.17)]. Nevertheless, for any fixed instant $\tau = s$, we can define a constant function $\mathcal{O}[f|\tau = s] : \mathcal{M} \to \mathbb{R}$, $\mathcal{O}[f|\tau = s](\tau) = f(s)$ that coincides with f at $\tau = s$. This constant worldline scalar is trivially invariant, $\delta_{\epsilon(\tau)}\mathcal{O}[f|\tau = s] = 0$, and it is called the invariant extension of $f(\tau)$ at $\tau = s$.

Second, let us consider an auxiliary phase-space function without explicit time dependence, $f(q(\tau), p(\tau); e(\tau)) \equiv f(\mathcal{S}(\tau))$. Under a gauge transformation, $\mathcal{S}(\tau) \mapsto \phi^*\mathcal{S}(\tau)$, the function is transformed, $f \mapsto \phi^* f \equiv f(\phi^*\mathcal{S}(\tau))$. We may regard $f(\mathcal{S}(\tau))$ as a function on the gauge orbit $[\mathcal{S}(\tau)]$, in which case the gauge-fixed function $f' := \phi^*_{\mathcal{S}} f = f(\phi^*_{\mathcal{S}}\mathcal{S}(\tau)) = f(\mathcal{S}_0(\tau))$ corresponds to the image of a single point in the orbit. Due to (1.74) and (1.75), this point can be seen as an invariant choice of origin in $[\mathcal{S}(\tau)]$, and thus $f(\mathcal{S}_0(\tau))$ is also invariant. More precisely, we can define the constant map $\mathcal{O}[f|\chi = \tau] : [\mathcal{S}(\tau)] \to [\mathcal{S}(\tau)]$, $\mathcal{O}[f|\chi = \tau](\mathcal{S}(\tau)) := f(\mathcal{S}_0(\tau))$, of which the map (1.73) is a particular case. Notice that the image of $\mathcal{O}[f|\chi = s]$ is a function on the worldline that is not necessarily constant. Since $\mathcal{O}[f|\chi = \tau]$ is constant along the gauge orbit (by definition) and it coincides with f at the origin $\mathcal{S}_0(\tau)$, it is called the invariant extension of f in the gauge $\phi^*_{\mathcal{S}}\chi = \tau$ [33]. Notice that invariance here refers only to the fact that $\mathcal{O}[f|\chi = \tau]$ remains the same under changes in the functional form of the fields $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ generated by G [cf. (1.53)], but it does not concern a possible explicit time dependence that $\mathcal{O}[f|\chi = \tau]$ may acquire when expressed in terms of $\mathcal{S}(\tau)$ (see §1.8 and §1.9.1). For this reason, we expect that $\mathcal{O}[f|\chi = \tau]$ (understood as a function in the auxiliary phase space) weakly-Poisson commutes with the gauge generator, given that the Poisson brackets are written in terms of the $(q(\tau), p(\tau), e(\tau), p_e(\tau))$ fields [cf. (1.27)], but it may have a nonvanishing explicit time derivative. We will confirm this in §1.8 and §1.9.1. Intuitively, the invariance under changes in the functional form of the fields generated by G follows from the fact that, in fixing the generalized reference frame defined by χ, all other frames become "irrelevant".

Third, let us now consider the general case of an auxiliary phase-space function with an explicit time dependence, $f(q(\tau), p(\tau); e(\tau); \tau) \equiv f(\mathcal{S}(\tau); \tau)$. Combining the results of the two previous paragraphs, we conclude that the gauge-fixed observable $f' = f(q'(\tau), p'(\tau); e'(\tau); \tau) \equiv f(\mathcal{S}_0(\tau); \tau)$ may be promoted to a diffeomorphism invariant at a fixed instant of time $\tau = s$; i.e., we define its invariant extension as

$$\begin{aligned} \mathcal{O}[f|\chi = s]:\ & \mathcal{M} \to \mathbb{R} \\ & p \mapsto f'|_{\tau=s} = f(\mathcal{S}_0(s); s)\ , \end{aligned} \tag{1.81}$$

for a fixed value of s. In (1.81), the letter p stands for a point in the worldline, the coordinate representation of which is τ in the intrinsic chart $(\mathcal{U}_\chi, \tilde{\chi}')$ defined by the gauge condition (cf. §1.6). In this way, the quantity $\mathcal{O}[f|\chi = s]$ is a constant worldline scalar, which is defined from a solution to the field equations. It can also be understood as a constant function on the gauge orbit $[\mathcal{S}_0(\tau)]$, the image of which is the constant worldline scalar $f(\mathcal{S}_0(s); s)$ (as opposed to the function $f(\mathcal{S}_0(\tau); \tau)$, which is not necessarily constant on the worldline). Therefore, it trivially satisfies the invariance properties: $\dot{\mathcal{O}}[f|\chi = s] \approx 0$ and $\delta_{\epsilon(\tau)}\mathcal{O}[f|\chi = s] \approx 0$; i.e., it is a diffeomorphism invariant. In this sense, one recovers the "frozen time" picture $\dot{\mathcal{O}} \approx 0$ mentioned above. Nevertheless, this picture is hardly illuminating: time is frozen simply because one is focusing on a single instant. Indeed, the invariant extension encodes the value of the quantity f' in the instant in which the generalized clock χ has the value s.

As it represents f' in relation to a (fixed) value of the clock, it is more customary to refer to $\mathcal{O}[f|\chi = s]$ as a relational observable [57, 58]. It is also important to mention that, although gauge invariant, relational observables are gauge-dependent objects (in the sense explained in Definition A.2). This simply means that their physical interpretation and functional form refer to a choice of gauge (generalized clock), as a consequence of the fact that they are extensions of a gauge-fixed quantity $f' = f(\mathcal{S}_0(\tau); \tau)$. The gauge dependence of observables is expected because, as already mentioned, time is defined intrinsically from the dynamical degrees of freedom (cf. §1.6), and any observer will perceive the dynamics in a gauge-fixed (i.e., relational) way. As mentioned in Remark A.3, we use the terms 'relational', 'gauge-fixed' and 'gauge dependent' as synonyms.

The above discussion implies that the definition of observables as gauge-fixed quantities is reasonable, and it is, in fact, equivalent to a class of diffeomorphism invariants (the relational observables). However, it seems that emphasizing the invariance aspect of this definition is a matter of convenience (or even semantics) in the classical theory. One could decide to work solely with (1.80) and its solutions, without mentioning their equivalence to invariant extensions. This is often done in practical calculations. Furthermore, it is important to mention that some researchers even argue against the definition of observables as invariants, as they take the position that an analogy with gauge theories of internal symmetries is unjustified (see, for instance, the discussions in [59–61]). Following [59–61], we could simply define observables as worldline tensors, which are not invariant under general diffeomorphisms. Intuitively, observables would be quantities that transform "covariantly". How can we reconcile this with the above definition of relational observables? There are two points of reconciliation.

The gauge-fixed auxiliary phase-space function $f' = f(\mathcal{S}_0(\tau); \tau)$ is the component of a worldline tensor field evaluated in the intrinsic coordinate determined by the generalized clock. As we have seen, $\mathcal{S}_0(\tau)$ is an invariant along the gauge orbits, and $f'|_{\tau=s}$ defines a diffeomorphism invariant for each fixed instant s. As we will see in §1.9.1, however, the family of relational observables (for all instants in the domain of the intrinsic chart) does not correspond to a diffeomorphism invariant due to its explicit time dependence, which recovers the law $\dot{\mathcal{O}} = \partial\mathcal{O}/\partial\tau$ (see also the discussion in [11, 12]). Thus, although gauge-fixed observables correspond to invariants at each instant, the dynamics encoded in the family of observables is clearly "covariant", and this marks the first point of contact of the definition of relational observable with the view that observables should transform "covariantly".

The second point concerns the tensor character of f'. It is straightforward to verify that $f' = f(q', p'; e'; \tau)$ transforms as the solution $\mathcal{S}_0(\tau) = (q'(\tau), p'(\tau), e'(\tau))$ is mapped to another via a diffeomorphism ϕ_0. One finds that the transformation $f' \mapsto f'(\phi_0^* \mathcal{S}_0(\tau); \phi_0(\tau))$, where we assumed the explicit time dependence is of scalar type. However, this transformation merely corresponds to a change of origin in the gauge orbit, as was argued in the paragraphs that precede (1.14) and follow (1.74), respectively. Once the new origin is fixed, one can in principle establish its invariance as in (1.75) and proceed to construct new invariant extensions. This means that the "covariance" of observables may be assigned to the freedom in choosing the origin in the gauge orbit or, in particular, in choosing the complete gauge fixing, whereas the invariance refers to the irrelevance of the functional form of the fields $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ written in an arbitrary frame. In other words, G generates transformations in the arbitrary frame of the solution $(q(\tau), p(\tau), e(\tau))$, which do not affect $f' = f(q', p'; e'; \tau)$. A similar remark was made in [9, 11, 12]. Therefore, the views regarding the definition of observables discussed above (observables as gauge-fixed quantities; relational observables; observables as quantities that transform "covariantly") are, in fact, equivalent.

Despite the equivalence of the above definitions of observables, we will see that the quantum theory demands (under reasonable assumptions) that observables commute with the constraint operators. It is, therefore, worthwhile to understand how to construct and interpret objects that Poisson-commute with the constraint functions in the classical theory before we proceed to quantization. For this reason, the classical analysis of relational observables is worthwhile. In the next section, we discuss a convenient representation of relational observables.

1.8 Integral representations of relational observables

Let the domain of the intrinsic chart associated with the generalized clock be $\mathcal{U}_\chi$. Its coordinate representation is an interval $\mathcal{I}_\chi = (\tau_0, \tau_1)$ in which $\chi(q(\tau), p(\tau))$ is invertible. Therefore, we assume that τ_0 and τ_1 are chosen such that $\chi(q(\tau), p(\tau)) = s$ only once in $\mathcal{I}_\chi$, and $\chi(q(\tau_0), p(\tau_0)) \neq s$, $\chi(q(\tau_1), p(\tau_1)) \neq s$ by hypothesis. From its definition (1.81), we then note that we can rewrite the relational observable as

$$\begin{aligned}\mathcal{O}[f|\chi = s] &:= f(\phi^* q(s), \phi^* p(s); \phi^* e(s); s) \\ &= \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \delta(\tau - \phi(s)) f\left(q(\tau), p(\tau); \frac{\mathrm{d}\phi}{\mathrm{d}s} e(\tau); s\right) \;,\end{aligned} \tag{1.82}$$

where we recall that $\phi(s) = \chi^{-1}(s)$, which is the inverse function of $\chi(s) \equiv \chi(q(s), p(s))$, and the Dirac delta distribution (henceforth referred to as 'Dirac delta' or 'delta function') is a worldline scalar density defined by

$$\begin{aligned}\delta(\tau) = 0 \; (\tau \neq 0) \;, \\ \int_{-\infty}^{\infty} \mathrm{d}\tau \; \delta(\tau) f(\tau) = f(0) \;.\end{aligned} \tag{1.83}$$

We note that (1.82) is of the form (1.79), and it expresses the relational observable in terms of the solution $(q(\tau), p(\tau), e(\tau))$ to the field equations written in an arbitrary frame. The integral formula (1.85) holds for any type of worldline tensor due to (1.4).

Even though $\mathcal{O}[f|\chi = s]$ satisfies $\delta_{\epsilon(\tau)} \mathcal{O}[f|\chi = s] \approx 0$ by construction, it is now worth verifying that it is indeed a diffeomorphism invariant and, in particular, that it weakly Poisson-commutes with the constraint functions p_e and C. To this end, we first compute

$$\frac{\mathrm{d}\phi}{\mathrm{d}s} = \left(\frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right)^{-1}_{\tau = \phi(s)} \approx \frac{1}{\{\chi, eC\}_{\tau = \phi(s)}} \approx \frac{\omega(\phi^* q(s), \phi^* p(s))}{e(\phi(s))} \tag{1.84}$$

from (1.29) and the fact that $\phi(s) = \chi^{-1}(s)$. If we substitute (1.84) into (1.82), we find that $\mathcal{O}[f|\chi = s]$ does not, in fact, depend on $e(\tau)$ and, as a result, $\{\mathcal{O}[f|\chi = s], p_e\} = 0$. Furthermore, we can compute $\{\mathcal{O}[f|\chi = s], C\}$ in the following way: given the solution $(q(\tau), p(\tau), e(\tau))$ in an arbitrary frame, where $e(\tau)$ is some fixed, nonvanishing function (with constant sign), we can use the properties of the Dirac delta to cast (1.82) into the useful form

$$\mathcal{O}[f|\chi = s] = \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \, \left|\frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right| \delta\left(\chi(q(\tau), p(\tau)) - s\right) f\left(q(\tau), p(\tau); \frac{\mathrm{d}\phi}{\mathrm{d}s} e(\tau); s\right) , \quad (1.85)$$

where $\mathrm{d}\chi/\mathrm{d}\tau \approx e(\tau)\{\chi, C\}$ [cf. (1.29)]. If we use (1.84), we can rewrite the integrand in (1.85) as $\mathrm{sgn}(e)e(\tau)g(\tau; s)$, where $\mathrm{sgn}(e) = \pm 1$ is constant, $e(\tau)$ is a fixed function, and we have defined

$$g(\tau; s) \equiv g(q(\tau), p(\tau); s) := |\{\chi, C\}| \, \delta\left(\chi - s\right) f\left(q(\tau), p(\tau); \omega(q(\tau), p(\tau)); s\right) . \quad (1.86)$$

Notice that $g(\tau_0; s) = g(\tau_1; s) = 0$ because of the assumption that $\chi(q(\tau_0), p(\tau_0)) \neq s$ and $\chi(q(\tau_1), p(\tau_1)) \neq s$. For a fixed value of s, we also obtain $\mathrm{d}g/\mathrm{d}\tau \approx \{g, eC\}$ [cf. (1.29)]. In this way, we find

$$\begin{aligned} \{\mathcal{O}[f|\chi = s], C\} &\approx \mathrm{sgn}(e) \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \, \{g, eC\} \approx \mathrm{sgn}(e) \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \, \frac{\mathrm{d}g}{\mathrm{d}\tau} \\ &= \mathrm{sgn}(e) \left(g(\tau_1; s) - g(\tau_0; s)\right) = 0 \end{aligned} \quad (1.87)$$

from (1.85). Thus, the relational observables indeed weakly Poisson-commute with the constraint functions p_e and C, and thus with the gauge generator [cf. (1.55)]. It is important to emphasize, as before, that the Poisson brackets are evaluated with respect to the $(q(\tau), p(\tau), e(\tau))$ fields instead of the pulled back (gauge-fixed) variables. Thus, the weak Poisson-commutation property of $\mathcal{O}[f|\chi = s]$ follows from the fact that the gauge freedom has been fixed, as was discussed in the paragraphs preceding (1.81). Finally, we note that $\mathcal{O}[f|\chi = s]$ has no explicit time dependence for a fixed value of s, and $\delta^{\text{expl.}}_{\epsilon(\tau)}\mathcal{O}[f|\chi = s] = 0$ is trivially satisfied. Then, $\delta_{\epsilon(\tau)}\mathcal{O}[f|\chi = s] \approx \delta^{\text{expl.}}_{\epsilon(\tau)}\mathcal{O}[f|\chi = s] + \{\mathcal{O}[f|\chi = s], G\} \approx 0$; i.e., $\mathcal{O}[f|\chi = s]$ is a diffeomorphism invariant, as it should be.

Notice that $\mathrm{d}\chi/\mathrm{d}\tau \approx e(\tau)\{\chi, C\}$ is proportional to the Faddeev-Popov determinant [cf. discussion after (1.78)]. Due to the Dirac delta in (1.85), we can replace the Jacobian factor by its invariant extension; i.e., $|\mathrm{d}\chi/\mathrm{d}\tau| \mapsto \Delta_\chi := |\phi^* \mathrm{d}\chi/\mathrm{d}\tau|_{\tau = s}$. If there is no risk of confusion, we refer to Δ_χ itself as the Faddeev-Popov determinant.

Its inverse can be written as [cf. (A.78)]

$$\Delta_\chi^{-1} = \left|\phi^* \frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right|_{\tau=s}^{-1} = \int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \delta(\chi(q(\tau),p(\tau)) - s)\ . \tag{1.88}$$

Using (1.88), the integral formula (1.85) can be rewritten as

$$\begin{aligned} \mathcal{O}[f|\chi = s] &= \Delta_\chi \int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \delta\left(\chi(q(\tau),p(\tau)) - s\right) f\left(q(\tau),p(\tau); \frac{\mathrm{d}\phi}{\mathrm{d}s} e(\tau); s\right) \\ &= \frac{\int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \delta\left(\chi(q(\tau),p(\tau)) - s\right) f\left(q(\tau),p(\tau); \frac{\mathrm{d}\phi}{\mathrm{d}s} e(\tau); s\right)}{\int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \delta(\chi(q(\tau),p(\tau)) - s)}\ , \end{aligned} \tag{1.89}$$

which is an instance of the general formula (A.79). The formula (1.89) expresses the relational observable as an "average" over the intrinsic chart domain. It is an instance of a general averaging procedure that can be used in gauge theories [cf. the discussion after (A.79)].[30]

In addition to (1.81), we may take (1.82), (1.85), or (1.89) as alternative definitions of $\mathcal{O}[f|\chi = s]$. As important particular cases, we find that the relational observable associated with the generalized clock itself is trivial, $\mathcal{O}[\chi|\chi = s] = s$, whereas the invariant extension of the identity is still the identity; i.e., $\mathcal{O}[1|\chi = s] = 1$. This preservation of the identity is a crucial aspect of the formalism, one that will also be of importance in the quantum theory, and it is more commonly called the 'Faddeev-Popov resolution of the identity' [20, 21] for the generalized clock χ. Due to (1.88), the resolution of the identity can be expressed as

$$1 = \Delta_\chi \int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \delta(\chi(q(\tau),p(\tau)) - s)\ . \tag{1.90}$$

We have seen that the relational observables recover the "frozen time" picture of evolution, $\dot{\mathcal{O}} \approx 0$. In what follows, we will discuss how the law $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau$ may be recovered (cf. §1.9.1), as well as a picture of orbits in phase space that are generated by a suitable Hamiltonian vector field (cf. §1.9.2).

[30] Instead of using integral formulas such as (1.89), Pons *et al.* show in [11] that invariant extensions can be recovered from a limiting procedure for a one-parameter family of canonical transformations.

1.9 Dynamics of relational observables

1.9.1 Gauge-fixed evolution

As mentioned in §1.7, the relational observable $\mathcal{O}[f|\chi = s]$ is a worldline constant that captures a single instant and is, therefore, "frozen" in time. Nevertheless, the family of all relational observables that refer to the generalized clock χ, $\mathcal{O}[f|\chi(\mathcal{I}_\chi)] := \{\mathcal{O}[f|\chi = s], s \in \chi(\mathcal{I}_\chi)\}$, is clearly dynamical: it encodes the relational evolution of on-shell worldline tensor fields (i.e., solutions to the field equations) for all the different instants that are in the domain of the intrinsic chart. For this reason, one sometimes refers to (the family of) relational observables as 'evolving constants of motion' [17].

From the definition (1.81), we see that the family $\mathcal{O}[f|\chi(\mathcal{I}_\chi)]$ is equivalent to the (image of the) gauge-fixed function $f' = f(q', p'; e'; \tau)$, which is a solution to (1.80). In this way, each moment of time in the evolution of f' in the generalized reference frame of the observer is captured by the family of invariant extensions $\mathcal{O}[f|\chi(\mathcal{I}_\chi)]$. As each member of the family Poisson-commutes with the constraint functions (cf. §1.8), their evolution is captured by the equation [cf. (1.29)]

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{O}[f|\chi = s] \approx \frac{\partial}{\partial s}\mathcal{O}[f|\chi = s] + \{\mathcal{O}[f|\chi = s], H_T\} \approx \frac{\partial}{\partial s}\mathcal{O}[f|\chi = s] \ , \tag{1.91}$$

which recovers the law $\dot{\mathcal{O}} \approx \partial\mathcal{O}/\partial\tau$ discussed previously. As was mentioned in the paragraphs that follow (1.81), this explicit time dependence signals that the family of relational observables is not diffeomorphism invariant in a strict sense, as we may consider the explicit gauge transformation $\delta_{\epsilon(\tau)}\mathcal{O}[f|\chi = \tau] = \delta^{\text{expl.}}_{\epsilon(\tau)}\mathcal{O}[f|\chi = \tau]$. Strict invariance is only obtained for a fixed instant $\tau = s$ (i.e., for each member of the family).

Can we compute the value of $\partial\mathcal{O}[f|\chi = s]/\partial s$? The answer is yes. First, let us note that the partial derivative of the relational observable is not, in general, equal to relational observable associated with the partial derivative. To see this, consider the example of the function $f(q(\tau), p(\tau); \tau) = \chi(q(\tau), p(\tau)) + \tau$, which satisfies $\partial f/\partial\tau = 1$, and the associated relational observable is $\mathcal{O}[\partial f/\partial s|\chi = s] = \mathcal{O}[1|\chi = s] = 1$. In contrast, we obtain $\mathcal{O}[f|\chi = s] = f(\phi^* q(s), \phi^* p(s); s) = \phi^*\chi + s = 2s$, such that $\partial\mathcal{O}[f|\chi = s]/\partial s = 2 \neq 1$. Second, let us define the convenient abbreviated notation $f^e_s \equiv f(q(\tau), p(\tau); e(\tau); s)$. Third, we use the integral formula (1.82) together with (1.84) to compute

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{O}[f|\chi=s] &= \frac{\mathrm{d}}{\mathrm{d}s}\int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \delta(\tau-\phi(s))f\left(q(\tau),p(\tau);\omega(q(\tau),p(\tau));s\right) \\
&= \int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \left[f_s^\omega\frac{\mathrm{d}}{\mathrm{d}s}\delta(\tau-\phi(s))+\delta(\tau-\phi(s))\frac{\partial f_s^\omega}{\partial s}\right] \\
&= \int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \left[-f_s^\omega\frac{\mathrm{d}\phi}{\mathrm{d}s}\frac{\mathrm{d}}{\mathrm{d}\tau}\delta(\tau-\phi(s))+\delta(\tau-\phi(s))\frac{\partial f_s^\omega}{\partial s}\right] \\
&= \int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \delta(\tau-\phi(s))\left[\frac{\mathrm{d}\phi}{\mathrm{d}s}\frac{\mathrm{d}f_s^\omega}{\mathrm{d}\tau}+\frac{\partial f_s^\omega}{\partial s}\right]\ ,
\end{aligned}
\tag{1.92}
$$

where we denoted $\omega\equiv\omega(q(\tau),p(\tau))$ for brevity. The integration by parts needed to reach the last line in (1.92) is permissible because we assume that $\chi(q(\tau_0),p(\tau_0))\neq s$ and $\chi(q(\tau_1),p(\tau_1))\neq s$. Moreover, we obtain

$$
\begin{aligned}
\frac{\mathrm{d}f_s^\omega}{\mathrm{d}\tau} &= \frac{\mathrm{d}}{\mathrm{d}\tau}\int_{\omega-1}^{\omega+1}\mathrm{d}x\ \delta(x-\omega)f(q(\tau),p(\tau);x;s) \\
&= \delta(1)f_s^{\omega+1}-\delta(-1)f_s^{\omega-1}+\int_{\omega-1}^{\omega+1}\mathrm{d}x\ f_s^x\frac{\mathrm{d}}{\mathrm{d}\tau}\delta(x-\omega)+\int_{\omega-1}^{\omega+1}\mathrm{d}x\ \delta(x-\omega)\frac{\mathrm{d}f_s^x}{\mathrm{d}\tau} \\
&= \int_{\omega-1}^{\omega+1}\mathrm{d}x\ f_s^x(-\dot\omega)\frac{\mathrm{d}}{\mathrm{d}x}\delta(x-\omega)+\int_{\omega-1}^{\omega+1}\mathrm{d}x\ \delta(x-\omega)\{f_s^x,e(\tau)C\} \\
&= (-\dot\omega)\left[\delta(1)f_s^{\omega+1}-\delta(-1)f_s^{\omega-1}\right]+\int_{\omega-1}^{\omega+1}\mathrm{d}x\ \delta(x-\omega)\left[\{f_s^x,e(\tau)C\}+\dot\omega\frac{\mathrm{d}f_s^x}{\mathrm{d}x}\right] \\
&\approx \int_{\omega-1}^{\omega+1}\mathrm{d}x\ \delta(x-\omega)\left[e(\tau)\{f_s^x,C\}+\dot\omega\{f_s^e,p_e\}_{e=x}\right] \\
&= e(\tau)\{f_s^\omega,C\}+\dot\omega\{f_s^e,p_e\}_{e=\omega}\ ,
\end{aligned}
$$

such that (1.92) becomes

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{O}[f|\chi=s] \\
&\approx \int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \delta(\tau-\phi(s))\left[\frac{\mathrm{d}\phi}{\mathrm{d}s}e(\tau)\{f_s^\omega,C\}+\frac{\mathrm{d}\phi}{\mathrm{d}s}\dot\omega\{f_s^e,p_e\}_{e=\omega}+\frac{\partial f_s^\omega}{\partial s}\right] \\
&= \int_{\tau_0}^{\tau_1}\mathrm{d}\tau\ \delta(\tau-\phi(s))\left[\omega(\phi(s))\{f_s^\omega,C\}+\frac{\mathrm{d}\omega}{\mathrm{d}s}\{f_s^e,p_e\}_{e=\omega}+\frac{\partial f_s^\omega}{\partial s}\right]\ ,
\end{aligned}
\tag{1.93}
$$

where we used (1.84), and we denoted $\omega(\phi(s))\equiv\omega(\phi^*q(s),\phi^*p(s))$. The derivative of $\omega(\phi(s))$ with respect to s is $\mathrm{d}\omega/\mathrm{d}s=\dot\omega|_{\tau=\phi(s)}\mathrm{d}\phi/\mathrm{d}s\approx\{\omega,\omega C\}_{\tau=\phi(s)}$ [cf. (1.29) and (1.84)]. Finally, we can rewrite (1.93) in two equivalent ways. The first reads

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{O}[f|\chi=s]\\&\approx\mathcal{O}\left[\left.\frac{\partial f}{\partial s}\right|\chi=s\right]+\omega(\phi(s))\{f_s^{\omega},C\}_{\tau=\phi(s)}+\frac{\mathrm{d}\omega}{\mathrm{d}s}\{f_s^{e},p_e\}_{\tau=\phi(s),e=\omega(\phi(s))}\ .\end{aligned}\tag{1.94}$$

By virtue of (1.81) and (1.82), the evolution determined by (1.94) for the family of relational observables is the same as the evolution dictated by (1.80) for $f'=f(q',p';e';\tau)$, as it should be. As the evolution of gauge-fixed observables is well-defined, we see that the evolution encoded in the family of relational observables is deterministic. Furthermore, we note that the second way to rewrite (1.93) is

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{O}[f|\chi=s]\approx\mathcal{O}\left[\left.\frac{\partial f}{\partial s}+\{f,H_T^{\mathrm{gf}}\}\right|\chi=s\right]\ ,\tag{1.95}$$

where H_T^{gf} is the gauge-fixed Hamiltonian given in (1.65), with $\dot{\omega}\equiv\{\omega,\omega C\}$. Equation (1.95) is a central result of the classical theory of relational observables. In [11], Pons *et al.* used another method to arrive at essentially the same result (at the classical level). In fact, the same result can be derived for general canonical gauge systems [see (A.83)]. We also note that (1.95) is expected to be promoted to an operator equation in the quantum theory in analogy to the Heisenberg picture of the usual (non-invariant) treatments of quantum mechanics. In §2.5.1, we show that this expectation is fulfilled and we discuss the notion of time evolution in the quantum theory.

The equivalence of (1.80), (1.94) and (1.95) implies that each can be used as a description of dynamics in the generalized reference frame associated with the clock field χ. Nevertheless, in each of these equations, the Poisson brackets are evaluated with respect to the $(q(\tau),p(\tau),e(\tau))$ fields instead of the pulled back (gauge-fixed) variables. One enforces the gauge fixing $\tau=\phi(s)$, as well as the constraints $C=p_e=0$, only at the end of the computation. For this reason, the evolution of observables is captured by the law $\dot{\mathcal{O}}=\partial\mathcal{O}/\partial\tau$ [cf. (1.91)], and one does not make use of Poisson brackets of the invariants themselves; i.e., one does not impose the constraints before evaluating the brackets. In what follows, we will see how the evolution of gauge-fixed or relational observables can be captured by brackets of the invariant extensions.

1.9.2 The reduced phase space, the physical Hamiltonian, and the physical worldline

Due to the presence of constraints, the auxiliary phase space Γ plays only an ancillary role in the theory. All physical motions satisfy the constraints and, therefore, are defined in the subspace Σ (the constraint hypersurface) of Γ. It is then reasonable to seek a description of the dynamics that dispenses with the extra structure present in the auxiliary phase space. At first, one could attempt to define the theory on Σ or directly in the space of solutions $\mathcal{S}(\tau)$. However, we have seen in §1.9.1 that families of relational observables capture the dynamics in their explicit time dependence, and that relational observables (for a fixed instant) can be regarded as constant functions on each gauge orbit [cf. the discussion that follows (1.81)]. For this reason, we can alternatively understand the relational observables as functions on the space of orbits, i.e., on the space of equivalence classes $[\mathcal{S}(\tau)]$ of solutions under the gauge transformations generated by G. This brings us to the question: can we define a Poisson-bracket structure and a suitable Hamiltonian vector field on the space of orbits to describe the dynamics of relational observables? The answer is yes [33]. Let us now analyze how this can be achieved.

We refer to the space of orbits as the 'reduced phase space' or the 'physical phase space', and we denote it by $\Gamma_{\rm phys}$. We assume that $\Gamma_{\rm phys}$ is a smooth manifold and that there exists a continuous surjection π from the space of solutions $\mathcal{S}(\tau)$, which we denote by $\mathfrak{F}$, and the reduced phase space; i.e., $\pi : \mathfrak{F} \to \Gamma_{\rm phys}$. We can define the relational observable $\mathcal{O}[f|\chi = s]$ as the function

$$
\begin{aligned}
\mathcal{O}[f|\chi = s] : \Gamma_{\rm phys} &\to \mathbb{R} \\
[\mathcal{S}(\tau)] &\mapsto f'|_{\tau=s} = f(\mathcal{S}_0(s); s) \ ,
\end{aligned}
\tag{1.96}
$$

for each solution $\mathcal{S}_0(\tau)$. Notice that we use the same notation in (1.96) as in (1.81) without risk of confusion. Thus, there are three views on the relational observables: (1) they are worldline constants; (2) they are constant functions on the gauge orbits; (3) they are functions on the reduced phase space. In fact, any function that is invariant under the transformations generated by G is constant along each gauge orbit and, therefore, may be seen as a function on $\Gamma_{\rm phys}$.

To define the Poisson-bracket structure and a Hamiltonian vector field in the reduced phase space, it is convenient to adopt a system of local coordinates in $\Gamma_{\rm phys}$ that are related to the relational observables. We proceed in a series of steps.

First, let $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ be a solution to the field equations in an arbitrary frame, and let $\chi(q(\tau), p(\tau))$ be a choice of generalized clock. Without loss of generality, we can suppose that $\chi(q(\tau), p(\tau)) = q^1(\tau)$ (possibly after a canonical transformation). We also assume that we can solve the secondary constraint $C = 0$ for $p_1(\tau)$, the canonical momentum conjugate to the clock, to obtain

$$
p_1(\tau) = -H^{\sigma}_{\chi}(q(\tau), p(\tau)) \ , \tag{1.97}
$$

where σ denotes a possible discrete degeneracy of the solution.[31] Evidently, the auxiliary phase-space function $H^\sigma_\chi(q(\tau), p(\tau))$ does not depend on $p_1(\tau)$. The solutions (1.97) can be found if $0 \neq \partial C/\partial p_1 = \{\chi, C\}$, which is the same condition for the complete gauge fixing associated with the generalized clock to be admissible [cf. (1.77)]. As already mentioned, this condition is, in general, only satisfied in a certain region W of the auxiliary phase space Γ.

Second, let us collectively denote the canonical pairs that are different from (q^1, p_1) by $(\bar{q}, \bar{p})$. Then, a point in the auxiliary phase space reads $(q, p, e, p_e) = (q^1, p_1, \bar{q}, \bar{p}, e, p_e)$, whereas a point on the constraint hypersurface Σ can be written as $(q^1, -H^\sigma_\chi, \bar{q}, \bar{p}, e, 0)$ due to (1.97). We omit the last (vanishing) entry without loss of generality. Moreover, as discussed in §1.6, the complete gauge fixing associated with $\phi^*_{\mathcal{S}}\chi = \tau$ corresponds to a choice of origin $\mathcal{S}_0(\tau)$ in each gauge orbit. We can write this gauge-fixed solution as

$$\begin{aligned}\mathcal{S}_0(\tau) &= (\phi^*_{\mathcal{S}} q^1(\tau), \phi^*_{\mathcal{S}} p_1(\tau), \phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau), \phi^*_{\mathcal{S}} e(\tau)) \\ &= (\tau, -H^\sigma_\chi(\phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau); \tau), \phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau), \omega(\phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau); \tau)) \\ &\equiv (\tau, -\phi^*_{\mathcal{S}} H^\sigma_\chi, \phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau), \phi^*_{\mathcal{S}}\omega)\end{aligned} \tag{1.98}$$

where we used (1.84) and (1.97) to write

$$\phi^*_{\mathcal{S}} e(\tau) = \omega(\phi^*_{\mathcal{S}} q^1(\tau), \phi^*_{\mathcal{S}} p_1(\tau), \phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau)) \equiv \omega(\phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau); \tau) \ .$$

It is straightforward to see that $\mathcal{S}_0(\tau) \in \Sigma|_\chi \subset \Sigma$ for each value of τ. As $\phi^*_{\mathcal{S}} H^\sigma_\chi$ and $\phi^*_{\mathcal{S}}\omega$ are functions of τ and $\phi^*_{\mathcal{S}}\bar{q}(\tau), \phi^*_{\mathcal{S}}\bar{p}(\tau)$ only, we conclude that the independent initial values of the solution $\mathcal{S}_0(\tau)$ are given by $\phi^*_{\mathcal{S}}\bar{q}(s), \phi^*_{\mathcal{S}}\bar{p}(s)$ (for a fixed value of s), which correspond to (the images of) the relational observables $\mathcal{O}[\bar{q}|\chi = s]$ and $\mathcal{O}[\bar{p}|\chi = s]$. In this way, a complete set of independent relational observables can be seen as a set of invariant extensions of initial data [30, 31]. For this reason, we also refer to $\phi^*_{\mathcal{S}}\bar{q}(s), \phi^*_{\mathcal{S}}\bar{p}(s)$ as 'relative initial data', and we denote $\bar{Q} := (\phi^*_{\mathcal{S}}\bar{q}(s), \phi^*_{\mathcal{S}}\bar{p}(s))$. We assume, for simplicity, that the space of all possible values of $\bar{Q}$ is $\bar{\Gamma} \subset \mathbb{R}^{2(d-1)}$. Furthermore, a general relational observable can be written in terms of the relative initial data, $\mathcal{O}[f|\chi = s] = f(\mathcal{S}_0(s); s)$, due to (1.96) and (1.98). The idea is then to use the relative initial data as local coordinates in Γ_{phys}.

Third, as mentioned after (1.80), we assume that the gauge-fixed field equations (1.80), (1.94), or (1.95) are integrable, and that a unique solution $\mathcal{S}_0(\tau)$ exists for each choice of (independent) initial conditions. This means that there exists a bijection $\mathcal{E}_s$ between a choice of relative initial data at $\tau = s$ and a solution $\mathcal{S}_0(\tau)$; i.e., we define

[31] For example, the sectors of positive and negative frequencies in the case of the relativistic particle (see Chapter 3).

$\mathcal{E}_s(\bar{Q}) = \mathcal{S}_0$ and $\mathcal{E}_s^{-1}(\mathcal{S}_0) = \bar{Q}$, where $\mathcal{S}_0 : \mathcal{M} \to \mathbb{R}$ stands for the function given in (1.98) in the local coordinate τ. In this way, different choices of the initial values lead to different solutions $\mathcal{S}_0(\tau)$, which are mapped to different gauge orbits by the surjection π.[32] For example, we note that if one performs a global time translation solely in $\phi_{\mathcal{S}}^*\bar{q}(\tau), \phi_{\mathcal{S}}^*\bar{p}(\tau)$, one reaches the solution

$$\tilde{\mathcal{S}}_0(\tau) = (\tau, -\phi_{\mathcal{S}}^* H_\chi^\sigma, \phi_{\mathcal{S}}^*\bar{q}(\tau+\epsilon), \phi_{\mathcal{S}}^*\bar{p}(\tau+\epsilon), \phi_{\mathcal{S}}^*\omega) \ , \tag{1.99}$$

where ϵ is a nonvanishing constant and the dependence of $\phi_{\mathcal{S}}^* H_\chi^\sigma$ and $\phi_{\mathcal{S}}^*\omega$ on $\phi_{\mathcal{S}}^*\bar{q}(\tau + \epsilon), \phi_{\mathcal{S}}^*\bar{p}(\tau+\epsilon)$ has been suppressed. The solution (1.99) is different from (1.98) because the initial data differ, and it is not on the same gauge orbit of (1.98) because it does not correspond to a pullback of $\mathcal{S}_0(\tau)$ (only the relative initial data are globally translated, but not the clock $\phi_{\mathcal{S}}^*\chi = \tau$).

Finally, as was mentioned after (1.75), the complete gauge fixing also corresponds to a choice of section $\ell : \Gamma_{\text{phys}} \to \mathfrak{F}$, $\ell([\mathcal{S}(\tau)]) = \mathcal{S}_0$ such that $\pi \circ \ell : \Gamma_{\text{phys}} \to \Gamma_{\text{phys}}$ is the identity. In this way, we can consider the mapping $\Gamma_{\text{phys}} \ni [\mathcal{S}(\tau)] \overset{\ell}{\mapsto} \mathcal{S}_0 \overset{\mathcal{E}_s^{-1}}{\mapsto} \bar{Q} \in \bar{\Gamma}$ with the inverse $\bar{\Gamma} \ni \bar{Q} \overset{\mathcal{E}_s}{\mapsto} \mathcal{S}_0 \overset{\pi}{\mapsto} [\mathcal{S}(\tau)] \in \Gamma_{\text{phys}}$.[33] Assuming that it is, in fact, a homeomorphism, we interpret this mapping as a choice of local coordinates in Γ_{phys}, which are the relative initial data. Incidentally, this implies that the dimension of Γ_{phys} is $2(d-1)$, which is equal to the number of dimensions of the auxiliary phase space $(2d+2)$ minus the number of first-class constraints (2) minus the number of gauge conditions in a complete gauge fixing (2). This is the standard counting of the number of physical degrees of freedom in a system without second-class constraints [33]. As the relational observables $\mathcal{O}[f|\chi = s]$ can be written in terms of the relative initial data, it is sufficient to determine the Poisson-bracket structure in these local coordinates.

A straightforward way to simultaneously define the bracket structure and a Hamiltonian vector field in Γ_{phys} is to analyze the on-shell action, which is obtained from (1.32) when the paths are restricted to be solutions to the field equations (and, in particular, they are defined in the constraint hypersurface Σ). We find

$$S_{\text{on-shell}} = \int_a^b \mathrm{d}\tau \left[\sum_{i=2}^d p_i(\tau)\dot{q}^i(\tau) - H_\chi^\sigma(q(\tau), p(\tau))\dot{\chi}(\tau)\right] \ , \tag{1.100}$$

where we used (1.97). Notice that (1.100) coincides with the on-shell value of (1.39).

[32] It is worthwhile to emphasize that the gauge fixing is a fixation of the functional form of the fields via the pullback by $\phi_{\mathcal{S}}$, but it is not a fixation of the independent initial data that label different solutions.

[33] Notice that, although $\ell \circ \pi : \mathfrak{F} \to \mathfrak{F}$ is not the identity, we find that $\mathcal{E}_s^{-1} \circ \ell \circ \pi \circ \mathcal{E}_s$ is the identity because the image of $\mathcal{E}_s$ is a gauge-fixed solution (the origin of a gauge orbit) by definition.

Due to (1.11), we can rewrite (1.100) as

$$S_{\text{on-shell}} = \int_{\phi_{\mathcal{S}}^{-1}(a)}^{\phi_{\mathcal{S}}^{-1}(b)} \mathrm{d}s \left[\sum_{i=2}^{d} p_i(\phi_{\mathcal{S}}(s)) \frac{\mathrm{d}q^i(\phi_{\mathcal{S}}(s))}{\mathrm{d}s} - H_\chi^\sigma(q(\phi_{\mathcal{S}}(s)), p(\phi_{\mathcal{S}}(s))) \right] . \quad (1.101)$$

One readily recognizes (1.101) as the usual action of an unconstrained system with degrees of freedom comprised of the relative initial data $\bar{Q} = (\phi_{\mathcal{S}}^* \bar{q}(s), \phi_{\mathcal{S}}^* \bar{p}(s))$. For a fixed value of s, this leads to the definition of the Poisson bracket[34]

$$\{f, g\}_{\Gamma_{\text{phys}}} := \sum_{i=2}^{d} \left(\frac{\partial f}{\partial q^i(\phi_{\mathcal{S}}(s))} \frac{\partial g}{\partial p_i(\phi_{\mathcal{S}}(s))} - \frac{\partial f}{\partial p_i(\phi_{\mathcal{S}}(s))} \frac{\partial g}{\partial q^i(\phi_{\mathcal{S}}(s))} \right) \quad (1.102)$$

for any two reduced phase-space functions f, g in the local coordinates $\bar{Q}$ in Γ_{phys}. Furthermore, the on-shell action (1.101) also implies that the evolution of $\phi_{\mathcal{S}}^* \bar{q}(s), \phi_{\mathcal{S}}^* \bar{p}(s)$ with respect to changes in the value of s is a canonical transformation in Γ_{phys} generated by the vector field $\{\cdot, \phi_{\mathcal{S}}^* H_\chi^\sigma\}_{\Gamma_{\text{phys}}}$, where $\phi_{\mathcal{S}}^* H_\chi^\sigma$ is called the 'physical' or 'reduced' Hamiltonian. Notice that the functional form of the physical Hamiltonian will generally differ for different gauge fixings. Moreover, the physical Hamiltonian coincides with (the image of) a relational observable, $\phi_{\mathcal{S}}^* H_\chi^\sigma = \mathcal{O}[H_\chi^\sigma | \chi = s]$, which is the invariant extension of the on-shell value of $-p_1(\tau)$. As any relational observable $\mathcal{O}[f|\chi = s]$ can be written in terms of the relative initial data, we conclude that, instead of (1.95), we can describe the evolution of the family of relational observables with respect to changes in the value of s with the physical Hamiltonian vector field,

$$\frac{\mathrm{d}}{\mathrm{d}s} \mathcal{O}[f|\chi = s] = \frac{\partial}{\partial s} \mathcal{O}[f|\chi = s] + \{\mathcal{O}[f|\chi = s], \mathcal{O}[H_\chi^\sigma|\chi = s]\}_{\Gamma_{\text{phys}}} . \quad (1.103)$$

In this way, the evolution is described solely in terms of brackets of diffeomorphism invariants.[35]

Lastly, following the discussion in the **Introduction**, we define a region γ_χ of the 'physical worldline' $\mathcal{M}_{\text{phys}}$ as the image of the solution $\mathcal{S}_0(\tau)$ for a fixed choice of relative initial data. As $\mathcal{S}_0(\tau)$ is only valid in the intrinsic chart $(\mathcal{U}_\chi, \tilde{\chi}')$ associated

[34]A similar construction is reviewed in §A.3, where it is explained that the reduced phase space can also be understood as the quotient space of the constraint hypersurface Σ by the orbits generated by $\{\cdot, C\}$ and $\{\cdot, p_e\}$.

[35]In fact, the physical Hamiltonian can also be used to define the bijection $\mathcal{E}_s$ between the relative initial data at $\tau = s$ and the solution $\mathcal{S}_0(\tau)$. For example, suppose that $\mathcal{O}[H_\chi^\sigma|\chi = s]$ does not explicitly depend on s for simplicity. Then, given a choice of $\bar{Q} = (\phi_{\mathcal{S}}^* \bar{q}(s), \phi_{\mathcal{S}}^* \bar{p}(s))$, we obtain a trajectory in the reduced phase space via the invertible mapping $\bar{Q} \mapsto \bar{Q}(\tau) := \exp\left((\tau - s)\{\cdot, \mathcal{O}[H_\chi^\sigma|\chi = s]\}\right) \bar{Q}$, which can be composed with the map that takes the function (worldline scalar) $\tau \mapsto \bar{Q}(\tau)$ to the $(2d+1)$-tuple of functions (worldline scalars) that form $\tau \mapsto \mathcal{S}_0(\tau)$ [as given in (1.98)]. Notice that, for a fixed gauge fixing (a fixed choice of origin in each gauge orbit), this map is invertible.

with the complete gauge fixing, the image is $\gamma_\chi := \mathcal{S}_0(\tilde{\chi}'(\mathcal{U}_\chi))$, which is invariant under diffeomorphisms in $\mathcal{M}$, since $\tilde{\chi}'(\mathcal{U}_\chi)$ and $\mathcal{S}_0(\tau)$ are invariant [cf. (1.75) and discussion after (1.77)]. More precisely, let $\mathcal{A}$ be a smooth intrinsic atlas on $\mathcal{M}$. We note that $\tau \mapsto \mathcal{S}_0(\tau) \in \Sigma_\chi \subset \Sigma$ is a description of the physical trajectory as a parametrized curve in the constraint hypersurface, and for any two charts $(\mathcal{U}_{\chi_1}, \tilde{\chi}'_1)$, $(\mathcal{U}_{\chi_2}, \tilde{\chi}'_2)$ in $\mathcal{A}$ that are smoothly compatible (with $\mathcal{U}_{\chi_1} \cap \mathcal{U}_{\chi_2} \neq 0$), a change of intrinsic coordinates corresponds to a change of gauge, which induces a change $\mathcal{S}_0(\tau) = \phi_0^* \tilde{\mathcal{S}}_0(\tau)$ in the origin of the gauge orbit (it also induces a change in the local coordinates of Γ_{phys}, understood as relative initial data). This, in turn, is a reparametrization of the curve in Σ. As $\mathcal{S}_0(\tau)$ is a $(2d+1)$-tuple of worldline scalars [cf. (1.98)], its image is invariant under diffeomorphisms, such that γ_χ is insensitive to diffeomorphisms on the abstract worldline or changes of gauge conditions. Furthermore, we see from (1.98) that $\tau \mapsto \mathcal{S}_0(\tau)$ is a bijection onto its image; i.e., it is a bijection between $\mathcal{U}_\chi$ and γ_χ. We then assume that the union $\cup_{\mathcal{A}} \gamma_\chi =: \mathcal{M}_{\text{phys}}$ is a smooth, one-dimensional manifold, which we define to be the physical worldline. Note that $\mathcal{M}_{\text{phys}}$ is constructed from diffeomorphism-invariant (extensions of) quantities, which are the relational objects that are accessible to any observer (see also the discussion in the **Introduction**).

1.10 Hamilton-Jacobi formalism

Before we proceed to the quantum theory, is it useful to discuss one of its closest classical analogues: the Hamilton-Jacobi (HJ) formalism (cf. §A.3.3). It is defined by a canonical transformation to the set of independent initial conditions. The generating function reads $\mathcal{F} = \mathrm{S}(q, P; e, P_e; \tau) - Q^i P_i - e_0 P_e$, where the new canonical coordinates are $(Q, P; e_0, P_e)$ and S is Hamilton's principal function. The Lagrangian in (1.32) is transformed according to $p_i \dot{q}^i + p_e \dot{e} - H_T = P_i \dot{Q}^i + P_e \dot{e}_0 - K_T + \mathrm{d}\mathcal{F}/\mathrm{d}\tau$, where $\lambda(\tau)$ is considered as an arbitrary multiplier. If we require that the new total Hamiltonian vanishes identically, we find the HJ equations

$$p_i = \frac{\partial \mathrm{S}}{\partial q^i} \ , \ Q^i = \frac{\partial \mathrm{S}}{\partial P_i} \ , \tag{1.104}$$

$$p_e = \frac{\partial \mathrm{S}}{\partial e} \ , \ e_0 = \frac{\partial \mathrm{S}}{\partial P_e} \ , \tag{1.105}$$

$$0 = \frac{\partial \mathrm{S}}{\partial \tau} + H_T \left(q, \frac{\partial \mathrm{S}}{\partial q}; e, \frac{\partial \mathrm{S}}{\partial e}; \tau \right) \ . \tag{1.106}$$

As is well-known, Eq. (1.106) is the classical analogue to the Schrödinger equation. Using (1.106) and $H_T = eC + \lambda(\tau)p_e$, an ansatz for S is found to be

$$\begin{aligned} \mathrm{S}(q, P; e, P_e; \tau) := \mathrm{W}(q, P) + (P_e - E\tau)\left[e - \int^{\tau} \mathrm{d}\tau' \lambda(\tau')\right] \\ - E \int^{\tau} \mathrm{d}\tau' \int^{\tau'} \mathrm{d}\tau'' \lambda(\tau'') \ , \end{aligned} \tag{1.107}$$

where the multiplier $\lambda(\tau)$ is understood as an arbitrary function of τ, and we have defined W as a solution to

$$C\left(q, \frac{\partial \mathrm{W}}{\partial q}\right) = E \ , \ (E \in \mathbb{R}). \tag{1.108}$$

We can evaluate Hamilton's principal function on a solution $\mathcal{S}(\tau) = (q(\tau), p(\tau), e(\tau))$ to the field equations in order to find its on-shell value, $\mathrm{S}_{\text{on-shell}}$. For any given solution $\mathcal{S}(\tau)$, we must have $p_e = 0$ and $C = 0$. Due to (1.105) and (1.108), the primary constraint implies that $\partial \mathrm{S}/\partial e = 0$, whereas the secondary constraint implies that $E = 0$. If we impose these conditions on (1.107), we find

$$\mathrm{S}_{\text{on-shell}} = \mathrm{W}(q(\tau), P) \ . \tag{1.109}$$

We thus see that $\mathrm{S}_{\text{on-shell}}$ has no explicit time dependence; i.e., due to the imposition of the constraints, we find from (1.106) that $\partial \mathrm{S}_{\text{on-shell}}/\partial\tau = 0$. As we will discuss in Chapter 2, this has a direct analogue in the quantum theory: physical wave functions must be independent of τ, which is often interpreted as a lack of quantum dynamics [6]. However, the classical condition $\partial \mathrm{S}_{\text{on-shell}}/\partial\tau = 0$ does not preclude evolution. It simply implies that the on-shell value of Hamilton's principal function obeys

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{S}_{\text{on-shell}} = \frac{\partial \mathrm{W}_{\text{on-shell}}}{\partial q^i}\dot{q}^i \equiv p_i \dot{q}^i \ ; \tag{1.110}$$

i.e., W is what is usually referred to as Hamilton's characteristic function, and it is the antiderivative of the Lagrangian featured in the actions (1.39) and (1.100),

$$\mathrm{W}_{\text{on-shell}} = \int \mathrm{d}\tau \ p_i \dot{q}^i \ . \tag{1.111}$$

How are the new canonical coordinates $(Q, P; e_0, P_e)$ in the auxiliary phase space related to the independent initial conditions? First, we note that (1.105) together with (1.107) implies

$$e_0 = e - \int^{\tau} \mathrm{d}\tau' \lambda(\tau') \ , \ P_e = p_e + E\tau \ . \tag{1.112}$$

Thus, e_0 is simply the initial value of the einbein [cf. (1.30)], which is arbitrary due to the arbitrariness of the multiplier $\lambda(\tau)$. Moreover, $P_e = 0$ on shell. Second, to determine the interpretation of (Q, P), we note from (1.108) that the HJ analogue of (1.97) is

$$p_1 = \frac{\partial \mathrm{W}}{\partial q^1} = -H_{\chi}^{\sigma,E}\left(\bar{q}, \frac{\partial \mathrm{W}}{\partial \bar{q}}; q^1\right) \ , \tag{1.113}$$

where we allow a general value of E, although $E = 0$ for any solution to field equations. Notice that (1.113) is of the same form as the ordinary time-dependent HJ equation [cf. (1.106)]. Here, the clock q^1 plays the role of time, and W can be seen as Hamilton's principal function for the variables $(\bar{q}, \bar{p})$, even though it is Hamilton's characteristic function for the whole system because it has no explicit dependence on τ [cf. (1.109)]. From the discussion in §1.9.2, we know that the invariant extensions of $(\bar{q}, \bar{p})$ for a certain value of the generalized clock comprise the independent initial data of the system, which serve as local coordinates in the reduced phase space. Therefore, we can choose $d-1$ pairs among the (Q, P) to be (functions of) the relative initial data, i.e., the initial values of $(\bar{q}, \bar{p})$ relative to the clock. Let us denote these pairs by (x, k), such that $(Q, P) = (x, k; t, h)$.

What is the interpretation of the remaining pair (t, h)? To find the answer, let us first note that, in terms of the new canonical coordinates, the Poisson bracket of two functions in the auxiliary phase space reads

$$\{f, g\} = \sum_{i=2}^{d}\left(\frac{\partial f}{\partial x^i}\frac{\partial g}{\partial k_i} - \frac{\partial f}{\partial k_i}\frac{\partial g}{\partial x^i}\right) + \frac{\partial f}{\partial t}\frac{\partial g}{\partial h} - \frac{\partial f}{\partial h}\frac{\partial g}{\partial t} + \frac{\partial f}{\partial e_0}\frac{\partial g}{\partial P_e} - \frac{\partial f}{\partial P_e}\frac{\partial g}{\partial e_0} \ . \tag{1.114}$$

Moreover, the pairs (x, k) are invariants by definition and may be used as local coordinates in Γ_{phys}. Thus, the bracket (1.114) coincides with (1.102) if f and g only depend on (x, k) and are, therefore, invariants. Subsequently, let us rewrite (1.104) as

$$p_i = \frac{\partial \mathrm{W}}{\partial q^i} \ (i = 1, \ldots, d) \ , \tag{1.115}$$

$$x^j = \frac{\partial \mathrm{W}}{\partial k_j} \ (j = 2, \ldots, d) \ , \tag{1.116}$$

$$t = \frac{\partial \mathrm{S}}{\partial h} \ . \tag{1.117}$$

Due to (1.113), we assume that we can invert (1.116) and use (1.115) to find

$$q^j \equiv q^j(x,k;q^1;E,\sigma)\ ,\ p_j \equiv p_j(x,k;q^1;E,\sigma)\ (j=2,\dots,d) \tag{1.118}$$

for fixed values of E and σ. If we fix $q^1 = s$ and $E = 0$, the quantities in (1.118) become invariants (for a fixed value of s), which coincide with the relational observables. Due to (1.103), we know that their evolution with respect to s is generated by a physical Hamiltonian $\mathcal{O}[H^\sigma_\chi|\chi = s]$, which we assume may be written solely in terms of x, k and s due to (1.118).

Finally, let us compute (1.117). We note that, without loss of generality, we can consider that the parameter E in (1.108) is a function of the invariants x, k, as well as of h and s; i.e., $E \equiv E(h,x,k;s)$. The simplest case is $E = h$. In general, we assume that $E = E(h,x,k;s)$ can be inverted for h such that we obtain

$$h = -H^{\sigma'}(E,x,k;s)\ ,\ \frac{\partial E}{\partial h} \neq 0\ , \tag{1.119}$$

where σ' is a discrete degeneracy. This means that $\sigma'_1 \neq \sigma'_2$ implies that $H^{\sigma'_1}(E,x,k;s) \neq H^{\sigma'_2}(E,x,k;s)$ for all possible values of (E,x,k) and s. In this way, Eq. (1.119) is analogous to (1.97) and (1.113). In particular, we may choose $H^\sigma(E,x,k;s)$ such that its restriction to $E = 0$ coincides with the physical Hamiltonian $\mathcal{O}[H^\sigma_\chi|\chi = s]$, which is the invariant extension of H^σ_χ. As E coincides with the secondary constraint [cf. (1.108)], we conclude that $h = -H^{\sigma'}(0,x,k)$ is a representation of the hypersurface $C = 0$. For later reference, we also assume that the function $H^{\sigma'}(E,x,k;s)$ in (1.119) can be expanded in powers of E,

$$H^{\sigma'}(E,x,k;s) = H^{\sigma'}_0(x,k;s) + H^{\sigma'}_1(x,k;s)E + \mathcal{O}(E^2)\ , \tag{1.120}$$

$$H^{\sigma'}_1(x,k;s) \equiv -\left(\frac{\partial E}{\partial h}\right)^{-1} \neq 0\ . \tag{1.121}$$

Evidently, for a solution to the field equations, we have the on-shell values $E = 0$, $h = -H^\sigma(0,x,k;s) = -H^\sigma_0(x,k;s)$. Using (1.119), Eq. (1.117) then yields

$$t = \frac{\partial \mathrm{S}}{\partial h} = \chi - \frac{\partial E}{\partial h}\left[\tau\left(e - \int^\tau \mathrm{d}\tau'\lambda(\tau')\right) + \int^\tau \mathrm{d}\tau' \int^{\tau'} \mathrm{d}\tau''\lambda(\tau'')\right]\ , \tag{1.122}$$

where

$$\chi \equiv \chi(x,k;q^1;E,\sigma) := \frac{\partial \mathrm{W}}{\partial h} \tag{1.123}$$

can be considered a function of q^1, x, k, E and σ due to (1.118). Moreover, if we use (1.112) together with (1.2) and $\dot{e} = \lambda$, we can rewrite (1.122) in terms of proper time

$$\chi = t + \frac{\partial E}{\partial h}\eta(\tau) \ , \tag{1.124}$$

such that χ is a canonical representation of proper time (as an auxiliary phase-space function) if $E = h$, and t is its "initial" value, which is arbitrary due to the freedom to globally shift η. If $E \neq h$ and a more general relation is chosen [cf. (1.119)], then the interpretation of χ and t is less straightforward (see, however, the comments in §2.5.2). Nonetheless, if H^σ is chosen to coincide with $\mathcal{O}[H^\sigma_\chi|\chi = s]$ (at least for $E = 0$), then χ is a generalized clock that is conjugate to the physical Hamiltonian, which is the invariant extension of the on-shell value of p_1. In this case, χ is not necessarily equal to q^1 because p_1 is not generally invariant and, therefore, equal to its invariant extension. Nevertheless, one may invert (1.123) to find the evolution of q^1 in terms of χ or proper time [cf. (1.124)]

$$q^1 \equiv q^1\left(t + \frac{\partial E}{\partial h}\eta, x, k; E, \sigma\right) \ . \tag{1.125}$$

This implies that fixing $q^1 = s$ corresponds to fixing $\chi = \chi(x, k; s; E, \sigma)$. If one inserts (1.125) back into (1.118), one may also express the other variables in terms of proper time.

We have thus seen that relational observables and relative initial data can be recovered from the (off-shell) HJ formalism. In particular, the dynamics can be defined regardless of the condition $\partial \mathrm{S}_{\text{on-shell}}/\partial\tau = 0$. This is important because an analogous construction of relational observables will be available (under certain circumstances) in the quantum theory due to its similarity to the HJ formalism, and the τ-independence of on-shell quantum states will be irrelevant to the definition of the quantum dynamics.

If one wishes to find the classical solution to the field equations using the HJ formalism, we suggest the following strategy (which will have its quantum counterpart; cf. §2.5.5): first, find the solutions (1.118) and (1.125) using the simple choice $E = h$, such that χ is a canonical representation of proper time. For a fixed value of χ, these solutions only depend on invariants (x, k, E, σ), and thus constitute functions on the reduced phase space if $E = 0$. Second, a change of functional form of these solutions via the pullback by a diffeomorphism can be described by the integral formula (1.89), with which one may obtain the invariants relative to the generalized reference frame of an arbitrary observer, instead of relative to the value of χ.

Chapter 2

Quantum Diffeomorphism Invariance on the Worldline

We now discuss the quantization of the general theory presented in Chapter 1, and we present a formalism for the construction and interpretation of quantum relational observables by closely following the analogy with the classical theory and, in particular, the HJ formalism.[1]

2.1 The auxiliary Hilbert space

The canonical quantization of the classical system defined by the action (1.32) is obtained by promoting the fields $q(\tau), e(\tau)$ and their conjugate momenta $p(\tau), p_e(\tau)$ to self-adjoint operators $\hat{q}, \hat{e}, \hat{p}, \hat{p}_e$ acting on a Hilbert space $\mathcal{H}$, which we refer to as the auxiliary Hilbert space in analogy to the auxiliary phase space Γ. The inner product $\langle\cdot|\cdot\rangle$ in $\mathcal{H}$ is called the auxiliary inner product, and we assume that the secondary constraint function is also mapped to an operator $\hat{C}$ that is self-adjoint with respect to $\langle\cdot|\cdot\rangle$. The dynamics is given by the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial\tau}\left|\psi\right\rangle = \hat{H}_T\left|\psi\right\rangle \ , \tag{2.1}$$

where $|\psi\rangle$ is a state in $\mathcal{H}$, and [cf. (1.30)]

$$\hat{H}_T := \hat{e}\hat{C} + \lambda(\tau)\hat{p}_e \tag{2.2}$$

it the total Hamiltonian operator. The multiplier $\lambda(\tau)$ is taken to be an arbitrary c-number-valued function of τ, and $[\hat{e}, \hat{C}] = 0$. The Schrödinger equation (2.1) is the

[1]This Chapter is based on [30,31,62].

quantum counterpart to (1.106). Furthermore, we can also define the quantum gauge generator [cf. (1.55)]

$$\hat{G} := \xi(\tau)\hat{C} + \dot{\xi}(\tau)\hat{p}_e \ , \tag{2.3}$$

where $\xi(\tau)$ is an arbitrary c-number-valued function of τ. The quantum gauge orbits are defined to be solutions to the equation $\mathrm{i}\hbar\overline{\delta}\,|\psi\rangle = \hat{G}\,|\psi\rangle$ [cf. (A.89)], where $\overline{\delta}$ designates a variation of the state at a fixed instant of τ.

In this construction, the quantum analogues of the constraint equations have not yet been imposed. Classically, the primary constraint follows from the extremization of action (1.32) with respect to the multiplier $\lambda(\tau)$, whereas the secondary constraint follows from the preservation of the primary in time (ensured by the Rosenfeld-Dirac-Bergmann algorithm; cf. §A.2.3). In the quantum theory, it seems reasonable to impose the conditions

$$\hat{p}_e\,|\psi\rangle = 0 \ , \ \hat{C}\,|\psi\rangle = 0 \tag{2.4}$$

as analogues of the classical definition of the constraint hypersurface. The conditions (2.4) define the so-called 'Dirac quantization' procedure [cf. §A.3.4]. In analogy to the fact that classical solutions to the field equations must satisfy the constraints, we define the 'physical' or 'on-shell' quantum states to be solutions to the conditions (2.4), and we denote them as $|\Psi\rangle$. There are two paramount consequences of this definition. First, due to (2.3), physical states are automatically gauge invariant; i.e., $\hat{G}\,|\Psi\rangle = 0$. Second, due to (2.1) and (2.2), physical states are annihilated by the total Hamiltonian, and thus they are independent of τ, $\partial\,|\Psi\rangle\,/\partial\tau = 0$.

The independence of on-shell states on the worldline time coordinate τ leads to the notorious problem of time in the quantum theory, as it seems to indicate an absence of dynamics. However, we stress that $\partial\,|\Psi\rangle\,/\partial\tau = 0$ is the quantum counterpart to the classical condition $\partial \mathrm{S}_{\text{on-shell}}/\partial\tau = 0$. As we have seen in §1.10, this condition does not mean that there is no evolution, but rather that the evolution is relational. Indeed, we will see that the quantum evolution can be understood in direct analogy to the HJ formalism (and its connection to relational observables and relative initial data), and we will propose a method of construction and interpretation of quantum relational observables.

2.2 To constrain or not to constrain? Stückelberg's approach

Before we proceed to the definition of quantum observables and their dynamics, it is worthwhile to mention an alternative to the Dirac quantization conditions (2.4) that is sometimes considered in the literature [43–47]. As was discussed in §1.4, we can examine a class of theories that can be globally deparametrized due to the introduction of a "cosmological constant" Λ in the secondary constraint. Concretely, let

$$C = \frac{1}{2}G^{ij}(q)p_i p_j + V(q) \tag{2.5}$$

be the secondary constraint, and let the primary $p_e = 0$ be tacitly solved. Subsequently, introduce a "cosmological constant" term, $C \mapsto C_\Lambda = 1/2G^{ij}(q)p_i p_j + V(q) - \Lambda$. The idea is to take Λ to be a free parameter instead of a fixed constant. As C_Λ is an initial value constraint, the value of Λ is then determined by the initial conditions on the scalars q, p (rather than by law).[2] In this case, the role of the constraint is simply to assign a value to a constant (conserved quantity), which may be identified with the total energy of the system. Indeed, following the discussion at the end of §1.4, we see that this procedure corresponds to a deparametrization if we formally identify Λ with the opposite of the momentum conjugate to a proper-time field, such that the physical Hamiltonian that dictates the dynamics of the scalars is equal to $H_{\rm phys} := C = 1/2G^{ij}(q)p_i p_j + V(q)$ [cf. (2.5)]. If one quantizes $H_{\rm phys}$, the result is an ordinary (unconstrained) quantum theory, governed by the Schrödinger equation $\mathrm{i}\hbar \, \mathrm{d} \left|\psi\right\rangle / \mathrm{d}\tau = \hat{C} \left|\psi\right\rangle$.

The above deparametrization procedure results in the same quantum theory that is obtained if we start with the constraint function (2.5), but instead of imposing the Dirac condition (2.4), we allow the quantum states to be in arbitrary superpositions of the eigenstates of $\hat{C}$. In other words, the (secondary) quantum constraint is not imposed and off-shell states are permitted in the quantum theory. Why is this so? In the same way that the value of Λ (which is the classical value of C) is a constant of motion that is taken to depend on the initial conditions of the scalars, the expectation value (and other correlation functions) of $\hat{C}$ depend on the choice of initial quantum state $\left|\psi\right\rangle$. For certain peaked states, one can recover, for example, $\langle \hat{C} \rangle = 0$. Evidently, this procedure rests on the assumption that a "free cosmological constant" exists (it is determined by the initial conditions of the universe) or, equivalently, that a proper-time field exists, which respect to which a global deparametrization is possible.

This approach to the quantization of a constrained system was originally proposed by Stückelberg in [43], in the context of the quantization of the free relativistic particle. In this example, the "cosmological constant" is simply related to the particle's mass, $\Lambda = m^2/2$, which is considered not to be fixed a priori, but rather determined by the initial position and momentum of the particle. Over the years, Stückelberg's approach has been reincarnated in various different proposals [44–47]. Although it is certainly an interesting approach, it is a particular case of the general framework considered in this

[2]If Λ is considered as a fixed constant, it acquires the status of law in the sense that it defines the constraint C_Λ, and its value determines which independent initial conditions on the scalars are allowed by the theory.

thesis because it involves a certain choice of worldline time coordinate (complete gauge fixing) related to proper time, as was also mentioned in §1.4. We will see below that this choice of time coordinate (and possibly others) can be, in principle, accommodated in the quantum theory based on Dirac's conditions (2.4) if one follows the analogy with the HJ formalism discussed in §1.10.[3]

2.3 The physical Hilbert space

Our task is now to construct and examine the space of solutions of the Dirac conditions (2.4). Since $\hat{p}_e$ and $\hat{C}$ commute and are assumed to be self-adjoint operators with respect to the auxiliary inner product, it is possible to find a system of eigenstates that is complete and orthonormal with respect to $\langle\cdot|\cdot\rangle$; i.e.,

$$\hat{p}_e\,|p_e,E,\mathbf{k}\rangle = p_e\,|p_e,E,\mathbf{k}\rangle \ , \tag{2.6}$$

$$\hat{C}\,|p_e,E,\mathbf{k}\rangle = E\,|p_e,E,\mathbf{k}\rangle \ , \tag{2.7}$$

$$\langle p'_e,E',\mathbf{k}'|p_e,E,\mathbf{k}\rangle = \delta(p'_e,p_e)\delta(E',E)\delta(\mathbf{k}',\mathbf{k}) \ , \tag{2.8}$$

where $\mathbf{k}$ denotes degeneracies[4] that can be regarded as local coordinates in the reduced configuration or momentum space [i.e., they can be chosen to be either of the (x,k) coordinates considered in the HJ formalism, cf. (1.114)], and $\delta(\cdot,\cdot)$ is a Dirac (Kronecker) delta if the labels are continuous (discrete). Let us denote a basis on the space of solutions of (2.4) as $|\mathbf{k}\rangle \equiv |p_e=0,E=0,\mathbf{k}\rangle$. This basis can be used to define on-shell, gauge-invariant states. We find the auxiliary overlap

$$\langle\mathbf{k}'|\mathbf{k}\rangle \equiv \langle p_e=0,E=0,\mathbf{k}'|p_e=0,E=0,\mathbf{k}\rangle = \delta(0,0)\delta(0,0)\delta(\mathbf{k}',\mathbf{k}). \tag{2.9}$$

As the primary constraint operator $\hat{p}_e$ is assumed to have a continuous spectrum, the corresponding factor $\delta(0,0)$ in (2.9) diverges. This is physically irrelevant because the physical solutions are those that satisfy the constraints [cf. (2.4)]. The auxiliary Hilbert space $\mathcal{H}$ is taken to be a merely ancillary construct, similarly to the auxiliary phase space in the classical theory. The divergence in (2.9) is simply a consequence of the way $\mathcal{H}$ was defined. Moreover, if zero is in the continuous part of the spectrum of the secondary constraint operator, the second $\delta(0,0)$ in (2.9) also diverges. This shows that the auxiliary inner product is, in fact, inadequate, and we must regularize it in order to define the norm of physical states.

[3]It is also worthwhile to mention Komar's approach [63], in which the Dirac conditions (2.4) are imposed, but the constraints are not self-adjoint, and the evolution is defined by an operator which is proportional to the Hermitian conjugate of the constraints.

[4]We assume that the labels $\mathbf{k}$ are independent of p_e and E.

We can define the so-called Rieffel induced inner product $(\cdot|\cdot)$ by requiring that the states $|\mathbf{k}\rangle$ are orthogonal (see [64–71]). Thus, we define

$$\langle p_e', E', \mathbf{k}'|p_e, E, \mathbf{k}\rangle =: \delta(p_e', p_e)\delta(E', E)(p_e', E', \mathbf{k}'|p_e, E, \mathbf{k}) \ , \tag{2.10}$$

where, in particular, we obtain

$$(\mathbf{k}'|\mathbf{k}) \equiv (p_e' = 0, E = 0, \mathbf{k}'|p_e = 0, E = 0, \mathbf{k}) = \delta(\mathbf{k}', \mathbf{k}) \ . \tag{2.11}$$

The induced inner product can be used to define the overlap of arbitrary physical states. Given the superpositions

$$|\Psi_{(1,2)}\rangle = \sum_{\mathbf{k}} \Psi_{(1,2)}(\mathbf{k})\,|\mathbf{k}\rangle \ , \tag{2.12}$$

their induced overlap is

$$(\Psi_{(1)}|\Psi_{(2)}) = \sum_{\mathbf{k}} \Psi^*_{(1)}(\mathbf{k})\Psi_{(2)}(\mathbf{k}) \ . \tag{2.13}$$

If the labels $\mathbf{k}$ are continuous, an integration replaces the summation in (2.13). In this way, the induced inner product can be seen as the physical inner product on the space of the superpositions (2.12). More precisely, we define the vector space of solutions of (2.4) that have finite induced norm to be the physical Hilbert space $\mathcal{H}_{\text{phys}}$.

Although the auxiliary Hilbert space and inner product are not physical, it is often useful to express the induced inner product in terms of $\langle\cdot|\cdot\rangle$. Let us examine two possible ways in which this can be done. First, we define the (improper) projectors

$$\begin{aligned} \hat{P}_{p_e,E} &= \sum_{\mathbf{k}} \ |p_e, E, \mathbf{k}\rangle\,\langle p_e, E, \mathbf{k}| \ , \\ \hat{P}_{p_e',E'}\hat{P}_{p_e,E} &= \delta(p_e' - p_e)\delta(E', E)\hat{P}_{p_e,E} \ , \end{aligned} \tag{2.14}$$

such that physical states satisfy [cf. (2.12)]

$$\hat{P}_{p_e,E}\,|\Psi_{(1,2)}\rangle = \delta(p_e)\delta(E,0)\,|\Psi_{(1,2)}\rangle \ . \tag{2.15}$$

Notice that $|p_e, E, \mathbf{k}\rangle = |p_e\rangle \otimes |E, \mathbf{k}\rangle$, and we can also define

$$\begin{aligned} \hat{P}_{p_e} &:= |p_e\rangle\langle p_e| \equiv \sum_{E,\mathbf{k}} |p_e, E, \mathbf{k}\rangle\langle p_e, E, \mathbf{k}| \ , \quad \int \mathrm{d}p_e \hat{P}_e = \hat{1} \ , \\ \hat{P}_E &:= \sum_{\mathbf{k}} |E, \mathbf{k}\rangle\langle E, \mathbf{k}| \equiv \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \mathrm{d}p_e \ |p_e, E, \mathbf{k}\rangle\langle p_e, E, \mathbf{k}| \ , \ \sum_E \hat{P}_E = \hat{1} \ , \end{aligned} \tag{2.16}$$

where an integral replaces the sum if E is continuous. Let us now adopt the sign $\bullet$ to denote the action of operators with respect to $(\cdot|\cdot)$, and let us use the short-hand notation $\hat{P}_0 \equiv \hat{P}_{p_e=0,E=0}$. Then, from (2.14), (2.15) and (2.11), we find

$$\begin{aligned} \hat{P}_0 \bullet |\Psi_{(1,2)}\rangle &= |\Psi_{(1,2)}\rangle \ , \\ \hat{P}_0 \bullet \hat{P}_0 &= \hat{P}_0 \ . \end{aligned} \tag{2.17}$$

This means that $\hat{P}_0$ is the identity in $\mathcal{H}_{\text{phys}}$. Now suppose that

$$\Psi_{(1,2)}(\mathbf{k}) = \langle p_e = 0, E = 0, \mathbf{k} | \psi_{(1,2)}\rangle \ ,$$

for some off-shell states $|\psi_{(1,2)}\rangle$. Then, Eqs. (2.12) and (2.13) imply that

$$\begin{aligned} |\Psi_{(1,2)}\rangle &= \hat{P}_0 |\psi_{(1,2)}\rangle \ , \\ (\Psi_{(1)}|\Psi_{(2)}) &= \left\langle \psi_{(1)} \middle| \hat{P}_0 \middle| \psi_{(2)} \right\rangle \ . \end{aligned} \tag{2.18}$$

This establishes a relation between the induced and auxiliary inner products. Incidentally, Eq. (2.18) is related to what is often called the "group averaging" procedure [69]. To see this, let us consider the particular case in which E spans the real line, such that

$$\begin{aligned} \hat{P}_0 &= \int_{-\infty}^{\infty} \mathrm{d}p_e \int_{-\infty}^{\infty} \mathrm{d}E \ \delta(p_e)\delta(E) \sum_{\mathbf{k}} |p_e, E, \mathbf{k}\rangle\langle p_e, E, \mathbf{k}| \\ &= \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}\lambda \mathrm{d}\tau \mathrm{d}p_e \mathrm{d}E \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda \hat{p}_e} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \sum_{\mathbf{k}} |p_e, E, \mathbf{k}\rangle\langle p_e, E, \mathbf{k}| \\ &= \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} \mathrm{d}\lambda \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda \hat{p}_e} \int_{-\infty}^{\infty} \mathrm{d}\tau \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \ , \end{aligned} \tag{2.19}$$

due to the fact that $|p_e, E, \mathbf{k}\rangle$ are a complete system. Then, Eq. (2.18) becomes the "group averaging" formula[5]

$$(\Psi_{(1)}|\Psi_{(2)}) = \left\langle \psi_{(1)} \left| \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} \mathrm{d}\lambda\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda\hat{p}_e} \int_{-\infty}^{\infty} \mathrm{d}\tau\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \right| \psi_{(2)} \right\rangle \ . \tag{2.20}$$

Another way to express $(\cdot|\cdot)$ in terms of $\langle\cdot|\cdot\rangle$ is obtained is by "gauge fixing" in the following sense: let us define the states

$$|e,t,\mathbf{k}\rangle := \frac{1}{\sqrt{2\pi\hbar}} \sum_E \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et} |e,E,\mathbf{k}\rangle = \sum_E \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_e}{2\pi\hbar}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}ep_e} |p_e,E,\mathbf{k}\rangle \ . \tag{2.21}$$

These states satisfy the properties

$$\langle p_e = 0, E = 0, \mathbf{k}'|e,t,\mathbf{k}\rangle = \frac{1}{2\pi\hbar}\delta(\mathbf{k}',\mathbf{k}) \ , \tag{2.22}$$

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda\hat{p}_e}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}} |e,t,\mathbf{k}\rangle = |e-\lambda, t-\tau, \mathbf{k}\rangle \ . \tag{2.23}$$

The second property is called 'covariance' [72–75]. Note that the values of t should be chosen so as to parametrize the unitary flow of $\hat{C}$ [75]. However, depending on the properties of the spectrum of $\hat{C}$ and its unitary flow, it may be impossible to construct a complete orthonormal system (in the auxiliary Hilbert space $\mathcal{H}$) from the states $|e,t,\mathbf{k}\rangle$ [72, 75]. Nevertheless, it is sufficient for our purposes to assume that a set of states with the properties given in (2.22) and (2.23) exists. Completeness and orthonormality with respect to the auxiliary inner product are not mandatory due to the ancillary character of $\mathcal{H}$. Let us then define the operator

$$\hat{\mu} := (2\pi\hbar)^2 \sum_{\mathbf{k}} |e=e_0, t=t_0, \mathbf{k}\rangle \langle e=e_0, t=t_0, \mathbf{k}| = 2\pi\hbar \hat{P}_{e=e_0, t=t_0} \ , \tag{2.24}$$

for arbitrary values of e_0 and t_0. Due to (2.22), we see that the induced overlap of two physical states can be written as

$$(\Psi_{(1)}|\Psi_{(2)}) = \langle\Psi_{(1)}|\hat{\mu}|\Psi_{(2)}\rangle \ , \tag{2.25}$$

and this yields another relation between the induced and auxiliary inner products. This can be regarded as a "gauge fixing", in the sense that the states $|e,t,\mathbf{k}\rangle$ can be

[5] If the spectrum of $\hat{C}$ is discrete, it may be possible to obtain a formula that is analogous to (2.20), where the integral over τ is performed over a finite interval. For example, if E spans the integers, we can integrate τ over the interval $(0, 2\pi)$.

used to define operators that are formally conjugate to the constraints if they form a complete system [72, 73, 75]. Thus, fixing arbitrary values of e_0 and t_0 is analogous to a classical gauge fixing procedure in which one fixes the values of the einbein and of a canonical representation of proper time [cf. (1.122)]. Even in the case in which the set of states $|e, t, \mathbf{k}\rangle$ is not complete and orthonormal (in the auxiliary Hilbert space), we still consider this analogy to be valid.

2.4 On-shell and invariant operators

The only operators that are physically relevant are those that act solely on $\mathcal{H}_{\text{phys}}$ and, therefore, define linear transformations between physical states. We refer to such operators as 'on shell'. A general on-shell operator can be written as

$$\begin{aligned}\hat{\mathcal{O}} &= \sum_{\mathbf{k}',\mathbf{k}} \mathcal{O}(\mathbf{k}',\mathbf{k}) \left|\mathbf{k}'\right\rangle \left\langle\mathbf{k}\right| \\ &\equiv \sum_{\mathbf{k}',\mathbf{k}} \mathcal{O}(\mathbf{k}',\mathbf{k}) \left|p_e = 0, E = 0, \mathbf{k}'\right\rangle \left\langle p_e = 0, E = 0, \mathbf{k}\right| \ .\end{aligned} \tag{2.26}$$

Notice that $\hat{p}_e\hat{\mathcal{O}} = \hat{\mathcal{O}}\hat{p}_e = \hat{C}\hat{\mathcal{O}} = \hat{\mathcal{O}}\hat{C} = 0$. More generally, we can define invariant operators, which commute with the constraints, as

$$\hat{\mathcal{O}}_{\text{inv}} = \sum_{E}\sum_{\mathbf{k}',\mathbf{k}} \int_{-\infty}^{\infty} \mathrm{d}p_e \ \mathcal{O}_{\text{inv}}(\mathbf{k}',\mathbf{k};p_e,E) \left|p_e, E, \mathbf{k}'\right\rangle \left\langle p_e, E, \mathbf{k}\right| \ . \tag{2.27}$$

Clearly, on-shell operators are obtained from invariants by the relation

$$\hat{\mathcal{O}} = \hat{P}_0\hat{\mathcal{O}}_{\text{inv}} \ , \tag{2.28}$$

such that $\mathcal{O}(\mathbf{k}',\mathbf{k}) = \mathcal{O}_{\text{inv}}(\mathbf{k}',\mathbf{k};0,0)$. Furthermore, given an operator $\hat{f}$ that does not commute with $\hat{p}_e$ nor with $\hat{C}$, we can define the invariant

$$\hat{\mathcal{O}}_{f;\text{inv}} := \sum_{E} \int_{-\infty}^{\infty} \mathrm{d}p_e \ \hat{P}_{p_e,E}\,\hat{f}\,\hat{P}_{p_e,E} \ , \tag{2.29}$$

for which $\mathcal{O}_{f;\text{inv}}(\mathbf{k}',\mathbf{k};p_e,E) = \langle p_e, E, \mathbf{k}'|\hat{f}|p_e, E, \mathbf{k}\rangle$. This is a well-defined operator if $\mathcal{O}_{f;\text{inv}}(\mathbf{k}',\mathbf{k};p_e,E) < \infty$. The associated on-shell operator has the induced matrix elements $\mathcal{O}_f(\mathbf{k}',\mathbf{k}) = \langle p_e = 0, E = 0, \mathbf{k}'|\hat{f}|p_e = 0, E = 0, \mathbf{k}\rangle$ and can be written as[6]

$$\hat{\mathcal{O}}_f = \hat{P}_0\,\hat{f}\hat{P}_0\ . \tag{2.30}$$

For our purposes, it will be sufficient to consider operators $\hat{f}$ that are defined solely from the scalars $\hat{q}$ and $\hat{p}$, which commute with $\hat{p}_e$ but not with $\hat{C}$. In this case, $\hat{f} \equiv f(\hat{q},\hat{p})$, and we define [cf. (2.16)]

$$\hat{\mathcal{O}}_{f;\mathrm{inv}} := 2\pi\hbar\sum_E \hat{P}_E\,\hat{f}\,\hat{P}_E \tag{2.31}$$

instead of (2.31). The associated on-shell operator is

$$\hat{\mathcal{O}}_f = 2\pi\hbar\hat{P}_0\,\hat{f}\,\hat{P}_{E=0} = 2\pi\hbar\hat{P}_{E=0}\,\hat{f}\,\hat{P}_0 \tag{2.32}$$

instead of (2.30). What is the classical analogue of (2.31) and (2.32)? To find the answer, let us consider again the particular case in which E spans the real line, such that (2.31) becomes[7]

$$\begin{aligned}
\hat{\mathcal{O}}_{f;\mathrm{inv}} &:= 2\pi\hbar\int_{-\infty}^{\infty}\mathrm{d}E\ \hat{P}_E\,\hat{f}\,\hat{P}_E\\
&= 2\pi\hbar\int \mathrm{d}E\mathrm{d}E'\ \delta(E'-E)\hat{P}_{E'}\,\hat{f}\,\hat{P}_E\\
&= \int \mathrm{d}E\mathrm{d}E'\mathrm{d}\tau\ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau(E'-E)}\hat{P}_{E'}\,\hat{f}\,\hat{P}_E\\
&= \int \mathrm{d}E\mathrm{d}E'\mathrm{d}\tau\ \hat{P}_{E'}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}}\,\hat{f}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}}\,\hat{P}_E\\
&= \int_{-\infty}^{\infty}\mathrm{d}\tau\ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}}\,\hat{f}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}}\ ,
\end{aligned} \tag{2.33}$$

where we used (2.16) to reach the last line. Notice that the integrand in (2.33) can be regarded as an auxiliary Heisenberg-picture operator, that encodes the evolution of $\hat{f} \equiv f(\hat{q},\hat{p})$ in terms of proper time.[8] In this way, Equation (2.33) is a quantum version of (1.79), where the worldline time coordinate τ is chosen to be the proper time (1.2), and the integration limits are $\tau_0 \to -\infty$ and $\tau_1 \to \infty$. For this reason, we take (2.29), (2.30), (2.31) and (2.32) to be the quantum counterparts to the classical invariants (1.79) (even in the case in which the spectrum of $\hat{C}$ does not coincide with

[6] In [33], on-shell operators were considered with a different notation and they were called 'projected kernels' (see Eq. 13.32 in [33]).

[7] See also [30, 53].

[8] The corresponding classical evolution is dictated by the gauge-fixed total Hamiltonian (1.65) with $\omega \equiv 1$, such that $H_T^{\mathrm{gf}} = C$. This is referred to as the 'proper-time gauge'.

the reals[9]).

As we have argued in §1.7, the classical invariants that have a clear physical interpretation are the relational observables. Therefore, we set out to construct quantum relational observables as on-shell operators of the form (2.30) or (2.32). We present three closely related methods of construction, and we examine the quantum dynamics of the ensuing observables.

2.5 Quantum relational observables

We expect that quantum relational observables will satisfy a quantum version of the classical evolution dictated by (1.95), which is based on the picture of observables evolving according to an explicit time dependence [cf. (1.91)]. As was argued in §1.9.1, one evades the classical "problem" of time due to the fact that families of relational observables encode the gauge-fixed evolution in their explicit dependence on the worldline time parameter and, as such, these families are not diffeomorphism invariant in a strict sense (although each member Poisson-commutes with the constraints and is, moreover, a worldline constant that encodes a fixed instant). In similar way, we will see that one can construct a family of operators that commute with the constraints [and, therefore, with the total Hamiltonian (2.2)], the dynamics of which is encoded in their explicit τ dependence.

Furthermore, it is also reasonable to anticipate that quantum observables will obey a counterpart of the classical reduced phase-space equation (1.103), which encodes their evolution in the orbits generated by the physical Hamiltonian. Correspondingly, we will see that one can, in principle, define a physical propagator in the quantum theory.

2.5.1 Proper-time evolution

Let us begin with the 'proper-time gauge' in which the classical, gauge-fixed total Hamiltonian coincides with C [cf. (1.65) with $\omega \equiv 1$]. More general gauges will be analyzed in §2.5.2 and §2.5.6. In the proper-time gauge, the classical einbein is equal to unity [cf. (1.63)], and we consider that the corresponding quantum observable is simply the identity operator [or, more precisely, the corresponding on-shell operator is the identity in $\mathcal{H}_{\text{phys}}$, which corresponds to $\hat{P}_0$; cf. (2.17) and (2.28)]. Let us then take a general operator $\hat{f} \equiv f(\hat{q}, \hat{p}; s)$ that depends solely on the scalar fields and on a parameter s together with the "gauge-fixed" measure (2.24) with $e_0 = 1$ and $t_0 = s$ to

[9] As was mentioned in footnote 5, it may be possible to obtain a formula similar to (2.33), where the integral is performed over a finite interval if the spectrum of $\hat{C}$ is discrete. For instance, if E spans the integers, the integral over τ may be performed from 0 to 2π.

define the invariant operator [cf. (2.29)]

$$\hat{\mathcal{O}}_{\text{inv}}[f|\chi = s] := \frac{1}{2}\sum_E \int \mathrm{d}p_e \ \hat{P}_{p_e,E} \, [\hat{f},\hat{\mu}]_+ \, \hat{P}_{p_e,E} \ , \tag{2.34}$$

where $[\cdot,\cdot]_+$ is the anticommutator. Let us now use the fact that $\hat{f}$ commutes with $\hat{p}_e$ together with (2.16), (2.21), and (2.24) to rewrite (2.34) as

$$\begin{aligned} \hat{\mathcal{O}}_{\text{inv}}[f|\chi = s] &:= \pi\hbar \sum_E \hat{P}_E \, [\hat{f},\hat{P}_{t=s}]_+ \, \hat{P}_E \ , \\ \hat{P}_{t=s} &:= \sum_{\mathbf{k}} |t = s, \mathbf{k}\rangle \langle t = s, \mathbf{k}| \ . \end{aligned} \tag{2.35}$$

In the particular case in which the spectrum of $\hat{C}$ is $\mathbb{R}$, we can develop (2.35) in a similar way as (2.33) to obtain

$$\hat{\mathcal{O}}_{\text{inv}}[f|\chi = s] = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \, [\hat{f},\hat{P}_{t=s}]_+ \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \ . \tag{2.36}$$

Finally, we can rewrite (2.36) as[10]

$$\begin{aligned} \hat{\mathcal{O}}_{\text{inv}}[f|\chi = s] &:= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \hat{f}\hat{P}_{t=s} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}} + \text{h.c.} \\ &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \ \hat{f}(\tau)\hat{P}_{t=s-\tau} + \text{h.c.} \ , \end{aligned} \tag{2.37}$$

where we used (2.23). We take $\hat{P}_{t=s-\tau}$ to be the quantum analogue of the gauge-fixing Dirac delta in (1.89), even if the states $|t,\mathbf{k}\rangle$ are not orthonormal.[11] In this way, Eq. (2.37) is the quantum analogue of (1.89) for the particular case in which $\tau_0 \to -\infty, \tau_1 \to \infty$, and the generalized clock $\chi(\tau) = t + \tau$ is a canonical representation of proper time [cf. (1.124)],[12] such that the Faddeev-Popov determinant is unity [cf. (1.88)]. For this reason, we consider that (2.35) is the quantum counterpart to the classical relational observable (1.89) in the proper-time gauge, even in the case in which the states $|e,t,\mathbf{k}\rangle$ do not form a complete orthononormal system in the auxiliary Hilbert space $\mathcal{H}$ and the spectrum of $\hat{C}$ does not coincide with $\mathbb{R}$. As was remarked after (2.23), the requirement of completeness and orthornormality in $\mathcal{H}$ is not obligatory due to its auxiliary character.

[10]The abbreviation “h.c.” is a short-hand for “Hermitian conjugate”. Here, the term Hermitian refers to the auxiliary inner product.

[11]Specifically, $\hat{P}_{t=s-\tau} = \sum_{\mathbf{k}} \int \mathrm{d}t \ \delta(t - s + \tau) \, |t,\mathbf{k}\rangle \langle t,\mathbf{k}|$.

[12]Notice that $T(\tau) = s$ implies that $t = s - \tau$, which is the condition enforced by $\hat{P}_{t=s-\tau}$.

From (2.35), we define the on-shell quantum relational observables in the proper-time gauge as [cf. (2.32)]

$$\hat{\mathcal{O}}[f|\chi = s] = \pi\hbar\hat{P}_0\,[\hat{f}, \hat{P}_{t=s}]_+\,\hat{P}_{E=0}\ . \tag{2.38}$$

In particular, if $\hat{f} = \hat{1}$, we can use (2.21) and (2.22) to find the quantum Faddeev-Popov resolution of the identity,

$$\hat{\mathcal{O}}[1|\chi = s] = 2\pi\hbar\hat{P}_0\hat{P}_{t=s}\hat{P}_{E=0} = \hat{P}_0\ , \tag{2.39}$$

which is the counterpart of (1.90) because $\hat{P}_0$ acts as the identity in $\mathcal{H}_{\text{phys}}$ [cf. (2.17)]. Equation (2.39) also implies that, if $\hat{f}$ is itself an invariant, then (2.38) becomes

$$\hat{\mathcal{O}}[f|\chi = s] = \hat{P}_0\hat{f}\ ; \tag{2.40}$$

i.e., the on-shell relational observable associated with an invariant $\hat{f} \equiv f(\hat{q}, \hat{p})$ is simply its restriction to the physical Hilbert space, as expected.

The quantum dynamics of (2.38) can be found by using (2.4), (2.23) and (2.32) to obtain

$$\begin{aligned}
\hat{\mathcal{O}}[f|\chi = s] &= \pi\hbar\hat{P}_0\,\hat{f}\hat{P}_{t=s}\,\hat{P}_{E=0} + \text{h.c.} \\
&= \pi\hbar\hat{P}_0\,\hat{f}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{C}}\hat{P}_{t=t_0}\,\hat{P}_{E=0} + \text{h.c.} \\
&= \pi\hbar\hat{P}_0\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{C}}\hat{f}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{C}}\hat{P}_{t=t_0}\,\hat{P}_{E=0} + \text{h.c.} \\
&= \pi\hbar\hat{P}_0\,\hat{f}(s-t_0)\hat{P}_{t=t_0}\,\hat{P}_{E=0} + \text{h.c.}\ ,
\end{aligned} \tag{2.41}$$

where, in the last line, we defined the auxiliary Heisenberg-picture operator $\hat{f}(s-t_0) := \exp(\mathrm{i}(s-t_0)\hat{C}/\hbar)\hat{f}\exp(-\mathrm{i}(s-t_0)\hat{C}/\hbar)$. If we now differentiate (2.41) with respect to s, we find

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\hat{\mathcal{O}}[f|\chi = s] &= \pi\hbar\hat{P}_0\,\left[\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\hat{f}(s-t_0)\,,\,\hat{P}_{t=t_0}\right]_+\,\hat{P}_{E=0} \\
&= \pi\hbar\hat{P}_0\,\left[\mathrm{i}\hbar\,\frac{\partial\hat{f}}{\partial s}\bigg|_{s-t_0} + [\hat{f},\hat{C}]|_{s-t_0}\,,\,\hat{P}_{t=t_0}\right]_+\,\hat{P}_{E=0} \\
&= \hat{\mathcal{O}}\left[\mathrm{i}\hbar\frac{\partial f}{\partial s} + [\hat{f},\hat{C}]\bigg|\,\chi = s\right]\ ,
\end{aligned} \tag{2.42}$$

which is the quantum version of (1.95) in the proper-time gauge.[13]

We can also define an analogue of (1.103) in terms of a physical propagator. More precisely, just as (1.103) expresses the evolution of classical relational observables in terms of orbits in the reduced phase space Γ_{phys}, we now seek a description of the evolution of quantum relational observables in terms of orbits related to a unitary flow in $\mathcal{H}_{\text{phys}}$. First, notice that (2.38) is symmetric with respect to the auxiliary inner product by construction. It is also symmetric with respect to the induced inner product because, given two physical states $|\Psi_{(1,2)}\rangle = |p_e = 0\rangle \otimes |\tilde{\Psi}_{(1,2)}\rangle$ [cf. (2.12)], we obtain[14]

$$\begin{aligned} |\mathcal{O}\Psi_{(1,2)}\rangle &:= \hat{\mathcal{O}}[f|\chi = s] \bullet |\Psi_{(1,2)}\rangle = \pi\hbar\, |p_e = 0\rangle \otimes \hat{P}_{E=0}[\hat{f}, \hat{P}_{t=s}]_+ |\tilde{\Psi}_{(1,2)}\rangle \ , \\ (\mathcal{O}\Psi_{(1)}|\Psi_{(2)}) &= (\Psi_{(1)}|\mathcal{O}\Psi_{(2)}) = \pi\hbar\, \langle\tilde{\Psi}_{(1)}|[\hat{f}, \hat{P}_{t=s}]_+|\tilde{\Psi}_{(2)}\rangle \ . \end{aligned} \tag{2.43}$$

If we assume that $\hat{\mathcal{O}}[f|\chi = s]$ is not only symmetric but, in fact, self-adjoint with respect to $(\cdot|\cdot)$ (or that a self-adjoint extension can be defined) for all possible values of s, then we can write its spectral decomposition as

$$\hat{\mathcal{O}}[f|\chi = s] =: \sum_{f,\mathbf{n}} f \ |f, \mathbf{n}; s\rangle \langle f, \mathbf{n}; s| \ , \tag{2.44}$$

where the sums are formal and $\mathbf{n}$ are degeneracies. The states $|f, \mathbf{n}; s\rangle$ form a complete and orthonormal system in $\mathcal{H}_{\text{phys}}$ for all possible values of s by hypothesis; i.e., we have

$$(f', \mathbf{n}'; s|f, \mathbf{n}; s) = \delta(f', f)\delta(\mathbf{n}', \mathbf{n}) \ , \tag{2.45}$$

$$\sum_{f,\mathbf{n}} |f, \mathbf{n}; s\rangle \langle f, \mathbf{n}; s| = \hat{P}_0 \ . \tag{2.46}$$

Incidentally, Eq. (2.46) is another representation of the Faddeev-Popov resolution of the identity (2.39).

Given two instants s and s_0, we define the physical proper-time propagator to be the overlap $(f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0)$. Formally, this has the correct properties: (1) due to (2.45), it reduces to the identity kernel function in the limit $s \to s_0$; (2) it corresponds to a unitary transformation in $\mathcal{H}_{\text{phys}}$ in the following sense: if we define the physical states $|\Psi\rangle := \sum_{f,\mathbf{n}} \Psi(f, \mathbf{n})\, |f, \mathbf{n}; s_0\rangle$ and $|\Psi; s\rangle := \sum_{f,\mathbf{n}} \Psi(f, \mathbf{n}; s)\, |f, \mathbf{n}; s_0\rangle$, where

$$\Psi(f, \mathbf{n}; s) := \sum_{f_0,\mathbf{n}_0} (f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0)\Psi(f_0, \mathbf{n}_0) \ , \tag{2.47}$$

[13] Notice that $\hat{P}_0[\hat{f}, \hat{C}]\hat{P}_{t=t_0}\hat{P}_{E=0} = \hat{P}_0\hat{f}\hat{C}\hat{P}_{t=t_0}\hat{P}_{E=0}$.

[14] In the particular case in which $\hat{f} = \hat{1}$, the second line of (2.43) coincides with (2.25).

then they have the same induced norm

$$\begin{aligned}(\Psi; s|\Psi; s) &= \sum_{f,\mathbf{n}} |\Psi(f, \mathbf{n}; s)|^2 \\ &= \sum_{f,\mathbf{n},f_0,\mathbf{n}_0,f_0',\mathbf{n}_0'} \Psi^*(f_0', \mathbf{n}_0') \left(f_0', \mathbf{n}_0'; s_0|f, \mathbf{n}; s\right) \\ &\quad \times (f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0) \, \Psi(f_0, \mathbf{n}_0) \\ &= \sum_{f_0,\mathbf{n}_0,f_0',\mathbf{n}_0'} \Psi^*(f_0', \mathbf{n}_0') \left(f_0', \mathbf{n}_0'; s_0|f_0, \mathbf{n}_0; s_0\right) \Psi(f_0, \mathbf{n}_0) \\ &= \sum_{f_0,\mathbf{n}_0} |\Psi(f_0, \mathbf{n}_0)|^2 = (\Psi|\Psi)\end{aligned} \tag{2.48}$$

due to (2.45) and (2.46). We can regard $|\Psi; s\rangle$ as the physical Schrödinger-picture state with initial condition $|\Psi; s_0\rangle = |\Psi\rangle$, and its evolution given by the physical propagator $(f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0)$ is unitary due to (2.48). Moreover, we can write the matrix element of (2.44) as

$$\begin{aligned}&\left(f', \mathbf{n}'; s_0 \left|\hat{\mathcal{O}}[f|\chi = s]\right| f, \mathbf{n}; s_0\right) \\ &= \sum_{f'',\mathbf{n}''} f'' \, (f', \mathbf{n}'; s_0|f'', \mathbf{n}''; s)(f'', \mathbf{n}''; s|f, \mathbf{n}, s_0) \ ,\end{aligned} \tag{2.49}$$

which has the form of a kernel function for a (physical) Heisenberg-picture operator. In this way, we see that the physical proper-time propagator $(f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0)$ encodes the evolution of $\hat{\mathcal{O}}[f|\chi = s]$ as a unitary flow in the physical Hilbert space, in analogy to the physical Hamiltonian in (1.103), which encodes the evolution of the classical observable as an orbit in the reduced phase space.

Before we proceed to discuss other gauges, a few comments regarding (2.45), (2.46), and the definition of the physical propagator are in order. First, the physical propagator constructed above may be trivial. For example, as the observable $\mathcal{O}[1|\chi = s] = \hat{P}_0$ coincides with the identity in $\mathcal{H}_{\text{phys}}$ [cf. (2.39)], its spectral decomposition is simply $\sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}|$ [cf. (2.14)], and the overlap $(\mathbf{k}'|\mathbf{k}) = \delta(\mathbf{k}', \mathbf{k})$ of its eigenstates is independent of s. This does not signal that the evolution cannot be defined in the physical Hilbert space but rather that the observable in question is constant [cf. (2.44)]. Second, in the classical case (1.103), it was possible for the observable $\mathcal{O}[f|\chi = s]$ to exhibit an explicit time dependence in addition to its variation along the orbits generated by the physical Hamiltonian vector field. This is also, in principle, possible in the quantum theory, but the physical propagator $(f, \mathbf{n}; s|f_0, \mathbf{n}_0; s_0)$ constructed above encodes both the explicit and implicit time dependence of $\hat{\mathcal{O}}[f|\chi = s]$ [cf. (2.44)] because it is constructed directly from the spectral decomposition (2.44) and we assume self-adjointness of the observable.[15] Third, if we compute the propagators from two different observables in the proper-time gauge, the resulting overlaps may be different. We take them to be simply different representations of the physical propagator in different bases (complete orthonormal systems in $\mathcal{H}_{\text{phys}}$, which are determined by the spectral decompositions), also in the case in which the observables have an explicit time dependence.

The above subtleties regarding the physical propagator are consequences of the fact that we started with the proper-time gauge but did not quantize a physical Hamiltonian directly. Alternatively, we could start by defining some invariant operator to be the quantum physical Hamiltonian, such that, instead of solely the physical propagator, we could derive explicitly the physical Heisenberg equations that are analogous to (1.103). A possible formalism for this is discussed next.

2.5.2 Evolution in other gauges

Following the construction of observables in the HJ formalism (cf. §1.10), we can identify the states $|\mathbf{k}\rangle$ and $|\mathbf{x}\rangle = \sum_{\mathbf{k}} \exp(-\mathrm{i}\mathbf{x}\cdot\mathbf{k}/\hbar)\, |\mathbf{k}\rangle / \sqrt{2\pi\hbar}$ as the quantum analogues of the (x,k) coordinates used in (1.114). The counterpart of the h and t coordinates can be defined as follows. For a moment, let us assume that zero is in the continuous part of the spectrum of $\hat{C}$, in order to follow the analogy with HJ formalism. We then define $\hat{h}$ as the invariant [cf. (2.27)]

$$\hat{h} = \sum_{\mathbf{k}',\mathbf{k}} \int \mathrm{d}E\mathrm{d}p_e\ h(\mathbf{k}',\mathbf{k};p_e,E)\, |p_e,E,\mathbf{k}'\rangle \langle p_e,E,\mathbf{k}| \ , \tag{2.50}$$

which obeys the symmetry condition $h(\mathbf{k}',\mathbf{k};p_e,E) = h^*(\mathbf{k},\mathbf{k}';p_e,E)$. As $\hat{h}$ commutes with the constraints, it is possible to find a simultaneous eigenbasis $|p_e,h,\mathbf{n}\rangle$ such that

$$\begin{aligned} \hat{p}_e\, |p_e,h,\mathbf{n}\rangle &= p_e\, |p_e,h,\mathbf{n}\rangle \ , \\ \hat{C}\, |p_e,h,\mathbf{n}\rangle &= C(h,\mathbf{n})\, |p_e,h,\mathbf{n}\rangle \ , \\ \hat{h}\, |p_e,h,\mathbf{n}\rangle &= h\, |p_e,h,\mathbf{n}\rangle \ , \end{aligned} \tag{2.51}$$

where $C(h,\mathbf{n}) \in \mathbb{R}$ is the expression of the eigenvalue of $\hat{C}$ in terms of the eigenvalue of $\hat{h}$ and the degeneracies $\mathbf{n}$. As in the classical theory (cf. §1.10), we may choose $\hat{h}$ to be the invariant extension of some operator with respect to a certain previously defined gauge (e.g., the proper-time gauge analyzed in §2.5.1). In particular, if we choose $\hat{h} = \hat{C}$, then we recover the proper-time gauge. In general, we assume that we

[15] Instead of (2.44), one could consider, in principle, a decomposition in which the eigenvalue f also has an explicit dependence on s. This is not discussed here. See, however, the developments of §2.5.2.

can solve $C(h,\mathbf{n}) = E$ to find the real solutions

$$h = -H^\sigma(E,\mathbf{n}) = -H_0^\sigma(\mathbf{n}) - H_1^\sigma(\mathbf{n})E + \mathcal{O}(E^2)\ , \tag{2.52}$$
$$H_1^\sigma(\mathbf{n}) \neq 0\ , \tag{2.53}$$

at least if E is in an interval that contains zero. Equation (2.52) is a quantum analogue of (1.119) and (1.120). Notice that the degeneracies $\mathbf{n}$ replace the classical (x,k) coordinates, and we have assumed for simplicity that $\hat{h}$ does not depend explicitly on s. Similarly to (1.121), we require that $H_1^\sigma(\mathbf{n}) \neq 0$ for all values of $\mathbf{n}$ and σ [cf. (2.53)]. As in the classical case, σ is a possible discrete multiplicity of the solution, with $H^{\sigma'}(E,\mathbf{n}) \neq H^\sigma(E,\mathbf{n})$ $(\forall E,\mathbf{n})$ if $\sigma' \neq \sigma$. If $\hat{h} = \hat{C}$, then $h = E$ and there is only one multiplicity sector, which can be formally set to $\sigma = 1$. Furthermore, we define

$$\frac{1}{\mathcal{N}}\,|p_e,E,\sigma,\mathbf{n}\rangle := |p_e,h,\mathbf{n}\rangle_{h=-H^\sigma(E,\mathbf{n})}\ , \tag{2.54}$$

where $\mathcal{N} \equiv \mathcal{N}(E,\sigma,\mathbf{n})$ is a normalization that can be determined by requiring that the states $|\sigma,\mathbf{n}\rangle := |p_e = 0, E = 0, \sigma, \mathbf{n}\rangle$ be orthonormal in the induced inner product. Indeed, using the auxiliary inner product [cf. (2.10)], we find

$$\begin{aligned}\langle p_e',h',\mathbf{n}'|p_e,h,\mathbf{n}\rangle &= \delta(p_e'-p_e)\delta(h'-h)\delta(\mathbf{n}',\mathbf{n})\\ &= \delta(p_e'-p_e)\delta(E'-E)\frac{(p_e',E',\sigma',\mathbf{n}'|p_e,E,\sigma,\mathbf{n})}{\mathcal{N}^2}\ ,\end{aligned} \tag{2.55}$$

where

$$(p_e',E',\sigma',\mathbf{n}'|p_e,E,\sigma,\mathbf{n}) := \mathcal{N}^2\delta_{\sigma',\sigma}\delta(\mathbf{n}',\mathbf{n})\left|\frac{\partial C}{\partial h}\right|_{h=-H_\chi^\sigma(E,\mathbf{n})}\ . \tag{2.56}$$

Notice that $\delta(h'-h)$ vanishes if h' and h are evaluated in different multiplicity sectors [cf. the explanation following (2.52)] and, for this reason, we include the Kronecker delta $\delta_{\sigma',\sigma}$ in (2.56). If we now choose

$$\mathcal{N} = \left|\frac{\partial C}{\partial h}\right|^{-\frac{1}{2}}_{h=-H_\chi^\sigma(E,\mathbf{n})}\ , \tag{2.57}$$

then, in particular, the on-shell states $|\sigma,\mathbf{n}\rangle$ satisfy $(\sigma',\mathbf{n}'|\sigma,\mathbf{n}) = \delta_{\sigma',\sigma}\delta(\mathbf{n}',\mathbf{n})$. Moreover, in a similar way to (2.14) and (2.16), we define

$$\hat{P}^\sigma_{p_e,E} := \sum_{\mathbf{n}} |p_e,E,\sigma,\mathbf{n}\rangle\,\langle p_e,E,\sigma,\mathbf{n}|\ , \tag{2.58}$$

$$\hat{P}_E^\sigma := \sum_{\mathbf{n}} |E,\sigma,\mathbf{n}\rangle\langle E,\sigma,\mathbf{n}| = \int_{-\infty}^{\infty} \mathrm{d}p_e\ \hat{P}^\sigma_{p_e,E}\ , \tag{2.59}$$

$$\hat{P}_{p_e,E} := \sum_\sigma \hat{P}^\sigma_{p_e,E}\ , \tag{2.60}$$

which are seen to obey $\hat{P}^{\sigma'}_{p'_e,E'}\hat{P}^\sigma_{p_e,E} = \delta_{\sigma',\sigma}\delta(p'_e - p_e)\delta(E'-E)\hat{P}^\sigma_{p_e,E}$ as a consequence of (2.55) and (2.56). Subsequently, we can define the states [cf. (2.21)]

$$|e,t,\mathbf{n}\rangle := \int \frac{\mathrm{d}h}{\sqrt{2\pi\hbar}}\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}ht}\,|e,h,\mathbf{n}\rangle = \int \frac{\mathrm{d}h\mathrm{d}p_e}{2\pi\hbar}\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}ht}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}ep_e}\,|p_e,h,\mathbf{n}\rangle\ . \tag{2.61}$$

which satisfy properties similar to (2.22) and (2.23)

$$\langle\sigma,\mathbf{n}'|e,t,\mathbf{n}\rangle = \frac{\mathcal{N}}{2\pi\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}tH^\sigma(0,\mathbf{n})}\delta(\mathbf{n}',\mathbf{n})\ , \tag{2.62}$$

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda\hat{p}_e}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{h}}\,|e,t,\mathbf{n}\rangle = |e-\lambda,t-\tau,\mathbf{n}\rangle\ , \tag{2.63}$$

where we used (2.54). As before, we do not require that these states be complete or orthonormal in the auxiliary Hilbert space, but we note that $|e,t,\mathbf{n}\rangle = |e\rangle\otimes|t,\mathbf{n}\rangle$, and the label t can be seen as an analogue of the coordinate t that is conjugate to h in the classical theory [cf. (1.117)].

To define relational observables, we start with the Faddeev-Popov resolution of the identity [cf. (1.90)]. We take the quantum counterpart of (1.88) to be the on-shell operator [cf. (2.30)]

$$\left(\hat{\Omega}_t^\sigma\right)^{-2} := (2\pi\hbar)^2\hat{P}_0^\sigma\hat{P}_{e=1,t=s}\hat{P}_0^\sigma\ , \tag{2.64}$$

where $\hat{P}_0^\sigma = \hat{P}^\sigma_{p_e=0,E=0}$ and $\hat{P}_{e=1,t=s} = \sum_{\mathbf{n}}|e=1,t=s,\mathbf{n}\rangle\langle e=1,t=s,\mathbf{n}|$. Using (2.62), we then find

$$\left(\hat{\Omega}_t^\sigma\right)^{-2} := \sum_{\mathbf{n}}\mathcal{N}^2\,|\sigma,\mathbf{n}\rangle\langle\sigma,\mathbf{n}|\ . \tag{2.65}$$

It is straightforward to verify that the operators

$$\left(\hat{\Omega}_t^\sigma\right)^{\rho} := \sum_{\mathbf{n}}(\mathcal{N})^{-\rho}\,|\sigma,\mathbf{n}\rangle\langle\sigma,\mathbf{n}|\ , \tag{2.66}$$

satisfy the relations

$$\hat{P}_0^\sigma\bullet\left(\hat{\Omega}_t^\sigma\right)^{\rho} = \left(\hat{\Omega}_t^\sigma\right)^{\rho}\bullet\hat{P}_0^\sigma = \left(\hat{\Omega}_t^\sigma\right)^{\rho}\ , \tag{2.67}$$

$$\hat{\Omega}_t^\sigma \bullet \left(\hat{\Omega}_t^\sigma\right)^{-1} = \left(\hat{\Omega}_t^\sigma\right)^{-1} \bullet \hat{\Omega}_t^\sigma = \hat{P}_0^\sigma \ . \tag{2.68}$$

due to (2.56) and (2.57). In particular, we refer to (2.66) with $\rho = 2$ as the σ-sector (on-shell) Faddeev-Popov operator. Equations (2.64), (2.67) and (2.68) lead to

$$\hat{P}_0^\sigma = (2\pi\hbar)^2 \hat{\Omega}_t^\sigma \hat{P}_{e=1,t=s} \hat{\Omega}_t^\sigma \ , \tag{2.69}$$

which is the Faddeev-Popov resolution of the identity in the σ-sector of $\mathcal{H}_{\text{phys}}$. Notice that (2.69) is a counterpart of (1.90). If $\hat{h} = \hat{C}$, then $\mathcal{N} = 1$ [cf. (2.57)], $\sigma \equiv 1$, and $\hat{\Omega}_t^\sigma \equiv \hat{P}_0$, such that (2.69) coincides with (2.39).[16]

Let us now define the corresponding relational observables. As before, we consider an operator $\hat{f}$ that depends solely on the scalars $\hat{q}$ and $\hat{p}$. The corresponding on-shell observable is defined to be

$$\hat{\mathcal{O}}[f|\chi = s] := \frac{(2\pi\hbar)^2}{2} \sum_\sigma \hat{\Omega}_t^\sigma [\hat{f}, \hat{P}_{e=1,t=s}]_+ \hat{\Omega}_t^\sigma \ . \tag{2.70}$$

In particular, due to (2.60) and (2.69), we find

$$\hat{\mathcal{O}}[1|\chi = s] = \hat{P}_0 \ , \tag{2.71}$$

as it should be. Furthermore, if the spectrum of $\hat{C}$ is not only continuous but coincides with $\mathbb{R}$, we can define [cf. $|p_e, E, \sigma, \mathbf{n}\rangle = |p_e\rangle \otimes |E, \sigma, \mathbf{n}\rangle$]

$$\left(\hat{\Delta}_\chi^\sigma\right)^{\frac{1}{2}} := \sum_{\mathbf{n}} \int \mathrm{d}E \ \frac{1}{\mathcal{N}(E, \sigma, \mathbf{n})} |E, \sigma, \mathbf{n}\rangle \langle p_e, E, \sigma, \mathbf{n}| \ ,$$

[16] It is important to emphasize that the quantum Faddeev-Popov resolution of the identity given in (2.39) or (2.69) is a key feature of our formalism. In this way, we differ, for example, from the other method proposed by Marolf in [53], where invariant extensions were defined in a way that did not invariantly extend the identity operator to the identity in $\mathcal{H}_{\text{phys}}$, and thus the Faddeev-Popov resolution of the identity was not reproduced. In the case of the relativistic particle (to be analyzed in Chapter 3), the formalism of [53] leads to $\hat{\mathcal{O}}_{\text{inv}}[1|q^0 = cs] = \text{sgn}(\hat{p_0}) \neq \hat{1}$. It is our opinion that reproducing the Faddeev-Popov resolution of the identity in the quantum theory should be the correct procedure. It is also worthwhile to note that (2.69) heuristically corresponds to “inserting a gauge condition operator” into the (auxiliary) inner product. This is a procedure that was suggested in [33, 76].

as well as the invariant observable [cf. (2.27)]

$$\hat{\mathcal{O}}_{\rm inv}[f|\chi = s] \\ := \frac{(2\pi\hbar)^2}{2} \sum_\sigma \int \mathrm{d}p_e \mathrm{d}E \; \hat{P}_{p_e,E} \left(\hat{\Delta}^\sigma_\chi\right)^{\frac{1}{2}} [\hat{f}, \hat{P}_{e=1,t=s}]_+ \left(\hat{\Delta}^\sigma_\chi\right)^{\frac{1}{2}} \hat{P}_{p_e,E} \; , \tag{2.72}$$

such that $\hat{\Omega}^\sigma_t = \hat{P}^\sigma_0 \left(\hat{\Delta}^\sigma_\chi\right)^{1/2}$ and $\hat{\mathcal{O}}[f|\chi = s] = \hat{P}_0 \hat{\mathcal{O}}_{\rm inv}[f|\chi = s]$ [cf. (2.28)]. As $\hat{f}$ depends only on the scalars, we can develop (2.72) in a similar way as (2.33) and (2.36) to find

$$\hat{\mathcal{O}}_{\rm inv}[f|\chi = s] = \int_{-\infty}^{\infty} \mathrm{d}\tau \; \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \; \hat{\omega}[f|\chi = s] \; \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}} \; , \tag{2.73}$$

$$\hat{\omega}[f|\chi = s] := \frac{1}{2} \sum_\sigma \left(\hat{\Delta}^\sigma_\chi\right)^{\frac{1}{2}} [\hat{f}, \hat{P}_{t=s}]_+ \left(\hat{\Delta}^\sigma_\chi\right)^{\frac{1}{2}} \; . \tag{2.74}$$

Equation (2.73) is a quantum version of (1.89) in the particular case in which $\tau_0 \to -\infty$, $\tau_1 \to \infty$, and the generalized clock $\chi(\tau)$ is conjugate to the invariant h. The initial value of $\chi(\tau)$ is t [cf. (1.124)], and we note that $\hat{P}_{t=s}$ is analogous to the gauge-fixing Dirac delta in (1.89), whereas $\left(\hat{\Delta}^\sigma_\chi\right)^{\frac{1}{2}}$ corresponds to the square root of the classical Δ_χ given in (1.88). Inspired by this particular case, we consider that (2.70) is the quantum version of the relational observable (1.89) in this particular χ-gauge, regardless of whether the states $|e, t, \mathbf{n}\rangle$ form a basis in the auxiliary Hilbert space or the spectrum of $\hat{C}$ coincides with $\mathbb{R}$. However, the derivation of (2.70) required the assumption that E is a continuous label. If this is not the case, one can, in principle, still fix the proper-time gauge as in §2.5.1. It may also be possible to derive a similar construction as the one presented here for more general gauges in the case of a discrete spectrum of $\hat{C}$, but we do not pursue this, as most examples we will consider feature a continuous spectrum (see, however, §2.7.2).

What can we say about the evolution of (2.70)? First, let us define the invariant operator [cf. (2.52)]

$$\hat{H}_0 := \sum_\sigma \sum_{\mathbf{n}} \int \mathrm{d}p_e \mathrm{d}E \; H^\sigma_0(\mathbf{n}) \, |p_e, E, \sigma, \mathbf{n}\rangle \langle p_e, E, \sigma, \mathbf{n}| \; , \tag{2.75}$$

such that [cf. (2.52) and (2.54)]

$$\begin{aligned} \left(\hat{h} + \hat{H}_0\right) |p_e, E, \sigma, \mathbf{n}\rangle &= E \left[-H^\sigma_1(\mathbf{n}) + \mathcal{O}(E)\right] |p_e, E, \sigma, \mathbf{n}\rangle \\ &= \hat{\omega}\hat{C} \, |p_e, E, \sigma, \mathbf{n}\rangle \; , \end{aligned} \tag{2.76}$$

where we also defined the invariant

$$\hat{\omega} := \sum_{\sigma}\sum_{\mathbf{n}}\int \mathrm{d}p_e \mathrm{d}E \; [-H_1^{\sigma}(\mathbf{n}) + \mathcal{O}(E)] \left|p_e, E, \sigma, \mathbf{n}\right\rangle \left\langle p_e, E, \sigma, \mathbf{n}\right| \; . \tag{2.77}$$

The interpretation of $\hat{H}_0$ and $\hat{\omega}$ will be discussed below. Notice that (2.75) and (2.77) imply that $\hat{H}_0$ and $\hat{\omega}\hat{C}$ commute. Moreover, due to (2.66), we obtain

$$\hat{\Omega}_t^{\sigma} = \hat{\Omega}_t^{\sigma} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{\omega}\hat{C}} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{\omega}\hat{C}} \hat{\Omega}_t^{\sigma} \tag{2.78}$$

for any c-number τ. Now, similarly to (2.41), we can use (2.63), (2.76) and (2.78) to write

$$\begin{aligned}
\hat{\mathcal{O}}[f|\chi = s] &= \frac{(2\pi\hbar)^2}{2} \sum_{\sigma} \hat{\Omega}_t^{\sigma} \hat{f} \hat{P}_{e=1,t=s} \hat{\Omega}_t^{\sigma} + \text{h.c.} \\
&= \frac{(2\pi\hbar)^2}{2} \sum_{\sigma} \hat{\Omega}_t^{\sigma} \hat{f} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{P}_{e=1,t=t_0} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{\Omega}_t^{\sigma} + \text{h.c.} \\
&= \frac{(2\pi\hbar)^2}{2} \sum_{\sigma} \hat{\Omega}_t^{\sigma} \hat{f}(s) \hat{\tilde{P}}_{e=1,t=t_0} \hat{\Omega}_t^{\sigma} + \text{h.c.} \; ,
\end{aligned} \tag{2.79}$$

where we defined

$$\hat{f}(s) := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{\omega}\hat{C}} \hat{f} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{\omega}\hat{C}} \; , \tag{2.80}$$

$$\hat{\tilde{P}}_{e=1,t=t_0} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{H}_0} \hat{P}_{t=t_0} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{H}_0} \; . \tag{2.81}$$

Notice that, since $\hat{H}_0$ only depends on the $\mathbf{n}$ labels [cf. (2.75)], Eq. (2.81) simply corresponds to a unitarity transformation (change of basis) associated with these labels. If we now differentiate (2.79) with respect to s, we find

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\hat{\mathcal{O}}[f|\chi = s] &= \frac{(2\pi\hbar)^2}{2} \sum_{\sigma} \hat{\Omega}_t^{\sigma} \left[\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\hat{f}(s-t_0) \, , \, \hat{\tilde{P}}_{e=1,t=t_0}\right]_+ \hat{\Omega}_t^{\sigma} \\
&= \frac{(2\pi\hbar)^2}{2} \sum_{\sigma} \hat{\Omega}_t^{\sigma} \left[\mathrm{i}\hbar \left.\frac{\partial \hat{f}}{\partial s}\right|_{s-t_0} + [\hat{f}, \hat{\omega}\hat{C}]|_{s-t_0} \, , \, \hat{\tilde{P}}_{e=1,t=t_0}\right]_+ \hat{\Omega}_t^{\sigma} \\
&= \hat{\mathcal{O}}\left[\mathrm{i}\hbar\frac{\partial f}{\partial s} + [\hat{f}, \hat{\omega}\hat{C}] \middle| \chi = s\right] \; ,
\end{aligned} \tag{2.82}$$

which is the quantum version of (1.95) in the χ-gauge. In this way, we conclude that $\hat{\omega}$ is the quantum analogue of the (invariant extension of the) gauge-fixed einbein, which was denoted by $\omega(\phi(s))$ in (1.94).[17] In particular, if $\hat{h} = \hat{C}$, then χ coincides with a canonical representation of proper time. In this case, Eqs. (2.52) and (2.77) imply that $\hat{\omega} = \hat{1}$, as it should be, such that (2.82) coincides with (2.42).

Subsequently, let us note that, if $\hat{H}_0 = \hat{0}$ (which is the case if, for example, $\hat{h} = \hat{C}$), then the physical propagator has to be defined from the spectral decomposition of the relational observables, as was done for the case of the proper-time gauge in §2.5.1. However, if $\hat{H}_0 \neq \hat{0}$, then we can explicitly derive a physical Heisenberg equation that is the quantum analogue of (1.103). To do so, we note that, in the classical case, Eq. (1.103) was derived from (1.101), which implies the physical Hamiltonian generates the evolution of the relative initial data. These data are invariant extensions of objects that Poisson-commute with the generalized clock χ and its conjugate momentum. In the quantum case, we therefore consider the case in which $\hat{f}$ commutes with $\hat{h}$, such that, instead of (2.79), we write

$$\begin{aligned} \hat{\mathcal{O}}[f|\chi = s] &= \frac{(2\pi\hbar)^2}{2} \sum_\sigma \hat{\Omega}_t^\sigma \hat{f} \hat{P}_{e=1,t=s} \hat{\Omega}_t^\sigma + \text{h.c.} \\ &= \frac{(2\pi\hbar)^2}{2} \sum_\sigma \hat{\Omega}_t^\sigma \hat{f} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{P}_{e=1,t=t_0} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{\Omega}_t^\sigma + \text{h.c.} \\ &= \frac{(2\pi\hbar)^2}{2} \sum_\sigma \hat{\Omega}_t^\sigma \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{f} \hat{P}_{e=1,t=t_0} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{h}} \hat{\Omega}_t^\sigma + \text{h.c.}\ . \end{aligned} \tag{2.83}$$

To cast this equation in a more useful form, we use the fact that (2.52), (2.51), and (2.75) imply $\hat{h}\,|\sigma, \mathbf{n}\rangle = -\hat{H}_0\,|\sigma, \mathbf{n}\rangle = -H_0^\sigma(\mathbf{n})\,|\sigma, \mathbf{n}\rangle$, which leads to

$$\left[\left(\hat{\Omega}_t^\sigma \right)^\rho, \hat{H}_0 \right] = 0\ , \tag{2.84}$$

due to (2.66). Thus, Eq. (2.83) becomes

$$\hat{\mathcal{O}}[f|\chi = s] = \frac{(2\pi\hbar)^2}{2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{H}_0} \sum_\sigma \hat{\Omega}_t^\sigma \hat{f} \hat{P}_{e=1,t=t_0} \hat{\Omega}_t^\sigma \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(s-t_0)\hat{H}_0} + \text{h.c.}\ . \tag{2.85}$$

Therefore, $\hat{H}_0$ can be interpreted as the quantum physical Hamiltonian that generates the evolution of the quantum relational observables with respect to s. In direct analogy to the derivation of (1.103), we find the "gauge-fixed" Heisenberg equation

$$\frac{\mathrm{d}}{\mathrm{d}s} \hat{\mathcal{O}}[f|\chi = s] = \frac{\partial}{\partial s} \hat{\mathcal{O}}\left[f|\,\chi = s \right] + \frac{1}{\mathrm{i}\hbar} [\hat{\mathcal{O}}[f|\chi = s], \hat{H}_0]\ , \tag{2.86}$$

[17] Notice that the evolution determined by the classical gauge-fixed Hamiltonian (1.65) is given by $\{f, H_T^{\mathrm{gf}}\} = \{f, \omega C\}$ if f only depends on the scalars.

from (2.85).[18] Incidentally, notice that (2.86) and (2.82) are equivalent. We thus conclude that, in the case in which $\hat{H}_0 \neq \hat{0}$, the physical propagator (for implicit time evolution) is simply (the kernel function of) $\exp(-\mathrm{i}(s-t_0)\hat{H}_0/\hbar)$. Due to (2.75), we see that $\hat{H}_0$ is by definition symmetric with respect to the auxiliary inner product and, because it is invariant, it is symmetric with respect to $(\cdot|\cdot)$. If we further assume that it is self-adjoint, then the evolution is manifestly unitary.

2.5.3 A useful particular case

At this stage, it is useful to consider a particular case that will be of interest in subsequent Chapters. Let us assume for a moment that the states $|e,t,\mathbf{n}\rangle$ form a complete orthonormal system in the auxiliary Hilbert space, such that the operator

$$\hat{\chi} := \sum_{\mathbf{n}} \int \mathrm{d}e\mathrm{d}t \; t \, |e,t,\mathbf{n}\rangle \langle e,t,n| \tag{2.87}$$

is self-adjoint with respect to $\langle\cdot|\cdot\rangle$ and can be interpreted as a noninvariant operator for the generalized clock. Furthermore, let us consider an $\hat{f}$ that commutes with $\hat{\chi}$ and that the states $|e,t,\mathbf{n}\rangle$ are the simultaneous eigenbasis of $\hat{f}$ and $\hat{\chi}$ (if they are not, then one can simply redefine them) such that

$$\hat{f} := \sum_{\mathbf{n}} \int \mathrm{d}e\mathrm{d}t \; f(t,\mathbf{n}) \, |e,t,\mathbf{n}\rangle \langle e,t,\mathbf{n}| \; . \tag{2.88}$$

In this particular case, Eq. (2.88) leads to the decomposition

$$\hat{\mathcal{O}}[f|\chi = s] = \sum_{\sigma,\mathbf{n}} f(s,\mathbf{n}) \;\; |\sigma,\mathbf{n};s\rangle \langle \sigma,\mathbf{n};s| \; , \tag{2.89}$$

where

$$|\sigma,\mathbf{n};s\rangle := 2\pi\hbar \, \hat{\Omega}_t^{\sigma} \, |e=1,t=s,\mathbf{n}\rangle \; . \tag{2.90}$$

From (2.62) and (2.66), we find that the states $|\sigma,\mathbf{n};s\rangle$ defined above are orthogonal with respect to the induced inner product for every possible value of s,

$$(\sigma',\mathbf{n}';s|\sigma,\mathbf{n};s) = \delta_{\sigma',\sigma}\delta(\mathbf{n}',\mathbf{n}) \; . \tag{2.91}$$

[18] Recall that we have made the simplifying assumption that $\hat{h}$ does not depend on s.

Moreover, the Faddeev-Popov resolution of the identity (2.69) implies that they are complete. Thus, $|\sigma, \mathbf{n}; s\rangle$ are the eigenstates of the relational observable (2.89), which is self-adjoint with respect to $(\cdot|\cdot)$. In this case, we can define the physical propagator as $(\sigma', \mathbf{n}'; s'|\sigma, \mathbf{n}; s)$.

Since the states (2.90) form a complete system, any on-shell state can be written as

$$|\Psi\rangle = \sum_{\sigma}\sum_{\mathbf{n}} \Psi_\sigma(\mathbf{n})\, |\sigma, \mathbf{n}; s_0\rangle \tag{2.92}$$

for a fixed value of $s = s_0$. If we consider the (Schrödinger-picture evolved) state

$$|\Psi; s\rangle = \sum_{\sigma}\sum_{\mathbf{n}} \Psi_\sigma(\mathbf{n}; s)\, |\sigma, \mathbf{n}; s_0\rangle \ , \tag{2.93}$$

where

$$\Psi_\sigma(\mathbf{n}; s) := \sum_{\sigma_0}\sum_{\mathbf{n}_0} (\sigma, \mathbf{n}; s|\sigma_0, \mathbf{n}_0; s_0)\, \Psi_{\sigma_0}(\mathbf{n}_0) \ , \tag{2.94}$$

we find that the completeness and orthogonality of (2.90) for all values of s implies

$$\begin{aligned}
(\Psi; s|\Psi; s) &= \sum_{\sigma}\sum_{\mathbf{n}} |\Psi_\sigma(\mathbf{n}; s)|^2 \\
&= \sum_{\sigma_0,\sigma_0',\sigma}\ \sum_{\mathbf{n}_0,\mathbf{n}_0',\mathbf{n}} \Psi^*_{\sigma_0'}(\mathbf{n}_0')\left(\sigma_0', \mathbf{n}_0'; s_0|\sigma, \mathbf{n}; s\right)(\sigma, \mathbf{n}; s|\sigma_0, \mathbf{n}_0; s_0)\, \Psi_{\sigma_0}(\mathbf{n}_0) \\
&= \sum_{\sigma_0,\sigma_0'}\ \sum_{\mathbf{n}_0,\mathbf{n}_0'} \Psi^*_{\sigma_0'}(\mathbf{n}_0')\left(\sigma_0', \mathbf{n}_0'; s_0|\sigma_0, \mathbf{n}_0; s_0\right) \Psi_{\sigma_0}(\mathbf{n}_0) \\
&= \sum_{\sigma_0}\sum_{\mathbf{n}_0} |\Psi_{\sigma_0}(\mathbf{n}_0)|^2 = (\Psi|\Psi) \ ,
\end{aligned}$$

similarly to (2.48). Thus, the norm of $|\Psi\rangle$ is conserved in the evolution determined by the physical propagator $(\sigma', \mathbf{n}'; s'|\sigma, \mathbf{n}; s)$.

2.5.4 An alternative factor ordering

It is worthwhile to mention that, instead of (2.70), one may choose to adopt an alternative factor ordering that has the appealing property that the invariant extension of an invariant is itself. More precisely, notice that, instead of (2.69), one could write the quantum Faddeev-Popov resolution of the identity as

$$\begin{aligned}
\hat{P}_0^\sigma &= 2\pi\hbar \left(\hat{\Omega}_t^\sigma\right)^2 \hat{P}_{t=s}\hat{P}_{E=0}^\sigma \\
&= 2\pi\hbar \hat{P}_{E=0}^\sigma \hat{P}_{t=s}\left(\hat{\Omega}_t^\sigma\right)^2 \ ,
\end{aligned} \tag{2.95}$$

such that the quantum observables would be alternatively defined as

$$\hat{\mathcal{O}}_{(II)}[f|\chi = s] := \pi\hbar \sum_{\sigma} \left(\hat{\Omega}_t^{\sigma}\right)^2 \hat{P}_{t=s}\hat{f}\hat{P}^{\sigma}_{E=0} + \text{h.c.} \ . \tag{2.96}$$

Then, given an invariant operator of the form

$$\hat{f} := \sum_{\sigma}\sum_{\mathbf{n}',\mathbf{n}} \int \mathrm{d}p_e \mathrm{d}E \ f^{\sigma}(p_e, E, \mathbf{n}', \mathbf{n}) \left|p_e, E, \sigma, \mathbf{n}'\right\rangle \left\langle p_e, E, \sigma, \mathbf{n}\right| \ , \tag{2.97}$$

where we assume the integrals can be performed, we find $\hat{\mathcal{O}}_{(II)}[f|\chi = s] = \hat{P}_0\hat{f}$. This is, in fact, the result obtained for the proper-time gauge [cf. (2.40)], but for more general gauges the factor orderings (2.70) and (2.96) will generally differ. Nonetheless, we will not consider (2.96) in what follows because it is not straightforwardly related to conditional probabilities, whereas we will see that (2.70) is (cf. §2.7). Since we consider conditional probabilities to be an appealing and intuitively clear approach to the quantum dynamics, we will thus favor (2.70).

2.5.5 A strategy

In analogy to the strategy suggested at the end of §1.10, we propose that (integrable) models with quantum diffeomorphism invariance [in the sense of (2.4)] can be treated as follows: first, one solves the eigenvalue problem for the constraint operators and determines the spectrum. Second, the dynamical solutions can be found in the proper-time gauge following §2.5.1. Third, If the spectrum of $\hat{C}$ is continuous, one can use the method of §2.5.2 to find the dynamical solutions in more general gauges (i.e., with respect to more general generalized clocks). To do so, it may be useful to choose $\hat{h}$ to be the invariant extension of an operator with respect to the previously computed proper-time gauge. This corresponds to choosing a new generalized clock which is conjugate to $\hat{h}$. This may seem to be a restrictive choice of clock because only clocks that are conjugate to invariant operators are obtained in this way. However, as every physically meaningful solution can be expressed in terms of the relational observables (invariant extensions), this is, in fact, a sufficiently general procedure. We consider that a quantum choice of gauge is admissible if it is defined from an $\hat{h}$ operator as in (2.52) and, in particular, it must obey (2.53), which is the quantum counterpart to the classical condition (1.77). Moreover, the solution (2.52) should be valid for all possible values of $\mathbf{n}$, without introducing restrictions on the span of these labels.

Notice that, once the solutions are found in the proper-time gauge, choosing a (new) $\hat{h}$ among the observables in this solution (and, therefore, a new clock) is the analogous procedure of a diffeomorphism of a certain solution $\mathcal{S}_0(\tau)$ in the classical theory, which corresponds to a change in the origin of the gauge orbit (cf. §1.6). We take this analogy seriously, and we further discuss the physical interpretation of the quantum dynamical solutions (relational observables) and the interrelation between different gauges in §2.6.

2.5.6 A perturbative procedure

There may be situations in which it is difficult or even impossible to determine the eigenstates of the constraint $\hat{C}$ exactly. In Chapters 5 and 6, we will examine the case in which the on-shell states can be defined in perturbation theory. Although it is, in principle, still possible to define the induced inner product as in (2.10) or (2.20), and the observables as in (2.38) or (2.70), these constructions often became complicated in the perturbative case. For this reason, it is worthwhile to consider similar constructions, which, as we will see in Chapters 5 and 6, can be defined in perturbation theory via an iterative procedure. In analogy to the classical Faddeev-Popov resolution of the identity (1.90) and to our previous quantum definition (2.64), we suggest that the perturbative inner product for a pair of perturbatively defined on-shell wave functions $\Psi_{(1,2)}(q)$ be of the form

$$\left(\Psi_{(1)}\middle|\Psi_{(2)}\right) := \sum_\sigma \int \mathrm{d}q \, \left(\hat{\mu}_\sigma^{\frac{1}{2}}\Psi_{(1)}\right)^* |J|\delta(\chi(q)-s)\hat{\mu}_\sigma^{\frac{1}{2}}\Psi_{(2)} \,, \tag{2.98}$$

where $\mathrm{d}q \equiv \prod_i \mathrm{d}q^i$, $\chi(q)$ is a configuration space function that serves as a choice of generalized clock,[19] and J is the Jacobian determinant $\frac{\partial(\chi,F)}{\partial q}$ for the invertible configuration-space coordinate transformation $q \mapsto (\chi, F)$. The label σ is a possible discrete multiplicity, in analogy to (2.64), whereas $\hat{\mu}_\sigma$ is a 'measure' [analogous to (2.66)] that should be determined in perturbation theory and should: (1) ensure that (2.98) is positive-definite; (2) ensure that (2.98) is conserved relative to changes in s, such that the dynamics is unitary.

In Chapter 5, it will be proven that a perturbative measure that satisfies the two criteria above can be defined and, furthermore, that it corresponds to a quantization of the classical Faddeev-Popov determinant associated with the choice of $\chi(q)$ as a generalized clock [cf. (5.68)], such that it is indeed analogous to the $\hat{\Omega}_t^\sigma$ operator defined in (2.66). It is important to note that similar definitions to (2.98) have been considered in [33, 51, 76, 77]. In [51], the unitarity of the perturbative theory and its connection to path integrals were examined in an expansion in powers of $\hbar$ (up to the "one-loop" order $\hbar^1$). In Chapters 5 and 6, we will not develop perturbation theory relative to $\hbar$, but rather relative to a heavy mass scale (e.g., the Planck mass). Moreover, the previous proposals did not discuss the definition of relational observables.[20] Here, we propose that, in analogy to (2.70), the quantum observables be defined via their matrix

[19] Although it is possible to choose more general (phase-space) functions as generalized clocks, the choice of $\chi(q)$ will be sufficient in the perturbation theory developed in Chapters 5 and 6.

[20] See, however, [78] for a related discussion.

elements as

$$\left(\Psi_{(1)}\middle|\hat{\mathcal{O}}[f|\chi=s]\middle|\Psi_{(2)}\right) := \sum_{\sigma}\int \mathrm{d}q\,\left(\hat{\mu}_{\sigma}^{\frac{1}{2}}\Psi_{(1)}\right)^{*}\hat{f}|J|\delta(\chi(\alpha,\phi)-t)\hat{\mu}_{\sigma}^{\frac{1}{2}}\Psi_{(2)}\;. \quad (2.99)$$

This definition will be useful in the perturbative formalism of Chapters 5 and 6.

2.6 A tentative set of postulates

Given the preceding formalism for the construction of the physical Hilbert space, the quantum relational observables and their dynamics, we now require a physical interpretation. As was mentioned in §2.5.5, we take the analogy to classical theory (and, in particular, the HJ formalism) seriously, which leads us to the conclusions: (1) the quantum dynamics should be understood in relational terms; (2) observers may choose generalized clocks which define generalized reference frames, with respect to which they record the dynamics of the quantum fields. From these determinations, we suggest a set of tentative postulates below.

2.6.1 Proper-time quantum mechanics

First, the results of §2.5.1 [in particular (2.42)] show that one can, in principle, define the quantum dynamics relative to the proper-time gauge. Even if no other choices of generalized clock are available in the quantum theory (e.g., due to the properties of the spectrum of $\hat{C}$), the possibility of analyzing the proper-time dynamics suggests the following set of postulates:

1. The quantum state of a diffeomorphism-invariant quantum system corresponds to a ray in the physical Hilbert space $\mathcal{H}_{\mathrm{phys}}$.
2. Observables are self-adjoint on-shell operators.
3. Observers who employ the proper-time clock (or, more precisely, a clock that keeps track of proper time) record the dynamics of worldline tensor fields according to the relational Heisenberg-picture operators [cf. (2.38)].
4. If the system is in the state $|\Psi\rangle$, a measurement of $\hat{f}$ relative to the proper-time clock results in an eigenvalue f of $\hat{\mathcal{O}}[f|\chi=s]$ with probability

$$p_{\Psi}(f) = \frac{|(f,\mathbf{n};s|\Psi)|^2}{(\Psi|\Psi)}\;, \quad (2.100)$$

   where $|f,\mathbf{n};s\rangle$ are the eigenstates of $\hat{\mathcal{O}}[f|\chi=s]$ [cf. (2.44)].
5. After the measurement, the state of the system is updated to $|f,\mathbf{n};s\rangle$.

The reader will readily notice that these postulates simply correspond to a kind of "proper-time Copenhagen interpretation", which clearly is to be taken with a certain degree of skepticism, as, most notably, the measurement problem is not solved. Nonetheless, the above set of postulates are admissible in the sense that they can reproduce the usual results of quantum mechanics if its "preferred" time parameter is identified with proper time (see, for instance, §2.7.2).

2.6.2 Quantum diffeomorphisms and changes of quantum reference frames

If more general clocks can be chosen (for example, by following the formalism of §2.5.2), we can modify the postulates of §2.6.1 as follows. Whereas postulates 1 and 2 are unaltered, we now suggest:

3. Observers who employ a certain generalized clock record the dynamics of worldline tensor fields according to the relational Heisenberg-picture operators [cf. (2.70)]. This defines the quantum generalized reference frame associated to the observer's choice of clock.

4. If the system is in the state $|\Psi\rangle$, a measurement of $\hat{f}$ relative to the generalized clock results in an eigenvalue $f(s, \mathbf{n})$ of $\hat{\mathcal{O}}[f|\chi = s]$ with probability

$$p_\Psi(f) = \sum_\sigma \frac{|(\sigma, \mathbf{n}; s|\Psi)|^2}{(\Psi|\Psi)} \, , \tag{2.101}$$

   where $|\sigma, \mathbf{n}; s\rangle$ are the eigenstates of $\hat{\mathcal{O}}[f|\chi = s]$ [although we use the notation of (2.89), we do not necessarily require that the particular case considered in §2.5.3 be realized].

5. After the measurement, the state of the system is updated to $|\sigma, \mathbf{n}; s\rangle$ in the generalized reference frame of the observer.

Evidently, these postulates are speculative. However, they are a straightforward extension of the usual formalism of quantum mechanics. In particular, the update (or 'collapse') postulate (the fifth postulate) refers to a specific generalized reference frame. This raises the question of what the state is perceived to be from the standpoint of other observers, who might employ different clocks and, therefore, refer their measurements to different reference frames. First, let us clarify that the update postulate is taken in the sense of a preparation of the state of the system. Once the system is prepared in a certain state, different observers in various reference frames might perform different measurements and, thus, lead to new preparations. Second, since we assume that the observables are self-adjoint, their eigenstates $|\sigma, \mathbf{n}; s\rangle$ form a complete orthonormal system with respect to which the components of any on-shell state may be computed. For this reason, we suggest that the induced overlap $(\sigma, \mathbf{n}; s|\Psi)$ should be regarded as the representation of $|\Psi\rangle$ in the quantum generalized reference frame associated with the χ-gauge. This leads to the conclusion that a transformation between quantum reference frames is simply a change of basis in $\mathcal{H}_{\text{phys}}$. Indeed, let us consider two admissible gauges, $\hat{\chi}_1$ and $\hat{\chi}_2$, such that the eigenstates of the corresponding relational observables are $|\sigma_1, \mathbf{n}_1; \chi_1\rangle$, $|\sigma_2, \mathbf{n}_2; \chi_2\rangle$. A state in the reference frame defined by $\hat{\chi}_1$ is expressed in the frame of $\hat{\chi}_2$ through the equation[21]

$$(\sigma_1, \mathbf{n}_1; \chi_1|\Psi) = \sum_{\sigma_2} \sum_{\mathbf{n}_2} (\sigma_1, \mathbf{n}_1; \chi_1|\sigma_2, \mathbf{n}_2; \chi_2)(\sigma_2, \mathbf{n}_2; \chi_2|\Psi) \ .$$

It is important to mention that the study of different notions of quantum reference frames and "relational quantum clocks" has been a topic of active research [73–75, 79–83]. Noteworthy is the approach of [75, 79–81], which establishes a framework in which different choices of reference frames can also be related, and in which the direct quantization of gauge-fixed field equations in different gauges leads to different Hilbert spaces that can be mapped to one another. Indeed, the main goal of [80] was to connect the physical Hilbert space constructed from the Dirac quantization procedure [cf. (2.4)] to the various Hilbert spaces that can be obtained if one quantizes the gauge-fixed field equations [without explicitly invariantly extending quantities through (1.89), for example]. The construction of these Hilbert spaces may be involved. They were related to one another in [80] by isometries called "trivialization maps".[22] The position taken in [80] was that one can only fully grasp the relationalism of the quantum theory if both the Dirac quantization and the various gauge-fixed Hilbert spaces are studied simultaneously and connected via isometries. It is interesting to note that, in a related early investigation [51], Barvinsky showed that the path integrals related to the physical Hilbert space of the Dirac quantization program can be related to the path integrals associated with the various gauge-fixed Hilbert spaces. He also analyzed the canonical (operator-based) quantum theory semiclassically (at "one-loop" order $\hbar^1$). Both [51] and [80] (and the related subsequent articles) can be seen as possible formalisms that relate different quantum reference frames.

We take a different position in comparison to [80]. In the framework described here, the Dirac quantization program and its associated physical Hilbert space are sufficient, and encode all the relational aspects of the quantum theory. There is no need to consider the various gauge-fixed Hilbert spaces in order to ascertain the different relational aspects of the theory. Notice that this is just as in the classical case: the

[21] Notice that the physical propagator $(\sigma, \mathbf{n}; s|\sigma_0, \mathbf{n}_0; s_0)$ is a particular case of the matrix $(\sigma_1, \mathbf{n}_1; \chi_1|\sigma_2, \mathbf{n}_2; \chi_2)$, but one changes the value of clock instead of switching clocks.

[22] These maps are akin to constructions that had been considered earlier in various contexts, such as those of non-Abelian gauge fields in [84] or quantum canonical transformations in [85].

relational observables can be seen as functions on the (single) reduced or physical phase space of the theory (cf. §1.9.2), just as the quantum relational observables are operators that act on the (single) physical Hilbert space. The different formalisms of [51,74,75,83] also signal, nevertheless, that it is possible to accommodate various choices of reference frames in a single Hilbert space (which was referred to as the "Dirac-Wheeler-DeWitt formulation" and the "perspective-neutral" or "reference-system-neutral" framework in [51] and [80], respectively). Our formalism provides a concrete realization of this idea, and it is based solely on standard concepts and techniques used in canonical gauge systems (cf. Appendix A).

In what follows, we assume that the particular case analyzed in §2.5.3 holds; i.e., one can define a self-adjoint $\hat{\chi}$ operator. In this case, we will show how the relational observables (2.70) can be related to conditional probabilities and, in particular, to the Page-Wootters formalism, which is one of the most popular approaches to the quantum mechanics of systems without an external (or preferred) time parameter. We also comment on the relation of our framework to other formalisms of the literature.

2.7 Conditional probabilities

Assuming the particular case of §2.5.3, let us take another point of view on the quantum relational dynamics. Instead of working with the invariant observables and the physical Hilbert space, let us define

$$p_\Psi(\mathbf{n}|\chi = s) = \frac{|\langle \chi = s, \mathbf{n}|\Psi\rangle|^2}{\sum_{\mathbf{n}} |\langle \chi = s, \mathbf{n}|\Psi\rangle|^2} \ , \tag{2.102}$$

to be the conditional probability of observing a value of $\mathbf{n}$ given that $\hat{\chi}$ is observed to be equal to s. In (2.102), we denote $|\chi = s, \mathbf{n}\rangle \equiv |e = 1, t = s, \mathbf{n}\rangle$. The idea is that the relational theory can be expressed in terms of conditional statements. This is reasonable because the classical relational observable $\mathcal{O}[f|\chi = s]$ can be regarded as a conditional quantity, as they encode the value of f based on the condition that $\chi = s$. From (2.102), the conditional expectation value of $\hat{f}$ is defined to be

$$\begin{aligned} \mathrm{E}_\Psi[f|\chi = s] &:= \sum_{\mathbf{n}} f(s, \mathbf{n}) \ p_\Psi(\mathbf{n}|\chi = s) \\ &= \frac{\left\langle \Psi \middle| \hat{f}\hat{P}_{\chi=s} \middle| \Psi \right\rangle}{\left\langle \Psi \middle| \hat{P}_{\chi=s} \middle| \Psi \right\rangle} \ , \end{aligned} \tag{2.103}$$

where we used (2.88) and $\hat{P}_{\chi=s} \equiv \hat{P}_{e=1,t=s}$. To make contact with the formalism based on the physical Hilbert space, we note that (2.103) can be rewritten in terms of the induced inner product as [cf. (2.17)]

$$\mathrm{E}_\Psi[f|\chi = s] = \frac{\left(\Psi \left| \hat{P}_{E=0} \hat{f} \hat{P}_{\chi=s} \hat{P}_{E=0} \right| \Psi\right)}{\left(\Psi \left| \hat{P}_{E=0} \hat{P}_{\chi=s} \hat{P}_{E=0} \right| \Psi\right)} \ . \tag{2.104}$$

Furthermore, due to (2.33), we also obtain

$$\mathrm{E}_\Psi[f|\chi = s] = \frac{\left(\Psi \left| \int_{-\infty}^{\infty} \mathrm{d}\tau \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \hat{f} \hat{P}_{\chi=s} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \right| \Psi\right)}{\left(\Psi \left| \int_{-\infty}^{\infty} \mathrm{d}\tau \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \hat{P}_{\chi=s} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau \hat{C}} \right| \Psi\right)} \ ,$$

which resembles the classical formula (1.89). Can we relate the quantum relational observables (2.70) to conditional quantities? The answer is yes. First, let the quantum average of an on-shell observable be

$$\left\langle \hat{\mathcal{O}} \right\rangle_\Psi := \frac{\left(\Psi \left| \hat{\mathcal{O}} \right| \Psi\right)}{(\Psi|\Psi)} \ , \tag{2.105}$$

where $|\Psi\rangle$ is the state of the system. Second, notice that the projectors (2.58) can also be written as [cf. (2.90)]

$$\hat{P}_0^\sigma := \sum_{\mathbf{n}} |\sigma, \mathbf{n}; s\rangle \langle \sigma, \mathbf{n}; s| \ . \tag{2.106}$$

In this way, the probability that the system is in the σ sector is

$$p_\Psi(\sigma) = \left\langle \hat{P}_{E=0}^\sigma \right\rangle_\Psi \ . \tag{2.107}$$

Now, using (2.70), we obtain

$$\left\langle \hat{\mathcal{O}}[f|\chi = s] \right\rangle_\Psi = \sum_\sigma p_\Psi(\sigma) \frac{\left(\Psi \left| \hat{\Omega}_t^\sigma \hat{f} \hat{P}_{\chi=s} \hat{\Omega}_t^\sigma \right| \Psi\right)}{\left(\Psi \left| \hat{\Omega}_t^\sigma \hat{P}_{\chi=s} \hat{\Omega}_t^\sigma \right| \Psi\right)} \ ,$$

and if we define

$$|\Psi_\sigma\rangle := \hat{\Omega}_t^\sigma \bullet |\Psi\rangle \ , \tag{2.108}$$

then we finally find

$$\left\langle \hat{\mathcal{O}}[f|\chi = s] \right\rangle_{\Psi} = \sum_{\sigma} p_{\Psi}(\sigma) \frac{\left(\Psi_{\sigma} \left| \hat{P}_{E=0} \hat{f} \hat{P}_{\chi=s} \hat{P}_{E=0} \right| \Psi_{\sigma} \right)}{\left(\Psi_{\sigma} \left| \hat{P}_{E=0} \hat{P}_{\chi=s} \hat{P}_{E=0} \right| \Psi_{\sigma} \right)} = \sum_{\sigma} p_{\Psi}(\sigma) \frac{\left\langle \Psi_{\sigma} \left| \hat{f} \hat{P}_{\chi=s} \right| \Psi_{\sigma} \right\rangle}{\left\langle \Psi_{\sigma} \left| \hat{P}_{\chi=s} \right| \Psi_{\sigma} \right\rangle} .$$

From (2.103), this leads us to the result

$$\left\langle \hat{\mathcal{O}}[f|\chi = s] \right\rangle_{\Psi} = \sum_{\sigma} p_{\Psi}(\sigma) \mathrm{E}_{\Psi_{\sigma}}[f|\chi = s] \ , \tag{2.109}$$

which means that the average of $\hat{\mathcal{O}}[f|\chi = s]$ is equal to a weighted sum of the conditional expectation values of $\hat{f}$ in each multiplicity sector with respect to the redefined states (2.108). In particular, if $|\Psi\rangle$ is in a definite multiplicity sector $\sigma = \sigma_0$, then $p_{\Psi}(\sigma) = \delta_{\sigma,\sigma_0}$ and the average of the relational observable is identical to a conditional expectation value. Furthermore, if we require that the state is normalized,

$$1 = (\Psi|\Psi) = \left(\Psi \left| \hat{P}^{\sigma_0}_{E=0} \right| \Psi \right) = 2\pi\hbar \left\langle \Psi_{\sigma_0} \left| \hat{P}_{\chi=s} \right| \Psi_{\sigma_0} \right\rangle \ , \tag{2.110}$$

then the representation of $|\Psi\rangle$ in the reference frame defined defined by the generalized clock $\hat{\chi}$ becomes a conditional probability amplitude,

$$|(\sigma_0, \mathbf{n}; s|\Psi)|^2 = 2\pi\hbar |\left\langle \chi = s, \mathbf{n}|\Psi_{\sigma_0} \right\rangle|^2 = p_{\Psi_{\sigma_0}}(\mathbf{n}|\chi = s) \ , \tag{2.111}$$

due to (2.102) and (2.110).

It is important to note that (2.109) implies that the quantum relational dynamics can be described in two equivalent ways. First, one can use the conditional expectation values of worldline tensor fields in a definite multiplicity sector. This is the 'gauge-fixed point of view'. Second, one can use the physical Hilbert space and the quantum relational observables (2.70), the averages of which manifestly invariant under diffeomorphisms. This is the 'invariant point of view'. These two perspectives were first discussed in [75] for a particular example that we examine in §2.7.2.

Despite the vast literature on conditional probabilities in timeless quantum mechanics [75, 86–93] and on the definition of observables [17, 33, 75, 76, 78–80, 94–98], the connection between these two topics has only recently been addressed in [99] and [75], where different formalisms to the one presented here are used. As we have already mentioned, our new formalism is, in principle, capable of dealing with general gauge choices for general (integrable) models, and it follows directly from standard techniques of canonical gauge systems (cf. Appendix A). Thus, we believe the connection established here between our method of construction of quantum relational observables and conditional probabilities adds to the literature, and further illuminates the interpretation of the relational character of the quantum dynamics.

Incidentally, Barvinsky also claims that the formalism he presented in [51] is related to conditional probabilities (cf. page 294 of [51]). Nonetheless, our formalism does not, in principle, require the restriction to a semiclassical expansion in powers of $\hbar$. Furthermore, the dynamics in [51] was restricted to what we call a definite multiplicity sector, $\sigma = \sigma_0$ and, as a result, a perturbative form of unitarity could be established. The case here is similar because the averages (2.109) (which evolve unitarily, cf. §2.5.3) are only equal to conditional expectation values in definite multiplicity sectors. Lastly, we note that if the perturbative inner product (2.98) is used, then the conditional probabilities may be defined as

$$p_\Psi := \frac{1}{(\Psi\,|\Psi)} \left(\hat{\mu}_\sigma^{\frac{1}{2}}\Psi\right)^* \hat{\mu}_\sigma^{\frac{1}{2}}\Psi\bigg|_{\chi(q)=s} \tag{2.112}$$

for a definite multiplicity sector, in analogy to (2.109).

2.7.1 Invariant extensions of states

Let us now suppose that one adopts the gauge-fixed point of view and works solely with conditional probabilities. In this case, it is important to note that definition of conditional probabilities from on-shell states is ambiguous. To see this, we use the factorization

$$\langle \chi = s, \mathbf{n} | \Psi \rangle = \xi(s)\psi(s, \mathbf{n}) \ , \tag{2.113}$$

suggested by Hunter in [100] in the context of Born-Oppenheimer systems (cf. Chapter 5 and Appendix B). We refer to $\psi(s, \mathbf{n})$ as a conditional wave function because the conditional probabilities (2.102) can be written solely in terms of $\psi(s, \mathbf{n})$,

$$p_\Psi(\mathbf{n}|\chi = s) = \frac{|\psi(s, \mathbf{n})|^2}{\sum_{\mathbf{n}} |\psi(s, \mathbf{n})|^2} \ . \tag{2.114}$$

The ambiguity in the definition of (2.114) is seen from the fact that it remains invariant, together with (2.113) under the redefinitions [see also (B.13)]

$$\begin{aligned} \xi(s) &\mapsto \mathrm{e}^{\alpha(s)+\mathrm{i}\beta(s)}\xi(s) \ , \\ \psi(s,\mathbf{n}) &\mapsto \mathrm{e}^{-\alpha(s)-\mathrm{i}\beta(s)}\psi(s,\mathbf{n}) \ , \end{aligned} \tag{2.115}$$

with $\alpha(s), \beta(s) \in \mathbb{R}$. What are the consequences of this ambiguity? Consider the case in which an observer is able to determine the conditional probability distribution that corresponds to a certain state preparation at an instant $s = s_0$ (cf. §2.6). This distribution determines all the conditional predictions the observer can make regarding the relational dynamics and, as a result, it is analogous to the classical relative initial data. In other words, just as the relational evolution is classically determined by a choice of relative initial data, the quantum relational evolution (at least for the particular case of §2.5.3) is determined from a certain conditional distribution at a moment $s = s_0$. This correspondence leads us to ask: if all that is known is the conditional distribution, is it possible to relate it to an on-shell state? If so, can we determine what the (Schrödinger-picture) state will be in the future? Below, we show that both questions can be answered affirmatively.

First, let us assume that $\psi(s_0, \mathbf{n}) = \langle \chi = s_0, \mathbf{n} | \psi \rangle$ is a conditional wave function that yields the known conditional distribution via (2.114) (i.e., up to the redefinitions (2.115)). Now consider the on-shell state

$$|\Psi_\sigma\rangle := (2\pi\hbar)^2 \hat{\Omega}_t^\sigma \bullet \hat{\Omega}_t^\sigma \hat{P}_{\chi=s_0} |\psi\rangle \ . \tag{2.116}$$

Equations (2.90) and (2.91) imply

$$(2\pi\hbar)^2 \hat{P}_{\chi=s_0} \hat{\Omega}_t^\sigma \bullet \hat{\Omega}_t^\sigma \hat{P}_{\chi=s_0} = \hat{P}_{\chi=s_0} \ , \tag{2.117}$$

which leads to

$$\hat{P}_{\chi=s_0} |\Psi_\sigma\rangle = \hat{P}_{\chi=s_0} |\psi\rangle \ , \tag{2.118}$$

which is the same as

$$\langle \chi = s_0, \mathbf{n} | \Psi_\sigma \rangle = \psi(s_0, \mathbf{n}) \ . \tag{2.119}$$

This means that the on-shell state $|\Psi_\sigma\rangle$ is an invariant extension of the initial conditional wave function. In other words, Eq. (2.116) produces an invariant state that coincides with $\psi(s, \mathbf{n})$ at the initial instant. In analogy to the classical theory, we then refer to $|\Psi_\sigma\rangle$ [or, in a slight abuse of terminology $\psi(s, \mathbf{n})$] as the relative initial data for the quantum evolution. Notice that the "invariantization" map is a projector,

$$(2\pi\hbar)^4\hat{\Omega}_t^\sigma \bullet \hat{\Omega}_t^\sigma \hat{P}_{\chi=s_0}\hat{\Omega}_t^\sigma \bullet \hat{\Omega}_t^\sigma \hat{P}_{\chi=s_0} = (2\pi\hbar)^2\hat{\Omega}_t^\sigma \bullet \hat{\Omega}_t^\sigma \hat{P}_{\chi=s_0} \ , \tag{2.120}$$

where we used (2.117). Furthermore, if we now evaluate

$$\langle\chi = s, \mathbf{n}|\Psi_\sigma\rangle = \sum_{\mathbf{n}_0}(\sigma, \mathbf{n}; s|\sigma, \mathbf{n}_0; s_0)\psi(s_0, \mathbf{n}_0) \ , \tag{2.121}$$

we see that, for $s \neq s_0$, the state Ψ_σ leads to an evolved conditional wave function, and its evolution is dictated by the physical propagator.

We can interpret the quantum relative initial data (invariant extensions of states) in a relational manner, similarly to the relational observables. They determine the conditional probability distributions in a diffeomorphism-invariant way, and correspond to the value of a certain conditional amplitude relative to the value s_0 of the generalized clock. It is worth mentioning that Woodard has suggested the use of an "invariantization" scheme to obtain solutions to the quantum constraint equation [76], but his approach did not specify the factor ordering that defines the Faddeev-Popov resolution of the identity [cf. (2.69)]. In the semiclassical approach of [51], Barvinsky has also suggested that gauge conditions (here, the generalized clock) should be used in the fixation of initial data for solutions to the quantum constraints. There have also been more recent proposals related to 'G-twirls' and 'relativization maps' that were put forth in the context of quantum information and quantum foundations [73, 74, 82, 83]. We will comment on how our formalism is related to them in §2.7.2.

2.7.2 Recovering the Page-Wootters formalism

The Page-Wootters formalism is one of the most actively researched approaches to timeless quantum mechanics [75, 86–93], and it is based on the use conditional probabilities. For this reason, it is paramount that we verify what the relation between our method and this approach is. We will see that our formalism can be regarded as a generalization of the standard Page-Wootters setting.

In most applications of the Page-Wootters formalism, one assumes that the constraint $\hat{C}$ is of the form

$$\hat{C} \equiv C(\hat{q}, \hat{p}) = C_{(1)}(\hat{q}^1, \hat{p}_1) + C_{(>1)}(\hat{q}, \hat{p}) \ , \tag{2.122}$$

where the operator $C_{(>1)}(\hat{q}, \hat{p})$ depends solely on $\hat{q}^i, \hat{p}_i$ for $i > 1$. This corresponds to the situation in which the variables $\hat{q}^1$ and $\hat{p}_1$ describe a "laboratory" ($\hat{C}_{(1)}$ is the "laboratory Hamiltonian"), whereas $\hat{q}^i, \hat{p}_i$ for $i > 1$ constitute degrees of freedom of the a system (with Hamiltonian $\hat{C}_{(>1)}$) to be studied relative to the standard of time of the laboratory. In other words, the purpose is to recover the usual Schrödinger equation for the subsystem based on an external "laboratory" time parameter. The typical procedure is to choose a variable $\hat{\chi} \equiv \chi(\hat{q}^1, \hat{p}_1)$ that is conjugate to $C_{(1)}(\hat{q}^1, \hat{p}_1)$ (and, therefore, to $\hat{C}$) as a generalized clock, conditioned on which the evolution is analyzed. In this way, we note that $\hat{\chi}$ corresponds to the "laboratory proper time" and, in fact, can be identified with the proper-time gauge discussed in §2.5.1 for whole system [in the particular case in which $\hat{C}$ is given by (2.122)].

It is important to mention that a connection between the Page-Wootters conditional probabilities and an approach to quantum relational observables was first noted in [75] (see also the earlier remarks in [93,99]) for the constraint (2.122) and generalized clocks that are formally conjugate to $C_{(1)}(\hat{q}^1, \hat{p}_1)$. Specifically, the case of $\hat{\chi}$ as a "covariant positive-operator valued measure (POVM)" was analyzed in [75]. Here, we will instead follow the formalism presented in §2.5.1 and §2.5.2.[23] Below, we disregard the primary constraint $\hat{p}_e$, which plays no role in the calculations.

First, we note that $\hat{C}_{(1)}$ is an invariant, and we may define $\hat{h} := \hat{C}_{(1)}$ (cf. §2.5.2). However, we do not need to assume in this case that the spectrum of $\hat{C}$ is continuous because of the simple form given in (2.122). Indeed, let us consider a complete orthonormal system of simultaneous eigenstates of $\hat{C}_{(1)}$ and $\hat{C}_{(>1)}$, which we denote by $|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle$. The counterparts of (2.51) and (2.52) are

$$\begin{aligned}
\hat{C}\,|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle &= (E_{(1)} + E_{(>1)})\,|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle \ , \\
\hat{h}\,|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle &= E_{(1)}\,|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle \ ,
\end{aligned}$$

and $h = -H(E, E_{(>1)}, \mathbf{n}) = E - E_{(>1)}$.[24] There is only one multiplicity sector ($\sigma \equiv 1$). Notice that, in this case, $H_0(E_{(>1)}, \mathbf{n}) = E_{(>1)}$, and the counterpart of (2.61) reads

$$|\chi, E_{(>1)}, \mathbf{n}\rangle = \frac{1}{\sqrt{2\pi\hbar}} \sum_{E_{(1)}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E_{(1)}\chi}\,|E_{(1)}, E_{(>1)}, \mathbf{n}\rangle \ . \tag{2.123}$$

If we define $\hat{P}_{E=0} = \sum_{E_{(>1)},\mathbf{n}} |E_{(1)} = -E_{(>1)}, E_{(>1)}, \mathbf{n}\rangle \langle E_{(1)} = -E_{(>1)}, E_{(>1)}, \mathbf{n}|$ and

[23] After the release of [31] (on which part of this Chapter is based) and its submission by the author of this thesis for publication, a generalization of [75] to "relativistic settings" appeared in [101]. The results therein are complementary to the ones presented in [31] and in the beginning of this section (§2.7), but, in contrast to [31] and §2.7, they are still restricted to a particular class of gauge choices (which have trivial Faddeev-Popov determinants). In the future, it would be interesting to compare the formalism presented here to the one proposed in [75, 101].

[24] We assume that E and $E_{(1)}$ are labels of the same type (discrete or continuous) and that the equation $E = E_{(1)} + E_{(>1)}$ can be solved for $E_{(1)}$. The solution is given by h. For example, if both E and $E_{(1)}$ are continuous labels, whereas $E_{(>1)}$ is discrete, then the restriction of h to the case in which $E = 0$ corresponds to a restriction of h to a set of discrete values given by $-E_{(>1)}$.

$\hat{P}_{\chi=s} = \sum_{E_{(>1)},\mathbf{n}} |\chi = s, E_{(>1)}, \mathbf{n}\rangle \langle \chi = s, E_{(>1)}, \mathbf{n}|$, we can define the relational observables as in the proper-time gauge [cf. (2.38)]

$$\begin{aligned}\hat{\mathcal{O}}_{\rm inv}[f|\chi = s] &= \pi\hbar \sum_E \hat{P}_E\, [\hat{f}, \hat{P}_{\chi=s}]_+\, \hat{P}_E \ ,\\ \hat{\mathcal{O}}[f|\chi = s] &= \pi\hbar \hat{P}_{E=0}\, [\hat{f}, \hat{P}_{\chi=s}]_+\, \hat{P}_{E=0} \ .\end{aligned} \tag{2.124}$$

Since there is only one multiplicity sector and the on-shell Faddeev-Popov operator is the identity in the physical Hilbert space [compare (2.124) to (2.70)], Eq. (2.109) reduces to

$$\left\langle \hat{\mathcal{O}}[f|\chi = s] \right\rangle_\Psi = \mathrm{E}_\Psi[f|\chi = s] \ , \tag{2.125}$$

such that the averages of relational observables coincide with conditional expectation values.

In particular, if E spans $\mathbb{R}$, we find

$$\hat{\mathcal{O}}_{\rm inv}[q^i|\chi = s] = \int_{-\infty}^{\infty} \mathrm{d}\tau\ \hat{q}^i(\tau) \otimes \hat{P}_{\chi=s-\tau} \ \ , \tag{2.126}$$

where

$$\hat{q}^i(\tau) := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\hat{C}_{(>1)}} \hat{q}^i \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\hat{C}_{(>1)}} \ ,$$

similarly to (2.37). Equation (2.126) is the result of the ‘G-twirl’ employed in [75],[25] and it also resembles the “relativization” operation used in [73, 74, 83]. Furthermore, the dynamics of $\hat{\mathcal{O}}[q^i|\chi = s]$ is found in analogy to (2.86),

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{\mathcal{O}}[q^i|\chi = s] = \frac{1}{\mathrm{i}\hbar}[\hat{\mathcal{O}}[q^i|\chi = s], \hat{C}_{(>1)}]\ (i > 1) \ .$$

These are simply the standard Heisenberg equations in the nonrelativistic quantum mechanics for the degrees of freedom $\hat{q}^i, \hat{p}_i$. Thus, we see that our formalism is capable of recovering the standard quantum theory. This is not, however, the standard derivation of the evolutionary law in the Page-Wootters approach. Usually, one focuses on what is, in our terminology, the Schrödinger picture for conditional wave functions. Here,

[25] The G-twirl operation is also sometimes used for spatial frames of reference (associated with generalized rods) [82].

this is obtained by noting that (2.123) leads to

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\left|\chi=s,q^i\right\rangle=\hat{C}_{(1)}\left|\chi=s,q^i\right\rangle\ , \tag{2.127}$$

where $|\chi=s,q^i\rangle$ is simply obtained by a change of basis in the space of the $\hat{q}^i,\hat{p}_i$ degrees of freedom,

$$|\chi=s,q^i\rangle=|\chi=s\rangle\otimes\sum_{E_{(>1)},\mathbf{n}}|E_{(>1)},\mathbf{n}\rangle\langle E_{(>1)},\mathbf{n}|q^j\rangle\ . \tag{2.128}$$

Then, for any on-shell state $|\Psi\rangle$, the evolution of the conditional wave function $\psi(s,q^i):=\langle\chi=s,q^i|\Psi\rangle$ [cf. (2.113)] reads

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\psi(s,q^i)&=\left\langle\chi=s,q^i\left|-\hat{C}_{(1)}\right|\Psi\right\rangle\\&=\left\langle\chi=s,q^i\left|\hat{C}_{(>1)}\right|\Psi\right\rangle\\&=\hat{C}_{(>1)}\left(q,\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right)\psi(s,q^i)\ ,\end{aligned} \tag{2.129}$$

which is the standard Schrödinger equation (with respect to the value s of the "laboratory proper time"). Eq. (2.129) is the usual Page-Wotters derivation. This is consistent with (2.121), which shows that (invariant extensions of) conditional wave functions (the quantum relative initial data) evolve according to the physical propagator. In this case, the propagator can be found by noticing that $\mathcal{O}[q^i|\chi=s]$ can be written in terms of the states [cf. (2.124)]

$$|q^i;s\rangle:=\sqrt{2\pi\hbar}\hat{P}_{E=0}\left|\chi=s,q^i\right\rangle\ , \tag{2.130}$$

which yield the expected result

$$\begin{aligned}\left(q'^i;s'|q^j;s\right)&=2\pi\hbar\left\langle\chi=s',q'^i\left|\hat{P}_{E=0}\right|\chi=s,q^j\right\rangle\\&=\sum_{E_{(>1)},\mathbf{n}}\langle q'^i|E_{(>1)},\mathbf{n}\rangle\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{(>1)}(s'-s)}\,\langle E_{(>1)},\mathbf{n}|q^j\rangle\\&=\left\langle q'^i\left|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{C}_{(>1)}(s'-s)}\right|q^j\right\rangle\ \ (i,j>1)\ ,\end{aligned} \tag{2.131}$$

due to the assumption that the states $|E_{(>1)},\mathbf{n}\rangle$ are complete and orthonormal in the space of the $\hat{q}^i,\hat{p}_i$ degrees of freedom.

Chapter 3

The Relativistic Particle as an Archetypical Example

In order to illustrate the formalism of Chapters 1 and 2 with a simple and well-known example, we now examine how the classical and quantum relational dynamics may be understood for the free relativistic particle. We emphasize that the dynamics is relational, both in classical and quantum levels, and we show how to obtain the nonrelativistic limit of (quantum) relational observables. This will serve as a prelude to the weak-coupling expansion method used in Chapter 5. Moreover, we will analyze other interesting examples in the context of cosmology in Chapter 4.[1]

The free relativistic particle is perhaps the most emblematic example of a system with worldline-diffeomorphism invariance. We first construct the classical relational observables for a relativistic particle with mass m and we discuss the nonrelativistic limit. Subsequently, we present the quantization of the system and discuss the quantum relational observables, their dynamics and their nonrelativistic counterparts. Incidentally, the nonrelativistic limit will also serve to introduce the concept of weak-coupling expansion, which will be paramount in Chapters 5 and 6.

3.1 Classical theory

3.1.1 Obsevables

The dynamics of a massive relativistic particle is defined by the action [cf. §1.4]

$$S = -mc\int_a^b \mathrm{d}\tau\, \sqrt{-\eta_{\mu\nu}\frac{\mathrm{d}q^\mu}{\mathrm{d}\tau}\frac{\mathrm{d}q^\nu}{\mathrm{d}\tau}}\ , \tag{3.1}$$

[1]This Chapter is based on [30].

where we assume that the particle moves in a Minkowski spacetime with $d+1$ dimensions [and signature $(-,+\cdots+)$]. The $d+1$ fields $q^\mu(\tau)=(ct,\mathbf{q})$ serve as the scalars considered in Chapters 1 and 2. The field equations

$$\dot{q}^\mu = \eta^{\mu\nu}p_\nu\sqrt{-\eta_{\rho\lambda}\dot{q}^\rho\dot{q}^\lambda}\ , \tag{3.2}$$

imply the initial value (primary) constraint

$$C = -\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}=0\ , \tag{3.3}$$

where the constants $p_\mu = \left(\frac{p_t}{c},\mathbf{p}\right)$ correspond to the canonical momenta. We can solve (3.2) in a relational way by expressing the evolution of the fields in terms of a generalized clock. For example, for an arbitrary worldline coordinate τ, if we choose $t(\tau)$ as the clock, we obtain

$$\mathbf{q}(\tau)=\mathbf{q}(a)-\frac{c^2\mathbf{p}}{p_t}(t(\tau)-t(a)) \quad (p_t\neq 0)\ , \tag{3.4}$$

and the boundary values correspond to invariant extensions in the $t(\tau)$ gauge,

$$\mathbf{q}(a)=\mathbf{q}(\tau)+\frac{c^2\mathbf{p}}{p_t}(t(\tau)-t(a))\ , \tag{3.5}$$

since

$$\begin{aligned}\delta_{\epsilon(\tau)}\left[\mathbf{q}(\tau)+\frac{c^2\mathbf{p}}{p_t}(t(\tau)-t(a))\right] &= \delta_{\epsilon(\tau)}\mathbf{q}(\tau)+\frac{c^2\mathbf{p}}{p_t}\delta_{\epsilon(\tau)}t(\tau)\\ = \epsilon(\tau)\sqrt{-\eta_{\rho\lambda}\dot{q}^\rho\dot{q}^\lambda}\left[\mathbf{p}-\frac{c^2\mathbf{p}}{p_t}\frac{p_t}{c^2}\right] = 0 &\end{aligned}$$

holds due to (3.2). It is also possible to invariantly extend $t(\tau)$ and $q^j(\tau)$ $(j=2,\ldots,d)$ with respect to the generalized clock defined by $q^1(\tau)$. The result is

$$\begin{aligned} t(a) &= t(\tau)+\frac{p_t}{c^2p_1}(q^1(\tau)-q^1(a))\ ,\\ q^j(a) &= q^j(\tau)-\frac{p_j}{p_1}(q^1(\tau)-q^1(a)) \ \ (j=2,\ldots,d)\ , \end{aligned} \tag{3.6}$$

with $p_1\neq 0$ (see, however, the discussion in §3.2.5). Since these gauges are conjugate to invariants, we can follow §1.10 and express the relational evolution in terms of the

Poisson brackets

$$\frac{\partial \mathbf{q}(a)}{\partial t(a)} = -\frac{c^2\mathbf{p}}{p_t} = \{p_t, \mathbf{q}(a)\} \ , \tag{3.7}$$
$$\frac{\partial t(a)}{\partial q^1(a)} = -\frac{p_t}{c^2 p_1} = \{p_1, t(a)\} \ , \tag{3.8}$$

with a similar result for $q^j(a)$ ($j = 2, \ldots, d$). In §3.2.3 and §3.2.5, the quantum versions of (3.7) and (3.8) will be derived. We can also rewrite (3.5) and (3.6) via the integral formula (1.89). For instance,

$$\begin{aligned}\mathbf{q}(a) = \mathbf{q}(\tau)|_{\tau=a} &= \int_{-\infty}^{\infty} \mathrm{d}\tau\ \delta(\tau - a)\mathbf{q}(\tau)\\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau\ \left|\frac{\mathrm{d}t}{\mathrm{d}\tau}\right| \delta(t(\tau) - t(a))\mathbf{q}(\tau)\\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau\ |p_t|\delta(t(\tau) - t(a))\mathbf{q}(\tau)\ .\end{aligned} \tag{3.9}$$

Lastly, it is worthwhile to note that the nonrelativistic limit of the invariant extensions can be obtained by performing an expansion in powers of $1/c^2$. The result is

$$\begin{aligned}\mathbf{q}(a) &= \mathbf{q}(\tau) - \frac{\sigma\mathbf{p}}{m\sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}}}(t(\tau) - t(a))\\ &= \mathbf{q}(\tau) - \frac{\sigma\mathbf{p}}{m}(t(\tau) - t(a)) + \mathcal{O}\left(\frac{1}{c^2}\right)\ ,\end{aligned} \tag{3.10}$$
$$\begin{aligned}t(a) &= t(\tau) - \frac{\sigma m\sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}}}{p_1}(q^1(\tau) - q^1(a))\\ &= t(\tau) - \frac{\sigma m}{p_1}(q^1(\tau) - q^1(a)) + \mathcal{O}\left(\frac{1}{c^2}\right)\ ,\end{aligned} \tag{3.11}$$
$$q^j(a) = q^j(\tau) - \frac{p_j}{p_1}(q^1(\tau) - q^1(a))\ . \tag{3.12}$$

One readily notices that the above quantities are the Newtonian relational observables; i.e., they are invariant extensions that encode the relational evolution of the field $\mathbf{q}(\tau)$ and $t(\tau)$ in the limit in which $t(\tau)$ evolves as a "preferred" clock. Moreover, Eq. (3.11) corresponds to the so-called time-of-arrival observable. It yields the value of $t(\tau)$ (Newtonian time) at which $q^1(\tau) = q^1(a)$ (see [80, 102] and references therein for a discussion).

3.1.2 On-shell action

In order to understand the nonrelativistic limit in the quantum theory, it is useful to first discuss the HJ formalism (cf. §1.10). To this end, it is sufficient to consider the on-shell action, which can be computed if we write the constant momenta p_μ in terms of the boundary values $q^\mu(a), q^\mu(b)$. Evaluating (3.3) and (3.4) at $\tau = b$, we obtain

$$p_t = -\sigma\sqrt{\mathbf{p}^2c^2 + m^2c^4} \quad , \quad \sigma = \pm 1 \; , \tag{3.13}$$

$$\left(1 + \frac{\mathbf{p}^2}{m^2c^2}\right)^{-1} = 1 - \frac{(\mathbf{q}(b) - \mathbf{q}(a))^2}{c^2(t(b) - t(a))^2} \; . \tag{3.14}$$

Notice that $\operatorname{sgn}(\dot{t}) = -\operatorname{sgn}(p_t) = \sigma = \text{const.}$ due to (3.13) and (3.2), and this implies that $|t(b) - t(a)| = \sigma(t(b) - t(a))$. If we insert the solution (3.4) in (3.1) and use (3.13) together with (3.14), we find the on-shell action

$$\begin{aligned} W(ct(b), \mathbf{q}(b); ct(a), \mathbf{q}(a)) := S_{\text{on-shell}} &= -\frac{\sigma mc^2}{\sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}}}(t(b) - t(a)) \\ &= -mc^2|t(b) - t(a)|\sqrt{1 - \frac{(\mathbf{q}(b) - \mathbf{q}(a))^2}{c^2(t(b) - t(a))^2}} \\ &= -mc\sqrt{c^2(t(b) - t(a))^2 - (\mathbf{q}(b) - \mathbf{q}(a))^2} \; , \end{aligned} \tag{3.15}$$

which is the well-known result from the special theory of relativity. Equation (3.15) also solves the HJ constraint [cf. (1.108)]

$$-\frac{1}{2c^2}\left(\frac{\partial W}{\partial t(b)}\right)^2 + \frac{1}{2}\left(\frac{\partial W}{\partial \mathbf{q}(b)}\right)^2 + \frac{m^2c^2}{2} = 0 \; . \tag{3.16}$$

If we now expand (3.15) in powers of $1/c^2$,

$$\begin{aligned} W(ct(b), \mathbf{q}(b); ct(a), \mathbf{q}(a)) &= -\sigma mc^2(t(b) - t(a))\sqrt{1 - \frac{(\mathbf{q}(b) - \mathbf{q}(a))^2}{c^2(t(b) - t(a))^2}} \\ &= -\sigma mc^2(t(b) - t(a))\left[1 - \frac{(\mathbf{q}(b) - \mathbf{q}(a))^2}{2c^2(t(b) - t(a))^2}\right] + \mathcal{O}\left(\frac{1}{c^2}\right) \\ &=: -\sigma mc^2(t(b) - t(a)) + S_\sigma(t(b), \mathbf{q}(b); t(a), \mathbf{q}(a)) \; , \end{aligned} \tag{3.17}$$

we find that

$$S_\sigma(t(b), \mathbf{q}(b); t(a), \mathbf{q}(a)) := \frac{\sigma m}{2}\frac{(\mathbf{q}(b) - \mathbf{q}(a))^2}{(t(b) - t(a))} + \mathcal{O}\left(\frac{1}{c^2}\right) \; . \tag{3.18}$$

is a solution to the HJ constraint in the Newtonian limit

$$\sigma\frac{\partial S_\sigma}{\partial t(b)}+\frac{1}{2m}\left(\frac{\partial S_\sigma}{\partial \mathbf{q}(b)}\right)^2=\mathcal{O}\left(\frac{1}{c^2}\right) \tag{3.19}$$

at order c^0. We note that the structure of the constraint (3.19) is identical to the ordinary time-dependent HJ equation (1.106), where $t(b)$ plays the role of a "preferred" time coordinate (with respect to which the system can be globally deparametrized). This implies that S_σ coincides with the on-shell action of the Newtonian theory. If we proceed to compute relativistic corrections (higher orders in $1/c^2$), we find that S_σ is a solution to a corrected constraint that can be regarded as a "Newtonian" HJ equation with an effective Hamiltonian, which follows from the expansion of (3.13). In the quantum theory, the corrected Newtonian HJ equation corresponds to a corrected Schrödinger equation with an effective quantum Hamiltonian. This is an elementary example of a general perturbative procedure ('weak-coupling expansion') that will be analyzed in Chapter 5 and applied to the early Universe in Chapter 6.

3.2 Quantum theory

Following the developments of Chapter 2, we first define the auxiliary Hilbert space $\mathcal{H}$ for the relativistic particle and, subsequently, discuss the definition of the induced inner product. In this case, we can simply define $\mathcal{H}=L^2(\mathbb{R}^{d+1},\mathrm{d}ct\mathrm{d}^dq)$, such that the auxiliary inner product reads[2]

$$\langle\psi_{(1)}|\psi_{(2)}\rangle=\int_{-\infty}^{\infty}c\mathrm{d}t\int_{\mathbb{R}^d}\mathrm{d}^dq\ \psi^*_{(1)}(ct,\mathbf{q})\psi_{(2)}(ct,\mathbf{q})\ .$$

The self-adjoint constraint operator

$$\hat{C}=-\frac{1}{2c^2}\hat{p}_t^2+\frac{1}{2}\hat{\mathbf{p}}^2+\frac{m^2c^2}{2}\ , \tag{3.20}$$

has the eigenstates

$$\langle ct,\mathbf{q}|\sigma,\mathbf{p},mc\rangle=\frac{1}{(2\pi\hbar)^{\frac{d+1}{2}}}\exp\left(-\frac{\mathrm{i}}{\hbar}\sigma\sqrt{\mathbf{p}^2c^2+m^2c^4}t\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{q}}\ . \tag{3.21}$$

[2] It is useful to perform a brief dimensional analysis. The dimensions of the central objects in the quantum theory are $[\hbar]=\frac{ML^2}{T},[q^\mu]=L,[p_\mu]=\frac{ML}{T},[|q^\mu\rangle]=L^{-\frac{1}{2}},[|p_\mu\rangle]=\frac{T^{\frac{1}{2}}}{L^{\frac{1}{2}}M^{\frac{1}{2}}}$, where L,M, and T are units of length, mass and time, respectively. Furthermore, if $\langle\psi|\psi\rangle=1$, then $[|\psi\rangle]=0$. Lastly, notice that $\Theta(x)$ (the Heaviside step function) is dimensionless.

The positive and negative frequency sectors are labeled by $\sigma = \pm 1$, respectively. From

$$\langle \sigma', \mathbf{p}', m'c | \sigma, \mathbf{p}, mc \rangle = \sqrt{\mathbf{p}^2 + m^2c^2} \delta_{\sigma',\sigma} \delta(\mathbf{p}' - \mathbf{p}) \delta\left(\frac{m'^2c^2}{2} - \frac{m^2c^2}{2} \right) , \tag{3.22}$$

we can define the induced inner product (cf. §2.3) [53, 67]

$$(\sigma', \mathbf{p}', mc | \sigma, \mathbf{p}, mc) := \sqrt{\mathbf{p}^2 + m^2c^2}\ \delta_{\sigma',\sigma} \delta(\mathbf{p}' - \mathbf{p}) , \tag{3.23}$$

and the improper projectors [cf. (2.14), (2.16) and (2.59)][3]

$$\hat{P}_{\sigma,m} := \int_{\mathbb{R}^d} \frac{\mathrm{d}^d p}{\sqrt{\mathbf{p}^2 + m^2c^2}} \, |\sigma, \mathbf{p}, mc\rangle \, \langle \sigma, \mathbf{p}, mc| \ , \tag{3.24}$$

which have the matrix elements

$$\begin{aligned} \left\langle \frac{p_t'}{c}, \mathbf{p}' \middle| \hat{P}_{\sigma,m} \middle| \frac{p_t}{c}, \mathbf{p} \right\rangle &= \delta\left(\frac{p_t'}{c} - \frac{p_t}{c} \right) \delta(\mathbf{p}' - \mathbf{p}) \\ &\times \delta\left(-\frac{p_t^2}{2c^2} + \frac{\mathbf{p}^2}{2} + \frac{m^2c^2}{2} \right) \Theta\left(-\frac{\sigma p_t}{c} \right) \ . \end{aligned} \tag{3.25}$$

3.2.1 The nonrelativistic limit of the induced inner product

If we now define $|ct, \mathbf{q}; \sigma, m\rangle := \hat{P}_{\sigma,m} |ct, \mathbf{q}\rangle$, then

$$(ct', \mathbf{q}'; \sigma', m | ct, \mathbf{q}; \sigma, m) = \delta_{\sigma',\sigma} \, \langle ct', \mathbf{q}' | \hat{P}_{\sigma,m} | ct, \mathbf{q} \rangle \ . \tag{3.26}$$

follows from (2.18). This amplitude is the quantum analogue of the on-shell action, as can be seen from an expansion in powers of $\hbar$. Alternatively, we are interested in an expansion in powers of $1/c^2$ and in the lowest order (the nonrelativistic limit). A straightforward calculation yields

$$\begin{aligned} &(ct', \mathbf{q}'; \sigma', m | ct, \mathbf{q}; \sigma, m) \\ &= \frac{\delta_{\sigma',\sigma}}{(2\pi\hbar)^{d+1} mc} \int_{\mathbb{R}^d} \frac{\mathrm{d}^d p}{\sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}}} \ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2 \sqrt{1 + \frac{\mathbf{p}^2}{m^2c^2}}(t'-t)} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{q}'-\mathbf{q})} \\ &= \frac{\delta_{\sigma',\sigma}}{2\pi\hbar mc} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2 (t'-t)} \int_{\mathbb{R}^d} \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma \frac{\mathbf{p}^2}{2m}(t'-t)} \end{aligned}$$

[3] The projector $\hat{P}_{\sigma,m}$ given in (3.24) has dimensions of $\left[\hat{P}_{\sigma,m}\right] = \left(\frac{ML}{T}\right)^{-2}$ (inverse momentum squared). For this reason, if $(\Psi|\Psi) = 1$, then $|\Psi\rangle$ has dimensions of momentum.

$$\times \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{q}'-\mathbf{q})} + \mathcal{O}\left(\frac{1}{c^3}\right)$$

$$= \frac{\delta_{\sigma',\sigma}}{2\pi\hbar mc} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t'-t)} K_\sigma(t', \mathbf{q}'; t, \mathbf{q}) + \mathcal{O}\left(\frac{1}{c^3}\right) \,, \tag{3.27}$$

where the pre-factor of $1/(\hbar mc)$ ensures that the dimensions are correct and

$$K_\sigma(t', \mathbf{q}'; t, \mathbf{q}) = \left(\frac{m}{2\pi\mathrm{i}\hbar\sigma(t'-t)}\right)^{\frac{d}{2}} \exp\left(-\frac{m(\mathbf{q}'-\mathbf{q})^2}{2\mathrm{i}\hbar\sigma(t'-t)}\right) \tag{3.28}$$

is the nonrelativistic propagator that solves the Schrödinger constraint, and it is analogous to the Newtonian on-shell action defined in (3.18). Moreover, Eq. (3.27) is analogous to (3.17). We conclude from this that the power series in $1/c^2$ yields similar results in the classical and the quantum theory. Although this is certainly expected, we will see in Chapter 5 that this power series is a particular example of a more general weak-coupling expansion, and we will see that the analogy between the classical and quantum theories is not only present in more general models, but also allow us to define the inner product and unitarity of the gauge-fixed quantum theory, as was discussed in §2.5.6. A central result will be the connection between the inner product that is conserved by the evolution given by the corrected version of (3.28) and the classical Faddeev-Popov determinant.

3.2.2 Quantum relational observables and their relation to the classical expressions I

As we will be interested in explicitly showing how the quantum relational observables for the relativistic particle are related to their corresponding classical expressions, we follow the formalism presented in §2.5.2, which is particularly useful for this purpose. For convenience, we define the states $|\frac{p_t}{c}, \mathbf{p}; \sigma, m) := \hat{P}_{\sigma,m}\,|\frac{p_t}{c}, \mathbf{p}\rangle$, such that the matrix elements of on-shell observables read

$$\left(\frac{p_t'}{c}, \mathbf{p}'; \sigma', m \left| \hat{\mathcal{O}}_\omega \right| \frac{p_t}{c}, \mathbf{p}; \sigma, m\right) = 2\pi\hbar \left\langle \frac{p_t'}{c}, \mathbf{p}' \left| \hat{P}_{\sigma',m}\hat{\omega}\hat{P}_{\sigma,m} \right| \frac{p_t}{c}, \mathbf{p} \right\rangle \,, \tag{3.29}$$

and the Faddeev-Popov resolution of the identity is

$$2\pi\hbar \left\langle \frac{p_t'}{c}, \mathbf{p}' \left| \hat{P}_{\sigma',m}\hat{\omega}[1|\chi = s]\hat{P}_{\sigma,m} \right| \frac{p_t}{c}, \mathbf{p} \right\rangle = \delta_{\sigma',\sigma} \left\langle \frac{p_t'}{c}, \mathbf{p}' \left| \hat{P}_{\sigma,m} \right| \frac{p_t}{c}, \mathbf{p} \right\rangle \,. \tag{3.30}$$

Let us begin by considering the classical gauge $ct(\tau) = cs$. As it is conjugate to the invariant p_t/c, the corresponding quantum gauge fixing can be defined from the results of §2.5.2, such that we obtain

$$\hat{\omega}\left[f(\mathbf{q})|ct=cs\right] := \sum_{\sigma=\pm}\int_{\mathbb{R}^d} \mathrm{d}^d q\ f(\mathbf{q})\,|\sigma,\mathbf{q};s\rangle\,\langle\sigma,\mathbf{q};s|\ , \tag{3.31}$$

$$|\sigma,\mathbf{q};s\rangle := \left|\frac{\hat{p}_t}{c}\right|^{\frac{1}{2}}\Theta\left(-\frac{\sigma\hat{p}_t}{c}\right)|ct=cs,\mathbf{q}\rangle\ . \tag{3.32}$$

One readily notices that (3.32) and (3.31) imply that (3.30) is fulfilled. Indeed, we can write

$$\begin{aligned}
&2\pi\hbar\left\langle\frac{p_t'}{c},\mathbf{p}'\left|\hat{P}_{\sigma',m}\hat{\omega}\left[1|ct=cs\right]\hat{P}_{\sigma,m}\right|\frac{p_t}{c},\mathbf{p}\right\rangle\\
&=\delta_{\sigma',\sigma}\int_{\mathbb{R}^d}\frac{\mathrm{d}^d q}{(2\pi\hbar)^d}\ \Theta\left(-\frac{\sigma p_t'}{c}\right)\Theta\left(-\frac{\sigma p_t}{c}\right)\left|\frac{p_t'p_t}{c^2}\right|^{\frac{1}{2}}\\
&\times\mathrm{e}^{\frac{\mathrm{i}}{\hbar}s(p_t-p_t')}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot(\mathbf{p}-\mathbf{p}')}\delta\left(-\frac{p_t'^2}{2c^2}+\frac{\mathbf{p}'^2}{2}+\frac{m^2c^2}{2}\right)\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\\
&=\delta_{\sigma',\sigma}\Theta\left(-\frac{\sigma p_t'}{c}\right)\Theta\left(-\frac{\sigma p_t}{c}\right)\left|\frac{p_t'p_t}{c^2}\right|^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}s(p_t-p_t')}\delta(\mathbf{p}-\mathbf{p}')\\
&\times\delta\left(-\frac{p_t'^2}{2c^2}+\frac{p_t^2}{2c^2}\right)\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\\
&=\delta_{\sigma',\sigma}\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\delta\left(\frac{p_t'}{c}-\frac{p_t}{c}\right)\delta(\mathbf{p}'-\mathbf{p})\Theta\left(-\frac{\sigma p_t}{c}\right)\\
&=\delta_{\sigma',\sigma}\left\langle\frac{p_t'}{c},\mathbf{p}'\left|\hat{P}_{\sigma,m}\right|\frac{p_t}{c},\mathbf{p}\right\rangle\ ,
\end{aligned}$$

where the result follows from the $\mathbf{q}$ integration and (3.25). Similarly, the matrix element of the relational observable of $\hat{\mathbf{q}}$ in the gauge $ct=cs$ is given by the kernel function [cf. (3.31)]

$$\begin{aligned}
&2\pi\hbar\left\langle\frac{p_t'}{c},\mathbf{p}'\left|\hat{P}_{\sigma',m}\hat{\omega}\left[\mathbf{q}|ct=cs\right]\hat{P}_{\sigma,m}\right|\frac{p_t}{c},\mathbf{p}\right\rangle\\
&=\delta_{\sigma',\sigma}\Theta\left(-\frac{\sigma p_t'}{c}\right)\Theta\left(-\frac{\sigma p_t}{c}\right)\left|\frac{p_t'p_t}{c^2}\right|^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}s(p_t-p_t')}\left[\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\mathbf{p}}\delta(\mathbf{p}-\mathbf{p}')\right]\\
&\times\delta\left(-\frac{p_t'^2}{2c^2}+\frac{\mathbf{p}'^2}{2}+\frac{m^2c^2}{2}\right)\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\ .
\end{aligned}\tag{3.33}$$

Although this may seem slightly complicated, it follows from the theory developed in §2.5.2, with which we can establish a relation between (3.33) and the corresponding classical observable (3.5) as follows: we choose a pair of test functions $\psi_{(1,2)}\left(\frac{p_t}{c},\mathbf{p}\right)$ that have compact support in momentum space and satisfy $\psi_{(1,2)}(0,\mathbf{p})=0$. For notational convenience, we also define

$$\psi^{\sigma}_{(1,2)}(\mathbf{p}) := \psi_{(1,2)}\left(-\sigma\sqrt{\mathbf{p}^2+m^2c^2},\mathbf{p}\right) \ .$$

The matrix element of the relational observables with respect to the test functions is [cf. (3.33)]

$$\begin{aligned}
&2\pi\hbar\sum_{\sigma',\sigma}\left\langle\psi_{(1)}\left|\hat{P}_{\sigma',m}\hat{\omega}\left[\mathbf{q}|ct=cs\right]\hat{P}_{\sigma,m}\right|\psi_{(2)}\right\rangle\\
&=\frac{\hbar}{\mathrm{i}}\sum_{\sigma=\pm}\int\frac{\mathrm{d}^d p'\mathrm{d}^d p\ \left(\psi^{\sigma}_{(1)}(\mathbf{p}')\right)^*\psi^{\sigma}_{(2)}(\mathbf{p})}{\left(\mathbf{p}'^2+m^2c^2\right)^{\frac14}\left(\mathbf{p}^2+m^2c^2\right)^{\frac14}}\\
&\quad\times\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}sc\sigma\left(\sqrt{\mathbf{p}^2+m^2c^2}-\sqrt{\mathbf{p}'^2+m^2c^2}\right)}\frac{\partial}{\partial\mathbf{p}}\delta(\mathbf{p}-\mathbf{p}')\\
&=\sum_{\sigma=\pm}\int_{\mathbb{R}^d}\frac{\mathrm{d}^d p}{\sqrt{\mathbf{p}^2+m^2c^2}}\ \left(\psi^{\sigma}_{(1)}(\mathbf{p})\right)^*\\
&\quad\times\left[\mathrm{i}\hbar\frac{\partial}{\partial\mathbf{p}}+\frac{c\mathbf{p}}{\sigma\sqrt{\mathbf{p}^2+m^2c^2}}s-\frac{\mathrm{i}\hbar\mathbf{p}}{2\left(\mathbf{p}^2+m^2c^2\right)}\right]\psi^{\sigma}_{(2)}(\mathbf{p}) \ .
\end{aligned} \tag{3.34}$$

Subsequently, notice that

$$\begin{aligned}
\frac{\partial}{\partial\mathbf{p}}\psi^{\sigma}_{(1,2)}(\mathbf{p}) = &\frac{\partial}{\partial\mathbf{p}}\psi_{(1,2)}\left(\frac{p_t}{c},\mathbf{p}\right)\bigg|_{\frac{p_t}{c}=-\sigma\sqrt{\mathbf{p}^2+m^2c^2}}\\
&+\frac{c^2\mathbf{p}}{p_t}\frac{\partial}{\partial p_t}\psi_{(1,2)}\left(\frac{p_t}{c},\mathbf{p}\right)\bigg|_{\frac{p_t}{c}=-\sigma\sqrt{\mathbf{p}^2+m^2c^2}}
\end{aligned}$$

implies that (3.34) is equal to

$$\begin{aligned}
&2\pi\hbar\sum_{\sigma',\sigma}\left\langle\psi_{(1)}\left|\hat{P}_{\sigma',m}\hat{\omega}\left[\mathbf{q}|ct=cs\right]\hat{P}_{\sigma,m}\right|\psi_{(2)}\right\rangle\\
&=\int\frac{\mathrm{d}p_t}{c}\mathrm{d}^d p\ \psi^*_{(1)}\left(\frac{p_t}{c},\mathbf{p}\right)\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\\
&\times\left[\mathrm{i}\hbar\frac{\partial}{\partial\mathbf{p}}+\mathrm{i}\hbar\frac{c^2\mathbf{p}}{p_t}\frac{\partial}{\partial p_t}-\frac{c^2\mathbf{p}}{p_t}s-\mathrm{i}\hbar\frac{c^2\mathbf{p}}{2p_t^2}\right]\psi_{(2)}\left(\frac{p_t}{c},\mathbf{p}\right) \ .
\end{aligned}$$

In other words, the matrix elements of the relational observable associated with $\hat{\mathbf{q}}$ in the gauge $c\hat{t}$ can be obtained if one inserts the operator

$$\mathrm{i}\hbar\frac{\partial}{\partial\mathbf{p}}+\mathrm{i}\hbar\frac{c^2\mathbf{p}}{p_t}\frac{\partial}{\partial p_t}-\frac{c^2\mathbf{p}}{p_t}s-\mathrm{i}\hbar\frac{c^2\mathbf{p}}{2p_t^2} \tag{3.35}$$

into the induced inner product $(\cdot|\cdot)$ in the momentum space representation of the pair of test functions $\psi_{(1,2)}\left(\frac{p_t}{c},\mathbf{p}\right)$. One readily verifies that (3.35) commutes with $\hat{C}$ and is symmetric with respect to $\langle\cdot|\cdot\rangle$, such that it is symmetric with respect to $(\cdot|\cdot)$. This is consistent with the developments of §2.5.2. If we identify $\mathbf{q}(\tau)\to \mathrm{i}\hbar\frac{\partial}{\partial \mathbf{p}}, t(\tau)\to \mathrm{i}\hbar\frac{\partial}{\partial p_t}, t(a)\to s$, then (3.35) is a symmetric quantization of the classical relational observable (3.5), as we wanted to show.

3.2.3 Dynamics and nonrelativistic limit I

The dynamics of $\hat{\mathcal{O}}\left[\mathbf{q}|ct=cs\right] := 2\pi\hbar\sum_{\sigma',\sigma}\hat{P}_{\sigma',m}\hat{\omega}\left[\mathbf{q}|ct=cs\right]\hat{P}_{\sigma,m}$ can also be ascertained with the use of the formalism of §2.5.2 and §2.5.3. In particular, we can use the decomposition (2.89) to conclude that the eigenstates of $\hat{\mathcal{O}}\left[\mathbf{q}|ct=cs\right]$ are $|\sigma,\mathbf{q};s,m\rangle := \sqrt{2\pi\hbar}\sum_{\sigma'}\hat{P}_{\sigma',m}\,|\sigma,\mathbf{q};s\rangle$, which lead to

$$
\begin{aligned}
\left\langle \frac{p_t}{c},\mathbf{p}\middle|\,\sigma,\mathbf{q};s,m\right\rangle &= \frac{1}{(2\pi\hbar)^{\frac{d}{2}}}\Theta\left(-\frac{\sigma p_t}{c}\right)\left|\frac{p_t}{c}\right|^{\frac{1}{2}}\\
&\times \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}sp_t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot\mathbf{p}}\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\ .
\end{aligned}
\tag{3.36}
$$

Notice that (3.36) can be regarded as eigenstates because they form a complete orthonormal system in $\mathcal{H}_{\text{phys}}$, as can be straightforwardly verified. This is essentially a consequence of the fact that one can solve $C(p_t,\mathbf{p}) = -p_t^2/(2c^2)+\mathbf{p}^2/2+m^2c^2/2 = 0$ for p_t without restricting the values of $\mathbf{p}$ and m (cf. discussion in §2.5.5).

It is worth mentioning that an expression resembling (3.36) was also presented in [103], and it followed from solving the eigenvalue problem of (3.35). Although this is a valid approach, we stress that, unlike [103], our computation does not require one to first solve the classical field equations in order to find the classical relational observables, which are then quantized. Indeed, this may be a difficult procedure for various models. The formalism presented in Chapter 2 is more general, and it is applicable to any theory with worldline diffeomorphism invariance for which the spectrum and eigenstates of $\hat{C}$ are known. As we have exemplified above, this formalism avoids the explicit construction of classical observables, and one only needs to work with on-shell states (i.e., the solutions to $\hat{C}\,|\Psi\rangle = 0$). Nevertheless, a relation of the quantum observables to the classical expression can, in principle, be established as in (3.35).

As discussed in §2.5.2 and §2.5.3, the evolution of the states (3.36) with respect to s is unitary, since

$$
\mathrm{i}\hbar\frac{\partial}{\partial s}\,|\sigma,\mathbf{q};s,m\rangle = \hat{p}_t\,|\sigma,\mathbf{q};s,m\rangle\,, \tag{3.37}
$$

where $\hat{p}_t$ is self-adjoint in $\mathcal{H}_{\text{phys}}$, implies that the observable

$$\hat{\mathcal{O}}[\mathbf{q}|ct = cs] = \sum_{\sigma=\pm} \int_{\mathbb{R}^d} \mathrm{d}^d q \; \mathbf{q} \, |\sigma, \mathbf{q}; s, m\rangle \langle \sigma, \mathbf{q}; s, m| \tag{3.38}$$

solves the Heisenberg equation

$$\mathrm{i}\hbar \frac{\partial}{\partial s} \hat{\mathcal{O}}[\mathbf{q}|ct = cs] = \left[\hat{p}_t, \hat{\mathcal{O}}[\mathbf{q}|ct = cs]\right] \;, \tag{3.39}$$

which is the quantum counterpart to (3.7).

In analogy to the classical theory and to (3.27), we can now compute the nonrelativistic limit of (3.38). By expanding (3.36), we obtain

$$\begin{aligned}
\langle\, ct, \mathbf{q}|\, \sigma, \tilde{\mathbf{q}}; s, m\rangle &= \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t-s)}}{\sqrt{2\pi\hbar mc}} \int_{\mathbb{R}^d} \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma \frac{\mathbf{p}^2}{2m}(t-s)} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{q}-\tilde{\mathbf{q}})} + \mathcal{O}\left(\frac{1}{c^{\frac{5}{2}}}\right) \\
&= \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t-s)}}{\sqrt{2\pi\hbar mc}} K_\sigma(t, \mathbf{q}; s, \tilde{\mathbf{q}}) + \mathcal{O}\left(\frac{1}{c^{\frac{5}{2}}}\right) \;,
\end{aligned}$$

where $K_\sigma(t, \mathbf{q}; s, \tilde{\mathbf{q}})$ was defined in (3.28). This implies that (3.38) becomes

$$\begin{aligned}
&\left\langle ct', \mathbf{q}' \left| \hat{\mathcal{O}}[\mathbf{q}|ct = cs] \right| ct, \mathbf{q} \right\rangle \\
&= \frac{1}{2\pi\hbar mc} \sum_{\sigma=\pm} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t'-t)} \int_{\mathbb{R}^d} \mathrm{d}^d\tilde{q} \; \tilde{\mathbf{q}} \; K_\sigma(t', \mathbf{q}'; s, \tilde{\mathbf{q}}) K_\sigma(s, \tilde{\mathbf{q}}; t, \mathbf{q}) + \mathcal{O}\left(\frac{1}{c^3}\right) \;,
\end{aligned}$$

which, apart from a WKB phase (cf. (3.27)), coincides with the Newtonian Heisenberg-picture operator for each σ-sector. Indeed, we can relate this result to the classical expression (3.10) in a similar fashion to what was done in (3.35). First, we write

$$K_\sigma(t', \mathbf{q}'; t, \mathbf{q}) = 2\pi\hbar \,\langle t', \mathbf{q}'|\hat{P}^{\text{nonrel}}_{\sigma,m}|t, \mathbf{q}\rangle \;, \tag{3.40}$$

where

$$\hat{P}^{\text{nonrel}}_{\sigma,m} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{2\pi\hbar} \; \exp\left[\frac{\mathrm{i}}{\hbar}\tau\left(\sigma\hat{p}_t + \frac{1}{2m}\hat{\mathbf{p}}^2\right)\right] \;. \tag{3.41}$$

In this way, we obtain the nonrelativistic observable

$$\frac{1}{2\pi\hbar} \int_{\mathbb{R}^d} \mathrm{d}^d\tilde{q} \; \tilde{\mathbf{q}} K_\sigma(t', \mathbf{q}'; s, \tilde{\mathbf{q}}) K_\sigma(s, \tilde{\mathbf{q}}; t, \mathbf{q}) = \left\langle t', \mathbf{q}' \left| \hat{\mathcal{O}}^{\text{nonrel}}_\sigma[\mathbf{q}|t = s] \right| t, \mathbf{q} \right\rangle \;,$$

with [cf. (3.38)]

$$\frac{1}{2\pi\hbar}\hat{O}^{\text{nonrel}}_{\sigma}[\mathbf{q}|t=s] := \int \mathrm{d}^d\tilde{q}\ \tilde{\mathbf{q}}\ \hat{P}^{\text{nonrel}}_{\sigma,m}\left|t=s,\tilde{\mathbf{q}}\right\rangle \left\langle t=s,\tilde{\mathbf{q}}\right| \hat{P}^{\text{nonrel}}_{\sigma,m}\ . \tag{3.42}$$

Second, the matrix element of (3.42) between a pair of compactly-supported test functions $\psi_{(1,2)}(p_t,\mathbf{p})$ is found to be

$$\begin{aligned}&\left\langle \psi_{(1)}\left|\hat{\mathcal{O}}^{\text{nonrel}}_{\sigma,m}[\mathbf{q}|t=s]\right|\psi_{(2)}\right\rangle \\ &= \int \mathrm{d}p_t\mathrm{d}^dp\ \psi^*_{(1)}(p_t,\mathbf{p})\delta\left(\sigma p_t+\frac{\mathbf{p}^2}{2m}\right)\left\{\mathrm{i}\hbar\frac{\partial}{\partial\mathbf{p}}-\mathrm{i}\hbar\frac{\sigma\mathbf{p}}{m}\frac{\partial}{\partial p_t}+\frac{\sigma\mathbf{p}s}{m}\right\}\psi_{(2)}(p_t,\mathbf{p})\ .\end{aligned} \tag{3.43}$$

If we make the identifications $\mathbf{q}(\tau)\to\mathrm{i}\hbar\frac{\partial}{\partial\mathbf{p}}, t(\tau)\to\mathrm{i}\hbar\frac{\partial}{\partial p_t}, t(a)\to s$, then (3.43) is a symmetric quantization of the classical nonrelativistic observable (3.10). Therefore, the formalism of §2.5.2 and §2.5.3 that is applied here yields the correct results in the relativistic theory and in its nonrelativistic limit as well.

3.2.4 Quantum relational observables and their relation to the classical expressions II

It is now worthwhile to repeat the preceding analysis for the generalized clock $\hat{q}^1$. As it is conjugate to the invariant $\hat{p}_1$, the formalism of §2.5.2 and §2.5.3 is again applicable, and we define

$$\left|\sigma,t,q^j;s\right\rangle := |\hat{p}_1|^{\frac{1}{2}}\,\Theta\left(\sigma\hat{p}_1\right)\left|ct,q^1=cs,q^j\right\rangle\ , \tag{3.44}$$

$$\hat{\omega}\left[1|q^1=cs\right] := \sum_{\sigma=\pm}\int_{-\infty}^{\infty}\mathrm{d}ct\int_{\mathbb{R}^{d-1}}\mathrm{d}^{d-1}q\ \left|\sigma,t,q^j;s\right\rangle\left\langle\sigma,t,q^j;s\right|\ . \tag{3.45}$$

The corresponding Faddeev-Popov resolution of the identity in $\mathcal{H}_{\text{phys}}$ is [cf. (3.30)]

$$\begin{aligned}&2\pi\hbar\left\langle\frac{p'_t}{c},\mathbf{p}'\left|\hat{P}_{\sigma',m}\hat{\omega}\left[1|q^1=cs\right]\hat{P}_{\sigma,m}\right|\frac{p_t}{c},\mathbf{p}\right\rangle\\ &=\sum_{\sigma''=\pm}\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\Theta\left(-\frac{\sigma p_t}{c}\right)\Theta\left(-\frac{\sigma' p_t}{c}\right)\\ &\times\Theta(\sigma''p'_1)\Theta(\sigma''p_1)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}cs(p_1-p'_1)}|p'_1p_1|^{\frac{1}{2}}\delta\left(\frac{p'^2_1}{2}-\frac{p_1^2}{2}\right)\delta(p_t-p'_t)\prod_{j=2}^{d}\delta(p_j-p'_j)\\ &=\left(\sum_{\sigma''=\pm}\Theta(\sigma''p_1)\right)\delta_{\sigma',\sigma}\delta(p_t-p'_t)\delta(\mathbf{p}-\mathbf{p}')\delta\left(-\frac{p_t^2}{2c^2}+\frac{\mathbf{p}^2}{2}+\frac{m^2c^2}{2}\right)\Theta\left(-\frac{\sigma p_t}{c}\right)\\ &=\delta_{\sigma',\sigma}\left\langle\frac{p'_t}{c},\mathbf{p}'\left|\hat{P}_{\sigma,m}\right|\frac{p_t}{c},\mathbf{p}\right\rangle\ .\end{aligned}$$

The relational observable associated with $\hat{t}$ in the gauge $\hat{q}^1$ is given by the kernel function

$$
\begin{aligned}
&2\pi\hbar \left\langle \frac{p_t'}{c}, \mathbf{p}' \middle| \hat{P}_{\sigma',m} \hat{\omega}\left[t|q^1 = cs\right] \hat{P}_{\sigma,m} \middle| \frac{p_t}{c}, \mathbf{p} \right\rangle = \sum_{\sigma''=\pm} \Theta\left(\sigma'' p_1'\right) \Theta\left(\sigma'' p_1\right) \left|p_1' p_1\right|^{\frac{1}{2}} \\
&\times \mathrm{e}^{\frac{\mathrm{i}}{\hbar} cs(p_1 - p_1')} \left[\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial p_t} \delta\left(\frac{p_t}{c} - \frac{p_t'}{c}\right)\right] \left[\prod_{j=2}^{d} \delta(p_j - p_j')\right] \Theta\left(-\frac{\sigma' p_t'}{c}\right) \Theta\left(-\frac{\sigma p_t}{c}\right) \\
&\times \delta\left(-\frac{p_t'^2}{2c^2} + \frac{\mathbf{p}'^2}{2} + \frac{m^2c^2}{2}\right) \delta\left(-\frac{p_t^2}{2c^2} + \frac{\mathbf{p}^2}{2} + \frac{m^2c^2}{2}\right) .
\end{aligned}
\tag{3.46}
$$

If we use this expression to compute the matrix element between a pair of compactly-supported test functions, we obtain the expected result

$$
\begin{aligned}
&2\pi\hbar \sum_{\sigma',\sigma} \left\langle \psi_{(1)} \middle| \hat{P}_{\sigma',m} \hat{\omega}\left[t|q^1 = cs\right] \hat{P}_{\sigma,m} \middle| \psi_{(2)} \right\rangle \\
&= \int \frac{\mathrm{d}p_t}{c} \mathrm{d}^d p \; \psi^*_{(1)}\left(\frac{p_t}{c}, \mathbf{p}\right) \delta\left(-\frac{p_t^2}{2c^2} + \frac{\mathbf{p}^2}{2} + \frac{m^2c^2}{2}\right) \\
&\times \left\{ \mathrm{i}\hbar \frac{\partial}{\partial p_t} + \mathrm{i}\hbar \frac{p_t}{c^2 p_1} \frac{\partial}{\partial p_1} - \frac{p_t s}{c p_1} - \mathrm{i}\hbar \frac{p_t}{2c^2 p_1^2} \right\} \psi_{(2)}\left(\frac{p_t}{c}, \mathbf{p}\right) ,
\end{aligned}
$$

where $\psi_{(1,2)}(0, \mathbf{p}) = \psi_{(1,2)}\left(\frac{p_t}{c}, p_1 = 0, p_j\right) = 0$. In this way, the matrix elements of the relational observable associated with $\hat{t}$ in the gauge $\hat{q}^1$ coincide with the insertion of the operator

$$
\mathrm{i}\hbar \frac{\partial}{\partial p_t} + \mathrm{i}\hbar \frac{p_t}{c^2 p_1} \frac{\partial}{\partial p_1} - \frac{p_t s}{c p_1} - \mathrm{i}\hbar \frac{p_t}{2c^2 p_1^2}
\tag{3.47}
$$

into the induced inner product in the momentum space representation of the pair of test functions. As before, we identify $t(\tau) \to \mathrm{i}\hbar\frac{\partial}{\partial p_t}, q^1(\tau) \to \mathrm{i}\hbar\frac{\partial}{\partial p_1}, q^1(a) \to cs$, such that (3.47) is a symmetric quantization of the invariant extension given in the first line of (3.6).

3.2.5 Dynamics and nonrelativistic limit II

As in §3.2.3, we write the observable $\hat{\mathcal{O}}[t|q^1 = cs] := 2\pi\hbar \sum_{\sigma',\sigma} \hat{P}_{\sigma',m}\hat{\omega}[t|q^1 = cs]\hat{P}_{\sigma,m}$ as [cf. (3.38)]

$$
\hat{\mathcal{O}}[t|q^1 = cs] = \sum_{\sigma=\pm} \int_{-\infty}^{\infty} \mathrm{d}ct \int_{\mathbb{R}^{d-1}} \mathrm{d}^{d-1}q \; t \left|\sigma, t, q^j; s, m\right\rangle \left\langle \sigma, t, q^j; s, m\right| ,
\tag{3.48}
$$

where

$$
\begin{aligned}
|\sigma, t, q^j; s, m\rangle &:= \sqrt{2\pi\hbar} \sum_{\sigma'} \hat{P}_{\sigma',m} |\sigma, t, q^j; s\rangle \ , \\
\left\langle \frac{p_t}{c}, \mathbf{p} \middle| \sigma, t, q^j; s, m \right\rangle &= \frac{|p_1|^{\frac{1}{2}}}{(2\pi\hbar)^{\frac{d}{2}}} \Theta\left(\sigma p_1\right) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} c s p_1} \\
&\quad \times \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} t p_t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \sum_{j=2}^{d} q^j p_j} \delta\left(-\frac{p_t^2}{2c^2} + \frac{\mathbf{p}^2}{2} + \frac{m^2 c^2}{2}\right) \ .
\end{aligned}
\tag{3.49}
$$

Notice that we cannot solve $C(p_t/c, \mathbf{p}) = -p_t^2/(2c^2) + \mathbf{p}^2/2 + m^2c^2/2 = 0$ for p_1 without a restriction on the values of the remaining invariants. Indeed, one must make the resctriction $p_t^2/c^2 - \sum_j p_j^2 - m^2c^2 \geq 0$ such that $p_1^2 \geq 0$. Following the discussion in §2.5.5, this implies that the quantum gauge $\hat{q}^1$ is not well-defined. We will discuss the consequences of this in the nonrelativistic limit. Nevertheless, it is still possible to verify that the states (3.49) obey

$$
\mathrm{i}\hbar \frac{\partial}{\partial s} |\sigma, t, q^j; s, m\rangle = c\hat{p}_1 |\sigma, t, q^j; s, m\rangle \ , \tag{3.50}
$$

such that the observable (3.48) solves the Heisenberg equation

$$
\mathrm{i}\hbar \frac{\partial}{\partial s} \hat{\mathcal{O}}[t|q^1 = cs] = c\left[\hat{p}_1, \hat{\mathcal{O}}[t|q^1 = cs]\right] \ , \tag{3.51}
$$

which is the counterpart to (3.8).

To consider the nonrelativistic limit of the observable (3.48) as in §3.2.3, we must first restrict it a fixed frequency sector by using the operator $\Theta\left(-\frac{\sigma\hat{p}_t}{c}\right)$ because the Newtonian theory is defined for a fixed sign of $\hat{p}_t$. We can then consider the expansion in powers of $1/c^2$ of the object

$$
\begin{aligned}
&\left\langle ct, \mathbf{q} \middle| \Theta\left(-\frac{\sigma\hat{p}_t}{c}\right) \middle| \tilde{\sigma}, \tilde{t}, \tilde{q}^j; s, m \right\rangle \\
&= \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^{\frac{2d+1}{2}}} \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma(t-\tilde{t})\sqrt{\mathbf{p}^2c^2+m^2c^4}}}{\sqrt{\mathbf{p}^2+m^2c^2}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_1(q^1-cs)} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sum_{j=2}^{d} p_j(q^j-\tilde{q}^j)} \Theta(\tilde{\sigma}p_1)|p_1|^{\frac{1}{2}} \\
&= \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t-\tilde{t})}}{\sqrt{2\pi\hbar}\ mc} \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d}\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma\frac{\mathbf{p}^2}{2m}(t-\tilde{t})} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_1(q^1-cs)} \\
&\quad \times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sum_{j=2}^{d} p_j(q^j-\tilde{q}^j)} \Theta(\tilde{\sigma}p_1)|p_1|^{\frac{1}{2}} + \mathcal{O}\left(\frac{1}{c^3}\right) \\
&= \sqrt{2\pi\hbar} \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t-\tilde{t})}}{mc} \left\langle t, \mathbf{q} \middle| \hat{P}^{\mathrm{nonrel}}_{\sigma,m} \Theta\left(\tilde{\sigma}\hat{p}_1\right) |\hat{p}_1|^{\frac{1}{2}} \middle| \tilde{t}, q^1 = cs, \tilde{q}^j \right\rangle + \mathcal{O}\left(\frac{1}{c^3}\right) \ ,
\end{aligned}
$$

where $\hat{P}^{\text{nonrel}}_{\sigma,m}$ is the projector defined in (3.41). This implies

$$\left\langle ct', \mathbf{q}' \left| \Theta\left(-\frac{\sigma \hat{p}_t}{c}\right) \hat{\mathcal{O}}_m[t|q^1 = cs] \Theta\left(-\frac{\sigma \hat{p}_t}{c}\right) \right| ct, \mathbf{q} \right\rangle \\ = \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma mc^2(t'-t)}}{mc} \left\langle t', \mathbf{q}' \left| \hat{\mathcal{O}}^{\text{nonrel}}_{\sigma,m}[t|q^1 = cs] \right| t, \mathbf{q} \right\rangle + \mathcal{O}\left(\frac{1}{c^3}\right),$$

where the nonrelativistic observable is defined as [cf. (3.42) and (3.48)]

$$\begin{aligned} &\hat{\mathcal{O}}^{\text{nonrel}}_{\sigma,m}[t|q^1 = cs] \\ &:= 2\pi\hbar \sum_{\tilde{\sigma}=\pm} \int_{-\infty}^{\infty} \mathrm{d}\tilde{t} \int_{\mathbb{R}^{d-1}} \mathrm{d}^{d-1}\tilde{q}\ \tilde{t}\ \hat{P}^{\text{nonrel}}_{\sigma,m} \Theta\left(\tilde{\sigma}\hat{p}_1\right) \left|\frac{\hat{p}_1}{m}\right|^{\frac{1}{2}} |\tilde{t}, q^1 = cs, \tilde{q}^j\rangle \\ &\times \langle \tilde{t}, q^1 = cs, \tilde{q}^j| \left|\frac{\hat{p}_1}{m}\right|^{\frac{1}{2}} \Theta\left(\tilde{\sigma}\hat{p}_1\right) \hat{P}^{\text{nonrel}}_{\sigma,m}\ . \end{aligned} \tag{3.52}$$

Following the derivation of the Faddeev-Popov resolution of the identity in §3.2.4, one can show that the states in the decomposition (3.52) formally constitute a complete system in the nonrelativistic physical Hilbert space. However, a straightforward calculation also shows that these states are not orthogonal, and this is compatible with the fact that the gauge $\hat{q}^1$ is not well-defined in the sense of §2.5.5.

As before, we can relate (3.52) to the corresponding classical expression by evaluating its matrix element between a pair of compactly-supported test functions $\psi_{(1,2)}(p_t, \mathbf{p})$ [with $\psi^{(1,2)}(p_t, p_1 = 0, p_j) = 0$]. As in (3.35), (3.43), and (3.47), we find

$$\begin{aligned} &\left\langle \psi^{(1)} \left| \hat{\mathcal{O}}^{\text{nonrel}}_{\sigma,m}[t|q^1 = cs] \right| \psi^{(2)} \right\rangle \\ &= \int \mathrm{d}p_t \mathrm{d}^d p\ \bar{\psi}^{(1)}(p_t, \mathbf{p}) \delta\left(\sigma p_t + \frac{\mathbf{p}^2}{2m}\right) \\ &\times \left\{ \mathrm{i}\hbar \frac{\partial}{\partial p_t} - \mathrm{i}\hbar \frac{\sigma m}{p_1} \frac{\partial}{\partial p_1} + \frac{\sigma m}{p_1} cs + \mathrm{i}\hbar \frac{\sigma m}{2p_1^2} \right\} \psi^{(2)}(p_t, \mathbf{p})\ . \end{aligned} \tag{3.53}$$

With $t(\tau) \to \mathrm{i}\hbar\frac{\partial}{\partial p_t}, q^1(\tau) \to \mathrm{i}\hbar\frac{\partial}{\partial p_1}, q^1(a) \to cs$, Eq. (3.53) is a symmetric quantization of the nonrelativistic time-of-arrival (3.11).

At this stage, we offer some remarks with the purpose of comparing the above developments to the earlier literature on the time-of-arrival operator (see, for instance, [80, 102]). The careful discussion in [102] established that it is necessary to regularize this operator if it is to be self-adjoint. However, the formalism of [102] did not include the operators $p_t, \mathrm{i}\hbar\frac{\partial}{\partial p_t}$, and instead focused on a "reduced" Hilbert space spanned by the eigenstates of $\hat{\mathbf{q}}, \hat{\mathbf{p}}$. The regularization proposed in [102] was later applied in [80] to the case in which the operators $p_t, \mathrm{i}\hbar\frac{\partial}{\partial p_t}$ are present; i.e., it was applied to the operator that is inserted in (3.53). In the present formalism, we see that the need to regularize stems from the fact that the states in (3.52) are not orthogonal, which is a signal that the gauge $\hat{q}^1$ is not well-defined according to the criteria of §2.5.5, as already mentioned. However, as was stressed in [98], we refrain from adopting such a regularization because our main focus is on the completeness of the states (in the sense of the Faddeev-Popov resolution of identity) that is obtained in our method. Furthermore, we take seriously the analogy with HJ formalism on which the formalism of Chapter 2 is based and the criteria for well-defined gauges discussed in §2.5.5. Nonetheless, one could apply the regularization of the time-of-arrival operator to (3.53), and it is certainly possible that the method described here will require further regularizations in more realistic examples (see also the discussion in §6.3.7).

Chapter 4

Homogeneous Classical and Quantum Cosmology

The simple examples discussed in Chapter 3 are certainly conceptually useful toy models and serve as a first introduction to the method developed in Chapter 2. However, in the interest of progressing towards quantum gravity, it is paramount that we consider quantum cosmology, which is the application of the canonical quantization of the theory of gravitation to the Universe, both in its late-time large-scale structure and in its early stages (cf. Chapter 6). This extrapolation is compelling because the gravitational interaction is predominant at large scales and, as was mentioned in the the **Introduction**, quantum theory appears to be universal. In this way, it is conceivable that the quantum nature of gravitation influences the origin and (relational) evolution of the Universe.

For simplicity, and in order to work with tractable equations, it is customary to perform symmetry reductions [6, 105, 106], which consist in the imposition of a certain group of symmetries at the level of the field equations. The 'reduction' follows from the consideration of invariant fields only. In the case of cosmological models, it is customary to impose homogeneity and, in certain cases, isotropy. We will only consider homogeneous models that obey the 'symmetric criticality principle' [6, 104–106], for which it is possible to apply the symmetry reduction directly at the level of the action. In this way, the critical points of the symmetry-reduced action are in correspondence to the critical points of the original (e.g., Einstein-Hilbert) action. Moreover, the imposition of homogeneity implies that the action becomes mechanical. In this case, one refers to the configuration space of the symmetry-reduced cosmology as 'minisuperspace', and the ensuing theory is a worldline theory of the type considered in Chapters 1 and 2.

Evidently, the quantization of symmetry-reduced models may fail to capture some crucial aspects of the full field theory. However, not only there are circumstances in which the reduction provides a reliable truncation or approximation of the theory (see Chapter 8 of [6], for example), but also the minisuperspace models serve as a fertile training ground to quantum gravity. Indeed, we consider homogeneous quantum cosmology to be a class of toy models of a theory of quantum gravitation, in which the general framework developed in Chapter 2 can be applied so as to illustrate how the definition of quantum relational observables as well as the postulates that were presented can lead to concrete results concerning the relational quantum dynamics of the Universe.[1]

4.1 Singularity avoidance

Before we proceed to the concrete examples of a closed FLRW universe in §4.2 and a Kasner model in §4.3, it is useful to explain how the quantum relational formalism of Chapter 2 can be used to determine whether the classical singularity is resolved in the quantum theory. In the models examined in §4.2 and §4.3, the singularity is reached when the scale factor of universe vanishes.

Let us denote by $\boldsymbol{s}$ the region of configuration space which corresponds to singular geometries. A popular criterion for singularity avoidance is that the solutions $|\Psi\rangle$ to the quantum constraint (WDW) equation should satisfy $\langle \boldsymbol{s}|\Psi\rangle = 0$. This is sometimes called the DeWitt criterion for singularity avoidance (see, for instance, [107]) because DeWitt proposed it as a boundary condition on the solutions to the WDW equation [25]. This criterion is certainly reasonable, but its meaning is unclear if the theory is not equipped with a probabilistic interpretation such as the one proposed in §2.6. Indeed, the criterion is often applied heuristically without a corresponding Hilbert space. For this reason, we suggest a slight modification that we call the 'conditional DeWitt criterion', as we explain below.

4.1.1 The wave function of the universe as relative initial data

Following the discussion in §2.7.1, the on-shell states (solutions to the quantum constraint equation) can be interpreted as invariant extensions of conditional wave functions, which are the relative initial data for the relational quantum evolution. In the case of cosmological models, a choice of on-shell state is usually called a 'wave function of universe'. As the physical Hilbert space is not trivial, there are many possible choices of on-shell states and, therefore, the wave function of the universe is not uniquely determined. For this reason, various proposals for boundary conditions have been put forth (see [6] for an overview).

We take a different view. According to §2.7.1, we can see the multitude of on-shell states as possible choices of relative initial data, each of which defines a different quantum evolution in the generalized reference frame adopted by an observer. Thus, it is the task of observers to determine what initial conditions should be chosen so as to describe the quantum universe they record with their generalized clocks and rods.

[1] This Chapter is based on [30, 31].

If the wave function of universe is seen as the relative initial data for the evolution of our universe, we are led to the question: what choice of initial data implies that there is no singularity from the perspective of a hypothetical observer in the early Universe? In other words, if the hypothetical observer uses some physical field as a generalized clock, is there an instant in which the scale factor vanishes?

To answer the above questions, we suggest that, in analogy to the conventional DeWitt criterion, one should impose that conditional probabilities vanish in $\boldsymbol{s}$; i.e., $p_\Psi(\boldsymbol{s}|\chi = s) = 0$, where χ is a generalized clock. We refer to this imposition as the conditional DeWitt criterion, and we consider that it is a completion of the conventional one. Clearly, the validity of this criterion rests on the assumption that Born rule is applicable to the induced overlap of on-shell states. In what follows, we will examine how this criterion can be used with the formalism of Chapter 2 in concrete examples.

4.2 Closed FLRW model

An instructive example is the model of a closed FLRW universe.[2] The simplest matter field that can be considered in this case is a minimally coupled, homogeneous and massless scalar field. As is well-known and we will see in what follows, the model exhibits a classical "recollapse", in the sense that the scale factor initially increases, reaches a maximum, and subsequently decreases. The quantization of the model was discussed by Kiefer in [108], where the behavior of wave packets of solutions to the quantum constraint equation was analyzed. However, the quantum observables and the physical Hilbert space were not defined. A general investigation of the definition of quantum observables and the induced inner product in recollapsing universes was carried out by Marolf in [109]. Our work differs from [109] mainly in two ways. First, we establish a connection to conditional probabilities (and relative initial data), which were not discussed in [109]. Second, as was mentioned in footnote 16 in Chapter 2, the definition of quantum observables in [109] did not yield the Faddeev-Popov resolution of the identity. In contrast, the identity $\mathcal{O}[1|\chi = s] = 1$ is a defining feature of our formalism. Thus, it is worthwhile to revisit this FLRW model in order to illustrate how the formalism presented here can reproduce the quantum observables for a recollapsing universe, and how their dynamics is connected to conditional probabilities.

4.2.1 Classical theory

The dynamics is defined by the action [6]

$$S = S_{\mathcal{M}} + S_{\partial\mathcal{M}} \ , \tag{4.1}$$

[2] A flat FLRW model will be discussed in Chapter 6 as the background on which cosmological perturbations are defined.

$$S_{\mathcal{M}} = \int_{\mathcal{M}} \mathrm{d}^4x\sqrt{-g}\left[\frac{1}{2\kappa}R - \frac{1}{2}\left(\nabla\phi\right)^2\right] \ , \tag{4.2}$$

$$S_{\partial\mathcal{M}} = -\frac{1}{\kappa}\int_{\partial\mathcal{M}} \mathrm{d}^3x\sqrt{h}\ K \ . \tag{4.3}$$

Here, $\mathcal{M}$ is a region of spacetime, $\kappa = 8\pi G/c^4$, and R is the Ricci scalar. Furthermore, the determinant of the induced metric on the boundary $\partial\mathcal{M}$ is denoted by h, whereas the trace of the extrinsic curvature of the boundary is K.

Given the line element on $\mathbb{S}^3$, $\mathrm{d}\Omega_3^2 = \mathrm{d}\chi^2 + \sin^2\chi\left(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\varphi^2\right)$, the line element for the closed FLRW model reads

$$\mathrm{d}s^2 = -N^2(\tau)\mathrm{d}\tau^2 + a^2(\tau)\mathrm{d}\Omega_3^2 \ , \tag{4.4}$$

and it leads to the equalities [6]

$$\sqrt{-g} = |N|a^3\sin^2\chi\sin\theta \ , \tag{4.5}$$

$$R = \frac{6}{N^2}\left[\frac{\ddot{a}}{a} - \frac{\dot{a}\dot{N}}{aN} + \left(\frac{\dot{a}}{a}\right)^2\right] + \frac{6}{a^2} \ , \tag{4.6}$$

$$K = \frac{3\dot{a}}{aN} \ . \tag{4.7}$$

For convenience, we assume that $N(\tau) > 0$. We can then integrate the first term in (4.6) to obtain the symmetry-reduced action

$$S = 2\pi^2\int_{\tau_0}^{\tau_1}\mathrm{d}\tau\left(-3\frac{a\dot{a}^2}{\kappa N} + \frac{3Na}{\kappa} + \frac{a^3}{2}\frac{\dot{\phi}^2}{N}\right) \ . \tag{4.8}$$

We can bring (4.8) to simpler form if we work with units in which $6\pi^2/\kappa = 1/2$, and we consider the redefinitions

$$\begin{aligned} a(\tau) &= \mathrm{e}^{\alpha(\tau)} \ , \\ N(\tau) &= \mathrm{e}^{3\alpha(\tau)}e(\tau) \ , \\ \phi(\tau) &\to \frac{1}{\sqrt{2}\pi}\phi(\tau) \ . \end{aligned} \tag{4.9}$$

Due to (4.9), we can rewrite (4.8) as

$$\begin{aligned} S &= \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \left(-\frac{\dot{\alpha}^2}{2e} + \frac{\dot{\phi}^2}{2e} + \frac{e}{2}\mathrm{e}^{4\alpha} \right) \\ &= \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \left(p_\alpha \dot{\alpha} + p_\phi \dot{\phi} - e(\tau) C \right) \ , \end{aligned} \tag{4.10}$$

which is of the form (1.40). The constraint is

$$C = -\frac{p_\alpha^2}{2} + \frac{p_\phi^2}{2} - \frac{\mathrm{e}^{4\alpha}}{2} \ , \tag{4.11}$$

and the field equations read

$$\begin{aligned} &\dot{\alpha} = -e(\tau) p_\alpha \ , \ \dot{p}_\alpha = 2e(\tau)\mathrm{e}^{4\alpha} \ , \\ &\dot{\phi} = e(\tau) p_\phi \ , \ \dot{p}_\phi = 0 \ , \\ &0 = -\frac{p_\alpha^2}{2} + \frac{p_\phi^2}{2} - \frac{\mathrm{e}^{4\alpha}}{2} \ . \end{aligned} \tag{4.12}$$

These equations can be solved relationally, i.e., by expressing the dynamics in terms of a generalized clock. By choosing $\phi(\tau)$ as the clock, the system (4.12) becomes

$$\begin{aligned} \dot{\alpha} = -\frac{p_\alpha}{p_\phi}\dot{\phi} \ , \ \dot{p}_\alpha &= \frac{2\mathrm{e}^{4\alpha}}{p_\phi}\dot{\phi} \ , \\ p_\phi = \sigma\sqrt{p_\alpha^2 + \mathrm{e}^{4\alpha}} &\equiv \sigma |k| \ , \end{aligned} \tag{4.13}$$

for an arbitrary initial choice of τ, and with $\sigma = \pm 1$. The symbol k in the last equation of (4.13) is a constant of integration. We can solve (4.13) in terms of the generalized clock $\phi(\tau)$ to find

$$\begin{aligned} a^2(\tau) &= \frac{|k|}{\cosh\left[2\sigma(\phi(\tau) - s) + \operatorname{arctanh}\left(\frac{p_\alpha|_{\phi(\tau)=s}}{|k|}\right)\right]} \ , \\ p_\alpha(\tau) &= |k| \tanh\left[2\sigma(\phi(\tau) - s) + \operatorname{arctanh}\left(\frac{p_\alpha|_{\phi(\tau)=s}}{|k|}\right)\right] \ . \end{aligned} \tag{4.14}$$

Notice that $|k|$ can be written in terms of the relative initial data

$$|k| = \sqrt{p_\alpha^2|_{\phi(\tau)=s} + a^4|_{\phi(\tau)=s}} \ ,$$

due to the last equation in (4.13). The values $p_\alpha^2\big|_{\phi(\tau)=s}$ and $\alpha\big|_{\phi(\tau)=s}$ can be seen as local coordinates in the reduced phase space (cf. §1.9.2), and they completely determine the solution (4.14). If we invert (4.14), we find expressions for $p_\alpha^2\big|_{\phi(\tau)=s}$ and $\alpha\big|_{\phi(\tau)=s}$ in terms of the variables $\alpha(\tau), \phi(\tau), p_\alpha(\tau)$ and $p_\phi(\tau)$ in an arbitrary worldline coordinate. These expressions are invariant extensions (relational observables). For instance, the relational observable associated with the square of the scale factor reads

$$\mathcal{O}[a^2|\phi = s] := a^2\big|_{\phi(\tau)=s} = \frac{|k|}{\cosh\left[2\sigma(s-\phi(\tau)) + \operatorname{arctanh}\left(\frac{p_\alpha(\tau)}{|k|}\right)\right]} \ , \tag{4.15}$$

and one can readily verify that it is a worldline-diffeomorphism invariant (for a fixed value of s). Indeed, as the on-shell identity

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left[2\sigma(s-\phi(\tau)) + \operatorname{arctanh}\left(\frac{p_\alpha(\tau)}{|k|}\right)\right] = 0 \tag{4.16}$$

holds due to (4.13), we obtain the transformation [cf. (1.17)]

$$\delta_{\epsilon(\tau)}\ a^2\big|_{\phi(\tau)=s} = \epsilon(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}\ a^2\big|_{\phi(\tau)=s} = 0 \ .$$

From (1.89), we know that we can write (4.15) as the integral formula

$$\begin{aligned}\mathcal{O}[a^2|\phi = s] &= \Delta_\phi \int_{-\infty}^{\infty} \mathrm{d}\tau\ \delta(\phi(\tau)-s)a^2(\tau) \\ &=: \frac{\int_{-\infty}^{\infty}\mathrm{d}\tau\ \delta(\phi(\tau)-s)a^2(\tau)}{\int_{-\infty}^{\infty}\mathrm{d}\tau\ \delta(\phi(\tau)-s)} \ .\end{aligned} \tag{4.17}$$

An invariant expression similar to (4.15) is found for $p_\alpha\big|_{\phi(\tau)=s}$, but it will not be needed. Furthermore, as $\phi(\tau)$ is conjugate to the invariant p_ϕ, we can use the formalism of §2.5.2 to write the evolution of (4.15) in terms of the auxiliary phase-space Poisson brackets,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\ a^2\big|_{\phi(\tau)=s} &= -\frac{\partial}{\partial\phi(\tau)}\ a^2\big|_{\phi(\tau)=s} \\ &= \left\{p_\phi, a^2\big|_{\phi(\tau)=s}\right\} \ .\end{aligned} \tag{4.18}$$

In §4.2.3, we show that the quantum relational observables satisfy the relational Heisenberg equation that is the quantum counterpart of (4.18).

Finally, if we evaluate (4.15) for different values of s, we obtain

$$a^2\big|_{\phi=s} = \frac{|k|}{\cosh\left[2\sigma(s-s_0) + \operatorname{arccosh}\left(\frac{|k|}{a^2|_{\phi=s_0}}\right)\right]} \ , \tag{4.19}$$

which expresses the evolution in terms of the local coordinates in the reduced phase-space; i.e., the dynamics with respect to s is written solely in terms of the relational observables. Incidentally, it is clear from (4.19) that the universe expands until the scale factor reaches a maximum value, after which the universe contracts. This signals that the classical universe recollapses.

4.2.2 Quantum theory I. The physical Hilbert space

The canonical quantization of (4.11) leads to the operator

$$\hat{C} := -\frac{\hat{p}_\alpha^2}{2} + \frac{\hat{p}_\phi^2}{2} - \frac{\mathrm{e}^{4\hat{\alpha}}}{2} \ , \tag{4.20}$$

which acts as a symmetric operator in the auxiliary Hilbert space $L^2(\mathbb{R}^2, \mathrm{d}\alpha\mathrm{d}\phi)$. Following Chapter 2, the induced inner product and the physical Hilbert space can be defined from the analysis of the spectrum of $\hat{C}$. Let us then examine the eigenvalue equation

$$\left(\frac{\hbar^2}{2}\frac{\partial^2}{\partial\alpha^2} - \frac{\hbar^2}{2}\frac{\partial^2}{\partial\phi^2} - \frac{\mathrm{e}^{4\alpha}}{2}\right)\Psi(\alpha,\phi) = E\Psi(\alpha,\phi) \ . \tag{4.21}$$

We will impose the boundary condition $\lim_{\alpha\to\infty}\Psi_{E,\sigma,k}(\alpha,\phi) = 0$. Moreover, the eigenstates can be expressed in terms of modified Bessel functions, which we denote by $K_{\mathrm{i}\nu}(x)$. Below, we will use the identities [110]

$$\overline{K_{\mathrm{i}\nu}(x)} = K_{-\mathrm{i}\nu}(x) = K_{\mathrm{i}\nu}(x) \ , \tag{4.22}$$

$$\int_{\mathbb{R}} \mathrm{d}\alpha K_{\mathrm{i}\nu'}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) K_{\mathrm{i}\nu}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) = \frac{\pi^2\delta(|\nu|-|\nu'|)}{4\nu\sinh(\pi\nu)}, \tag{4.23}$$

$$K_{\mathrm{i}\nu}(x) = \frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}y\ \mathrm{e}^{-x\cosh y}\cos(\nu y) \ . \tag{4.24}$$

If $E \geq 0$, we set $E = \frac{\lambda^2}{2}$, and the eigenstates read

$$\begin{aligned}\langle\alpha,\phi|E,\sigma,k\rangle &:= \Psi_{E,\sigma,k}(\alpha,\phi) \\ &= \exp\left(\frac{\mathrm{i}}{\hbar}\sigma\sqrt{k^2+\lambda^2}\phi\right) K_{\frac{\mathrm{i}k}{2\hbar}}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) \ ,\end{aligned} \tag{4.25}$$

where $\sigma = \pm 1$. Similarly, if $E \leq 0$, we find

$$\langle \alpha, \phi | E, \sigma, k \rangle := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma |k| \phi} K_{\mathrm{i}\nu(\lambda,k)}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) \ , \tag{4.26}$$

where $E = -\frac{\lambda^2}{2}$ and $\nu(\lambda, k) := \sqrt{k^2+\lambda^2}/(2\hbar)$. The auxiliary inner product of the eigenstates is

$$\langle E', \sigma', k' | E, \sigma, k \rangle = \delta\left(E' - E\right) \big(E, \sigma', k' | E, \sigma, k\big) \ , \tag{4.27}$$

where

$$\big(E, \sigma', k' | E, \sigma, k\big) = \begin{cases} \frac{2\pi^3\hbar^3\sqrt{k^2+\lambda^2}}{k \sinh\left(\frac{\pi k}{2\hbar}\right)} \delta_{\sigma',\sigma}\delta(|k'| - |k|) & \text{for } E', E \geq 0 \ , \\ \frac{2\pi^3\hbar^3}{\sinh\left(\frac{\pi\sqrt{k^2+\lambda^2}}{2\hbar}\right)} \delta_{\sigma',\sigma}\delta(|k'| - |k|) & \text{for } E', E \leq 0 \ , \end{cases} \tag{4.28}$$

due to (4.22) and (4.23). In this way, we can normalize the on-shell states

$$|\sigma, k) := \mathcal{N}(k) \, |E = 0, \sigma, k\rangle \tag{4.29}$$

according to

$$\mathcal{N}(k) := \left[\frac{\sinh\left(\frac{\pi|k|}{2\hbar}\right)}{4\pi^3\hbar^3}\right]^{\frac{1}{2}} \ . \tag{4.30}$$

Indeed, if we take the limit in which $\lambda \to 0$ in (4.28), we find the induced inner product

$$\big(\sigma', k' | \sigma, k\big) = \frac{1}{2}\delta_{\sigma',\sigma}\delta(|k'| - |k|) \ . \tag{4.31}$$

A superposition of (4.29) is said to be a 'normalizable on-shell state' if it is square-integrable in the induced inner product. The physical Hilbert space $\mathcal{H}_{\text{phys}}$ is the vector space of normalizable on-shell states equipped with $(\cdot|\cdot)$. The improper projector

$$\hat{P}_{E=0} := \sum_{\sigma=\pm} \int_{-\infty}^{\infty} \mathrm{d}k \ \ |\sigma, k\rangle \, \langle \sigma, k| \tag{4.32}$$

acts as the identity in the physical Hilbert space [cf. (2.69)].

4.2.3 Quantum theory II. Relational observables

The quantum counterpart of (4.15) can be constructed using the formalism of §2.5.2 because the generalized clock ϕ is conjugate to an invariant. To this end, we consider the commuting invariants $\hat{p}_\phi$ and $\hat{C}_\alpha = \frac{\hat{p}_\phi^2}{2} - \hat{C}$, where $\hat{C}_\alpha := \hat{p}_\alpha^2/2 + \exp(4\alpha)/2$. An orthonormal system of simultaneous eigenstates is defined by the relations

$$\begin{aligned} \hat{p}_\phi \left|k, p_\phi\right\rangle &= p_\phi \left|k, p_\phi\right\rangle \ , \\ \hat{C}_\alpha \left|k, p_\phi\right\rangle &= \frac{k^2}{2} \left|k, p_\phi\right\rangle \ , \\ \hat{C} \left|k, p_\phi\right\rangle &= \left(\frac{p_\phi^2}{2} - \frac{k^2}{2}\right) \left|k, p_\phi\right\rangle \ , \end{aligned} \tag{4.33}$$

such that

$$\langle \alpha, \phi | k, p_\phi \rangle := |k|^{\frac{1}{2}} \mathcal{N}(k) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} p_\phi \phi} K_{\frac{\mathrm{i}k}{2\hbar}} \left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) \ .$$

Equation (4.33) leads to [cf. (2.52), (2.54) and (2.57)]

$$\begin{aligned} p_\phi &= -H_\phi^\sigma = \sigma |k| \ (\sigma = \pm 1) \ , \\ |\sigma, k\rangle &= |k|^{-\frac{1}{2}} \left|k, p_\phi\right\rangle_{p_\phi = \sigma |k|} \ , \end{aligned} \tag{4.34}$$

where $|\sigma, k\rangle$ are given in (4.29). The Faddeev-Popov operator is straightforwardly computed [cf. (2.66)],

$$\hat{\Omega}_\phi^\sigma := \int_{\mathbb{R}} \mathrm{d}k \ |k|^{\frac{1}{2}} \left|\sigma, k\right\rangle \left\langle \sigma, k\right| \ , \tag{4.35}$$

and observables can defined as

$$\hat{\mathcal{O}}[f(\alpha)|\phi = s] := \sum_{\sigma = \pm} \int_{\mathbb{R}} \mathrm{d}\alpha f(\alpha) \left|\sigma, \alpha; s\right\rangle \left\langle \sigma, \alpha; s\right| \ , \tag{4.36}$$

with [cf. (2.90)]

$$|\sigma, \alpha; s\rangle := \sqrt{2\pi\hbar} \hat{\Omega}_\phi^\sigma \left|\alpha, \phi = s\right\rangle \ . \tag{4.37}$$

Notice that, due to (4.29) and (4.35), we can rewrite (4.37) as

$$\left(\sigma', k' | \sigma, \alpha; s\right) = \sqrt{2\pi\hbar} \delta_{\sigma', \sigma} \mathcal{N}(k') K_{\frac{\mathrm{i}k'}{2\hbar}} \left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) |k'|^{\frac{1}{2}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \sigma' |k'| s} \ . \tag{4.38}$$

The Faddeev-Popov resolution of the identity requires that $\hat{\mathcal{O}}[1|\phi = s]$ coincides with the identity in the physical Hilbert space [cf. (4.32)], and it means that the states $|\sigma, \alpha; s\rangle$ form a complete system in $\mathcal{H}_{\text{phys}}$. This can be verified if we use (4.23), (4.30), and (4.38) to write

$$\begin{aligned}\left(\sigma', k' \left|\hat{\mathcal{O}}[1|\phi = s]\right| \sigma, k\right) &= \sum_{\sigma''=\pm} \int_{\mathbb{R}} \mathrm{d}\alpha \left(\sigma', k'|\sigma'', \alpha; s\right) \left(\sigma'', \alpha; s|\sigma, k\right) \\ &= \frac{1}{2}\delta_{\sigma',\sigma}\delta(|k'| - |k|) \\ &= (\sigma', k'|\sigma, k) \ ,\end{aligned} \tag{4.39}$$

which coincides with (4.31). Furthermore, the dynamics of the observables (4.36) is also encoded in the states $|\sigma, \alpha; s\rangle$. Due to (4.25), (4.29), and (4.38), we obtain

$$\begin{aligned}\left(\sigma', k' \left|\mathrm{i}\hbar\frac{\partial}{\partial s}\right| \sigma, \alpha; s\right) &= \sigma'|k'| \left(\sigma', k'|\sigma, \alpha; s\right) \\ &= \left(\sigma', k' \left|\hat{p}_\phi\right| \sigma, \alpha; s\right) \ ,\end{aligned} \tag{4.40}$$

such that the observables (4.36) satisfy the Heisenberg equation [cf. (2.86)]

$$\mathrm{i}\hbar\frac{\partial}{\partial s}\hat{\mathcal{O}}[f(\alpha)|\phi = s] = \left[\hat{p}_\phi, \hat{\mathcal{O}}[f(\alpha)|\phi = s]\right] \ . \tag{4.41}$$

If we set $f(\alpha) = \mathrm{e}^{2\alpha}$, then (4.41) is the quantum counterpart of (4.18). The operator $-\hat{p}_\phi$ serves as a physical Hamiltonian and determines a unitary evolution in the physical Hilbert space, since it is an invariant that is also self-adjoint with respect to the auxiliary inner product.

4.2.4 Quantum theory III. Relational quantum dynamics

Let us illustrate how the relational quantum dynamics of this model universe may be understood in terms of the gauge-fixed propagation of relative initial data (cf. §2.7.1). For simplicity, we consider the conditional wave function

$$\langle\alpha, \phi = s_0|\psi\rangle = \psi(\alpha, s_0) = \int_{\mathbb{R}} \mathrm{d}k \ \psi(k, s_0) K_{\frac{\mathrm{i}k}{2\hbar}}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) \tag{4.42}$$

as the relative initial data at $\phi = s_0$. We assume that $\psi(k, s_0)$ is even in k. From (2.116) and (2.121), we can compute the σ-sector invariant extension of (4.42) by using the

σ-sector gauge-fixed propagator $(\sigma,\alpha;\phi|\sigma,\alpha_0;s_0)$,

$$\langle\alpha,\phi|\Psi_\sigma\rangle := \int_{\mathbb{R}} \mathrm{d}\alpha_0\ (\sigma,\alpha;\phi|\sigma,\alpha_0;s_0)\psi(\alpha_0)\ , \tag{4.43}$$

Notice that the useful formula

$$\begin{aligned}\frac{1}{2}\sum_\sigma(\sigma,\alpha;\phi|\sigma,\alpha_0;s_0) &:= \pi\hbar\sum_\sigma\left\langle\alpha,\phi\left|\hat{\Omega}^\sigma_\phi\bullet\hat{\Omega}^\sigma_\phi\right|\alpha_0,s_0\right\rangle\\ &= \pi\hbar\left\langle\alpha,\phi\left||\hat{p}_\phi|\hat{P}_{E=0}\right|\alpha_0,s_0\right\rangle\\ &= 2\pi\hbar\int_{\mathbb{R}}\mathrm{d}k\ \mathcal{N}^2|k|\cos\left[\frac{k}{\hbar}(\phi-s_0)\right]K_{\frac{\mathrm{i}k}{2\hbar}}(x)K_{\frac{\mathrm{i}k}{2\hbar}}(x_0)\ ,\end{aligned} \tag{4.44}$$

where $x\equiv\exp(2\alpha)/(2\hbar)$ and $x_0\equiv\exp(2\alpha_0)/(2\hbar)$, suggests that it is convenient to consider the state $|\Psi\rangle := \sum_\sigma|\Psi_\sigma\rangle/2$. Its invariant extension is an on-shell state [i.e., a solution to (4.20)] that coincides with (4.42) if $\phi=s_0$, and it reads

$$\langle\alpha,\phi|\Psi\rangle\equiv\Psi(\alpha,\phi)=\int_{\mathbb{R}}\mathrm{d}k\ \psi(k)\cos\left[\frac{k}{\hbar}(\phi-s_0)\right]K_{\frac{\mathrm{i}k}{2\hbar}}\left(\frac{\mathrm{e}^{2\alpha}}{2\hbar}\right) \tag{4.45}$$

due to (4.23), (4.42), and (4.44). For concreteness, let us set

$$\psi(k)=\frac{k}{\hbar}\sin\left(\frac{k}{\hbar}c_0\right)\ , \tag{4.46}$$

with $c_0\in\mathbb{R}$. This corresponds to the initial data [cf. (4.42)]

$$\psi(\alpha,s_0)=2\pi\mathrm{e}^{2\alpha}\sinh(2c_0)\exp\left[-\frac{\mathrm{e}^{2\alpha}}{2\hbar}\cosh(2c_0)\right]\ , \tag{4.47}$$

the invariant extension of which is

$$\Psi(\alpha,\phi)=-\pi\hbar\sum_{\sigma=\pm}\frac{\partial}{\partial c_0}\exp\left\{-\frac{\mathrm{e}^{2\alpha}}{2\hbar}\cosh\left[2\sigma\left(\phi-s_0\right)+2c_0\right]\right\} \tag{4.48}$$

due to (4.24) and (4.45). Each term in the sum in (4.48) is a conditional probability amplitude in a definite σ-sector for an arbitrary value $\phi=s$. Each of these amplitudes defines a conditional exponential distribution of a^2 with mean value

$$a^2\big|_{\mathrm{mean}}=\frac{2\hbar}{\cosh\left[2\sigma\left(s-s_0\right)+2c_0\right]}\ . \tag{4.49}$$

Notice that (4.49) is analogous to the classical solution (4.19), and it also leads to a 'mean recollapse' given by the condition $\lim_{s\to\pm\infty} a^2\big|_{\text{mean}} = 0$. Nevertheless, this does not imply that the singularity is still present. According to the conditional DeWitt criterion, the singularity is removed because the state (4.48) assigns zero conditional probabilities to the classical singularity,

$$\lim_{\alpha\to\pm\infty} p_\Psi(\alpha|\phi = s) = 0 \ . \tag{4.50}$$

In other words, given a certain observed value of the scalar field, the probability that the scale factor vanishes is zero.

4.3 The Kasner model

One of the most elementary yet instructive models of homogeneous quantum cosmology is the vacuum Bianchi I (Kasner) model, which is the simplest anisotropic cosmology. The reader is referred to [107, 111, 112] and references therein for a comprehensive overview and further details regarding anisotropic cosmologies. Here, we examine this example as another application of our method of construction of relational observables and, in particular, as another instance of the conditional DeWitt criterion for singularity avoidance.

4.3.1 Classical theory

To define the Bianchi I model, we start with the symmetry-reduced line element

$$\mathrm{d}s^2 = -N^2\mathrm{d}\tau^2 + a_x^2\mathrm{d}x^2 + a_y^2\mathrm{d}y^2 + a_z^2\mathrm{d}z^2 \ . \tag{4.51}$$

For convenience, we choose to work with the 'Misner variables' α, β_+, β_-, which are defined as

$$\begin{aligned} a_x &= \mathrm{e}^{\alpha+\beta_+ +\sqrt{3}\beta_-} \ , \\ a_y &= \mathrm{e}^{\alpha+\beta_+ -\sqrt{3}\beta_-} \ , \\ a_z &= \mathrm{e}^{\alpha-2\beta_+} \ . \end{aligned} \tag{4.52}$$

Notice that α, β_+, β_- are worldline scalars; i.e., we obtain $\delta_{\epsilon(\tau)}\alpha = \epsilon(\tau)\mathrm{d}\alpha/\mathrm{d}\tau$, and similarly for β_+ and β_-, for diffeomorphisms generated by a vector field $V = v(\tau)\mathrm{d}/\mathrm{d}\tau$ [cf. (1.17)]. In terms of the Misner variables, the scale factor reads $(a_x a_y a_z)^{\frac{1}{3}} = e^\alpha$.

In this section, we work with units in which $3c^6 V_0/(4\pi G) = 1$ [107]. After the symmetry reduction, the Einstein-Hilbert action then acquires the simple form [cf. (1.10)]

$$S = \frac{1}{2}\int d\tau \, \frac{e^{3\alpha}}{N}\left(-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2\right) \ . \tag{4.53}$$

The canonical theory is defined by the usual Legendre transformation [cf. §1.3.1]. The total Hamiltonian reads[3]

$$H_T = \frac{N e^{-3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2\right) \ , \tag{4.54}$$

where the momenta conjugate to the Misner variables are also worldline scalars. Without loss of generality, we can redefine the arbitrary lapse function as $N(\tau) = e^{3\alpha(\tau)}\omega(\tau)$, such that $\omega(\tau)$ plays the role of the einbein [cf. (1.40)]. In this way, the constraint is $C = -p_\alpha^2/2 + p_+^2/2 + p_-^2/2$, which coincides with the limit $m \to 0$ of the mass-shell constraint of a free relativistic particle in a $(2+1)$-dimensional Minkowski spacetime. From the total Hamiltonian (4.54) and the field equations (1.29), it is straightforward to find the trajectories in terms of proper time $\eta = \int d\tau \ \omega(\tau)$ [cf. (1.2)],

$$\begin{aligned} \alpha(\eta) &= \alpha - p_\alpha \eta \ , \ p_\alpha(\eta) = p_\alpha \ , \\ \beta_\pm(\eta) &= \beta_\pm + p_\pm \eta \ , \ p_\pm(\eta) = p_\pm \ . \end{aligned} \tag{4.55}$$

In order to illustrate the discussion about singularity avoidance (cf. §4.1) in the quantum theory, let us consider the relational observable associated with the scale factor in the gauge defined by the generalized clock $\beta_+(\eta)/p_+(\eta)$. We can write this observable in terms of the proper-time parametrization,

$$\mathcal{O}[e^\alpha|\beta_+ - p_+ s = 0] := \int_{-\infty}^{\infty} d\eta \ |p_+| \, \delta\left(\beta_+(\eta) - p_+(\eta)s\right) e^{\alpha(\eta)} \ . \tag{4.56}$$

Due to (4.55), we find

$$\mathcal{O}[e^\alpha|\beta_+ - p_+ s = 0] = \exp\left(\alpha + \frac{p_\alpha}{p_+}\beta_+ - p_\alpha s\right) \ . \tag{4.57}$$

It is straightforward to verify that (4.57) Poisson-commutes with C. We note that the singularity is reached when the scale factor is zero, which corresponds to the limit $p_\alpha s \to \infty$ in (4.57).

[3] As in Chapter 5, we eliminate the primary constraint $p_e = 0$ for simplicity, and we work with the partially gauge-fixed theory discussed in §1.3.2. Here, the arbitrariness of the multiplier ω in (1.38) corresponds to the arbitrariness in the choice of lapse function.

4.3.2 Quantum theory

The quantum theory can be constructed following the general formalism discussed in Chapter 2. The particular form of the physical Hilbert space follows from the relativistic particle construction in Chapter 3. Here, our main interest here is to determine how the classical singularity may be removed according to the criteria established in §4.1; i.e., if the relative initial data for the quantum scale factor assign zero probability to $\mathrm{e}^{\alpha} = 0$.

To begin with, we note that the argument of the Dirac delta in (4.56) corresponds to a family of gauge conditions labeled by the value of s. Each member is conjugate to p_+, which is an invariant [cf. (4.55)]. In this way, we can use the results of §2.5.2 to construct the quantum relational observables. Furthermore, a change in the value of s in $\chi(\eta) = \beta_+(\eta) - p_+(\eta)s$ is generated by $\{\cdot, p_+^2/2\}$. For this reason, we can define the states

$$|\chi, \alpha, \beta_-; s\rangle := \int \mathrm{d}p_+ \ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p_+\chi}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p_+^2}{2}s}\,|\alpha, p_+, \beta_-\rangle \ , \tag{4.58}$$

which form an orthonormal system in the auxiliary Hilbert space for a fixed value of s. Following Chapter 3, we can define the eigenstates of the invariant extension of the scale factor in the gauge $\chi = 0$ as

$$|\sigma, \alpha, \beta_-; s\rangle := \sqrt{2\pi\hbar}\sum_{\sigma'=\pm}\hat{P}_{\sigma',m=0}\,|\hat{p}_+|^{\frac{1}{2}}\,\Theta(\sigma\hat{p}_+)\,|\chi = 0, \alpha, \beta_-; s\rangle \ , \tag{4.59}$$

where $\hat{P}_{\sigma',m=0}$ was given in (3.24). From (4.59), one readily finds the physical transition amplitude

$$\begin{aligned}
&\big(\sigma', \alpha', \beta_-'; s'|\sigma, \alpha, \beta_-; s\big)\\
&= \delta_{\sigma',\sigma}\int \frac{\mathrm{d}p_\alpha \mathrm{d}p_- \mathrm{d}p_+}{(2\pi\hbar)^2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{p_+^2}{2}(s'-s)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_\alpha(\alpha'-\alpha)}\\
&\times \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_-(\beta_-'-\beta_-)}\Theta(\sigma p_+)|p_+|\delta\left(-\frac{p_\alpha^2}{2}+\frac{p_+^2}{2}+\frac{p_-^2}{2}\right)\\
&= \delta_{\sigma',\sigma}\int \frac{\mathrm{d}p_\alpha \mathrm{d}p_-}{(2\pi\hbar)^2}\mathrm{e}^{\frac{\mathrm{i}(s'-s)}{2\hbar}\left(p_\alpha^2-p_-^2\right)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_\alpha(\alpha'-\alpha)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_-(\beta_-'-\beta_-)}\\
&= \delta_{\sigma',\sigma}\overline{K}_{(\alpha)}(\alpha', s'; \alpha, s)K_{(-)}(\beta_-', s'; \beta_-, s) \ ,
\end{aligned} \tag{4.60}$$

where we defined the propagators

$$\begin{aligned}
K_{(\alpha)}(\alpha', s'; \alpha, s) &= \left[2\pi\hbar\mathrm{i}(s'-s)\right]^{-\frac{1}{2}}\exp\left(-\frac{(\alpha'-\alpha)^2}{2\mathrm{i}\hbar(s'-s)}\right) \ ,\\
K_{(-)}(\beta_-', s'; \beta_-, s) &= \left[2\pi\hbar\mathrm{i}(s'-s)\right]^{-\frac{1}{2}}\exp\left(-\frac{(\beta_-'-\beta_-)^2}{2\mathrm{i}\hbar(s'-s)}\right) \ .
\end{aligned} \tag{4.61}$$

Notice that (4.61) coincide with nonrelativistic propagators, and (4.60) simplifies to $\delta_{\sigma',\sigma}\delta(\alpha'-\alpha)\delta(\beta_-'-\beta_-)$ in the limit $s'\to s$. The states (4.59) also allows us to define the quantum relational observables [cf. (4.56)]

$$\hat{\mathcal{O}}[f(\alpha,\beta_-)|\chi(s)=0] := \sum_{\sigma=\pm}\int \mathrm{d}\alpha\mathrm{d}\beta_-\ f(\alpha,\beta_-)\,|\sigma,\alpha,\beta_-;s\rangle\,\langle\sigma,\alpha,\beta_-;s|\ , \tag{4.62}$$

such that $\hat{\mathcal{O}}[\mathrm{e}^{\alpha}|\chi(s)=0]$ is the invariant extension of the scale factor.

Let us now discuss a choice of relative initial data. We define the Gaussian wave packet

$$\begin{aligned}
|\psi,\sigma;s\rangle &:= \int \mathrm{d}\alpha\mathrm{d}\beta_-\ \psi_{(\alpha)}(\alpha)\psi_{(-)}(\beta_-)\,|\sigma,\alpha,\beta_-;s\rangle\ ,\\
\psi_{(\alpha)}(\alpha) &:= \left[\pi\mathcal{A}^2\right]^{-\frac{1}{4}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_\alpha^0(\alpha-\alpha_0)}\mathrm{e}^{-\frac{(\alpha-\alpha_0)^2}{2\mathcal{A}^2}}\ ,\\
\psi_{(-)}(\beta_-) &:= \left[\pi\mathcal{B}^2\right]^{-\frac{1}{4}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_-^0(\beta_--\beta_0)}\mathrm{e}^{-\frac{(\beta_--\beta_0)^2}{2\mathcal{B}^2}}\ ,
\end{aligned}$$

for simplicity. It satisfies $(\psi,\sigma';s|\psi,\sigma;s)=\delta_{\sigma',\sigma}$; i.e., it is normalized with respect to the induced inner product. We find the overalp

$$\begin{aligned}
(\sigma',\alpha',\beta_-';s|\psi,\sigma;s=0) &= \delta_{\sigma',\sigma}\left[\int_{-\infty}^{\infty}\mathrm{d}\alpha\ \overline{K}_{(\alpha)}(\alpha',s;\alpha,0)\psi_{(\alpha)}(\alpha)\right]\\
&\quad\times\left[\int_{-\infty}^{\infty}\mathrm{d}\beta_-\ K_{(-)}(\beta_-',s;\beta_-,0)\psi_{(-)}(\beta_-)\right]\\
&=: \delta_{\sigma',\sigma}\psi_{(\alpha)}(\alpha';s)\psi_{(-)}(\beta_-';s)\ ,
\end{aligned}\tag{4.63}$$

from (4.60) and (4.61). In (4.63), we defined

$$\begin{aligned}
&\psi_{(\alpha)}(\alpha;s)\\
&:= \left[\pi^{\frac{1}{2}}\left(\mathcal{A}-\frac{\mathrm{i}\hbar s}{\mathcal{A}}\right)\right]^{-\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_\alpha^0\left(\alpha-\alpha_0+\frac{1}{2}p_\alpha^0 s\right)}\exp\left[-\frac{(\alpha-\alpha_0+p_\alpha^0 s)^2}{2\mathcal{A}^2\left(1-\frac{\mathrm{i}\hbar s}{\mathcal{A}^2}\right)}\right]\ ,
\end{aligned}\tag{4.64}$$

$$\begin{aligned}
&\psi_{(-)}(\beta_-;s)\\
&:= \left[\pi^{\frac{1}{2}}\left(\mathcal{B}+\frac{\mathrm{i}\hbar s}{\mathcal{B}}\right)\right]^{-\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_-^0\left(\beta_--\beta_0-\frac{1}{2}p_-^0 s\right)}\exp\left[-\frac{(\beta_--\beta_0-p_-^0 s)^2}{2\mathcal{B}^2\left(1+\frac{\mathrm{i}\hbar s}{\mathcal{B}^2}\right)}\right]\ ,
\end{aligned}\tag{4.65}$$

for convenience. Following §2.6, the overlap (4.63) leads to the transition probability

$$\left|(\sigma',\alpha',\beta_-';s|\psi,\sigma;s=0)\right|^2 = \delta_{\sigma',\sigma}\left|\psi_{(\alpha)}(\alpha';s)\right|^2\left|\psi_{(-)}(\beta_-';s)\right|^2\ ,$$

which satisfies

$$\lim_{|\alpha'|\to\infty} \left|(\sigma', \alpha', \beta'_-; s|\psi, \sigma; s=0)\right|^2 = 0 \ , \tag{4.66}$$

due to (4.64) and (4.65). Equation (4.66) yields the probability that a transition occurs between the Gaussian relative initial data (at $s = 0$) and the eigenstate of the invariant extension of the scale factor with a vanishing (or diverging) eigenvalue. As this probability is zero, this is an instance of the conditional DeWitt criterion and we interpret it as an avoidance of the singularity by the physical quantum dynamics (of Gaussian wave packets).

Besides this criterion, it is also useful to analyze the behavior of expectation values. First, we note that the relative initial data $|\psi, \sigma; s=0\rangle$ is a "minimum uncertainty wave packet", as it implies [cf. (4.62)]

$$\begin{aligned} \Delta\mathcal{O}[\alpha|\chi(s=0)=0]\Delta p_\alpha &= \frac{\hbar}{2} \ , \\ \Delta\mathcal{O}[\beta_-|\chi(s=0)=0]\Delta p_- &= \frac{\hbar}{2} \ . \end{aligned} \tag{4.67}$$

The symbol Δ denotes the uncertainty of the observables, which is defined as

$$\Delta\mathcal{O} = \left\langle \left(\hat{\mathcal{O}} - \langle\hat{\mathcal{O}}\rangle\right)^2 \right\rangle^{\frac{1}{2}} \ , \tag{4.68}$$

where $\langle\cdot\rangle$ is the average in the induced inner product.

Second, we find the expectation value [cf. (4.62), (4.63)) and (4.64)]

$$\begin{aligned} \left\langle \hat{\mathcal{O}}[\mathrm{e}^\alpha|\chi(s)=0] \right\rangle &= \sum_{\sigma'=\pm} \int \mathrm{d}\alpha \mathrm{d}\beta_- \ \mathrm{e}^\alpha \left|(\psi, \sigma, s=0|\sigma', \alpha, \beta_-; s)\right|^2 \\ &= \int_{-\infty}^{\infty} \mathrm{d}\alpha \ \mathrm{e}^\alpha \ \left|\psi_{(\alpha)}(\alpha; s)\right|^2 \\ &= \exp\left[\alpha_0 - p_\alpha^0 s + \frac{1}{4}\left(\mathcal{A}^2 + \frac{\hbar^2 s^2}{\mathcal{A}^2}\right)\right] \ , \end{aligned} \tag{4.69}$$

which is the quantum counterpart of (4.57). In contrast to the classical value, the expectation (4.69) is different from zero for all values of s, and it leads to a quantum bounce. Indeed, the average scale factor has the minimum value

$$\left\langle \hat{\mathcal{O}}[\mathrm{e}^\alpha|\chi(s)=0] \right\rangle_{\min} = \exp\left[\alpha_0 - \frac{(p_\alpha^0)^2\mathcal{A}^2}{\hbar^2} + \frac{\mathcal{A}^2}{4}\right] \ , \tag{4.70}$$

which is realized when

$$s = s_{\text{bounce}} = \frac{2p_\alpha^0 \mathcal{A}^2}{\hbar^2} \ . \tag{4.71}$$

In this way, the quantum expectation (4.69) provides an alternative evidence that the quantum dynamics, at least for the minimum uncertainty relative initial data, may avoid the classical singularity.

Chapter 5

Weak-Coupling Expansion

If the relational quantum dynamics discussed in Chapter 2 and exemplified in Chapters 3 and 4 is to be applied to the early Universe, we must account for the inclusion of cosmological perturbations, which leads us outside of the scope of the homogeneous models examined in §4.2 and §4.3. In this case, can we still discuss the quantum theory in the relational terms of Chapter 2? The answer is yes.

The inclusion of cosmological perturbations, which will be analyzed in Chapter 6, leads to a description of the early Universe as a Born-Oppenheimer (BO) system, for which a natural separation of the degrees of freedom into "heavy" and "light" variables exists. The dynamics of the heavy fields is related to a certain energy scale $\sqrt{M}$, whereas the light degrees of freedom are restricted to scales $m \ll \sqrt{M}$. This suggests that a perturbative expansion of the field equations in a power series in the ratio m^2/M or, more formally, in $1/M$, is possible. We refer to this procedure as a 'weak-coupling expansion'. In this Chapter, we analyze this expansion for a general BO system, and we examine how the relational quantum dynamics can be understood in terms of the iterative procedure discussed in §2.5.6. A central result is the unitarity of the theory with respect to the physical inner product, which can be related to a quantization of the classical Faddeev-Popov determinant associated with a "heavy" generalized clock. The weak-coupling expansion is a generalization of the expansion in powers of $1/c^2$ that was analyzed in the classical and quantum theories of the relativistic particle (cf. Chapter 3).

Below, we will see how the weak-coupling expansion of a BO system selects a "preferred" class of clocks, which are the possible worldline time variables that describe the trajectories of the heavy variables when the light degrees of freedom are neglected. For this reason, the use of the weak-coupling expansion in the quantum theory of a BO system is sometimes seen as a solution to the problem of time. However, in light of the formalism presented in Chapter 2, we see that this is not the most general solution, but rather a particular case (cf. §2.5.6), since it is conceivable that a relational notion of time is valid beyond the (semi)classical level. In fact, the "preferred" class of clocks selected by the weak-coupling expansion is a generalization of the nonrelativistic limit of a free particle, in which the Newtonian time is selected as a "preferred" orderer of the dynamics.

The application of the weak-coupling expansion to describe cosmological perturbations defines the 'BO approach to quantum cosmology'. It provides a way to go beyond homogeneous quantum cosmology in a perturbative setting. In this cosmological case, the heavy variables often coincide with the homogeneous background associated with the Planck mass, whereas the light variables are the cosmological perturbations associated with energies below the Planck scale (see [62, 98, 113] for further details and [114–116] for applications of the BO approach).

It is worthwhile to emphasize that, despite the fact that the BO approach is a particular instance of a more general relational theory, it is nonetheless important for the phenomenology of quantum gravitation. Indeed, as we will see in Chapter 6, the weak-coupling expansion in cosmology yields corrections to the usual calculations of QFT in a fixed background spacetime. For this reason, the BO approach is of paramount importance to the analysis of quantum-gravitational corrections to phenomena in the early Universe, such as inflation [114–116].

The weak-coupling expansion is developed below in connection to the formalism of Chapter 2, and it does not immediately coincide with the traditional BO approach that is studied in the literature. We dedicate Appendix B to a comparison to the traditional approach, where we also establish the equivalence of both approaches, and we offer a critique of the usual formulation of the concept of 'backreation' in the traditional approach.[1]

5.1 Classical theory

Although the classical description of mechanical BO systems with diffeomorphism invariance is a particular case of the theory presented in Chapter 1, it is instructive to analyze how the weak-coupling expansion is related to a choice of gauge, as this will guide us in the construction and interpretation of the quantum theory. Let us establish our notation and assumptions. We consider that the heavy-sector configuration space is a smooth manifold with an indefinite metric $\mathbf{G}$ and local coordinates $Q^a, a = 1, \dots, n$, whereas the light-sector configuration space is endowed with a positive-definite metric $\mathbf{h}(Q)$ and local coordinates $q^\mu, \mu = 1, \dots, d$. We use the components of $\mathbf{G}$ and its inverse, G_{ab} and G^{ab}, to lower and raise the heavy-sector indices, while $h^{\mu\nu}$ and $h_{\mu\nu}$ raise and lower the light-sector indices. A summation over repeated indices is implied in the formulae below.

[1] This Chapter is based on [62, 98].

The action is taken to be of the form (1.40),[2]

$$S = \int \mathrm{d}\tau \, \left(P_a \dot{Q}^a + p_\mu \dot{q}^\mu - \omega(\tau) C\right) \, , \tag{5.1}$$

where the constraint has the following functional form:

$$\begin{aligned} C &= C_g(Q,P) + C_m(Q;p,q) = 0 \, , \\ C_g(Q,P) &= \frac{1}{2M} G^{ab}(Q) P_a P_b + M V(Q) \, , \\ C_m(Q;p,q) &= \frac{1}{2} h^{\mu\nu}(Q;q) p_\mu p_\nu + V_m(Q;q) \, . \end{aligned} \tag{5.2}$$

The subscripts g and m denote the heavy and light sectors, respectively.[3] The dependence of the light-sector Hamiltonian, $\omega(\tau) C_m(Q;p,q)$, on the heavy variables Q is only parametric. The heavy-sector potential term, $V(Q)$, is assumed to be nonvanishing, whereas the light-sector potential, $V_m(Q;q)$, is a non-negative C^∞-function. The light-sector canonical variables p_μ, q^μ are tacitly associated with an energy scale m such that $m^2 \ll M$.

From (5.1), one finds the field equations

$$\begin{aligned} &\dot{Q}^a \approx \frac{\omega(\tau)}{M} G^{ab}(Q) P_b \, , \; \dot{P}_a \approx -\omega(\tau) \left(\frac{1}{2M} \frac{\partial G^{cd}}{\partial Q^a} P_c P_d + M \frac{\partial V}{\partial Q^a} \right) - \omega(\tau) \frac{\partial C_m}{\partial Q^a} \, , \\ &\dot{q}^\mu \approx \omega(\tau) \frac{\partial C_m}{\partial p_\mu} \, , \; \dot{p}_\mu \approx -\omega(\tau) \frac{\partial C_m}{\partial q^\mu} \, , \\ &C = C_g + C_m \approx 0 \, , \end{aligned} \tag{5.3}$$

which we assume can be (perturbatively) integrated once a complete gauge fixing is chosen (cf. §1.6). However, it is convenient to consider the HJ equation [cf. (1.108)]

$$\frac{1}{2M} G^{ab}(Q) \frac{\partial \mathrm{W}}{\partial Q^a} \frac{\partial \mathrm{W}}{\partial Q^b} + M V(Q) + C_m \left(Q; \frac{\partial \mathrm{W}}{\partial q}, q \right) = 0 \tag{5.4}$$

because, given a solution W for Hamilton's characteristic function, we can work with

[2] In other words, we are working with the partially gauge-fixed theory analyzed in §1.3.2. The primary constraint $p_e = 0$ has thus been eliminated.

[3] We adopt this notation because, in minisuperspace cosmological models (cf. Chapters 4 and 6), the heavy sector usually coincides with the gravitational sector, whereas the light sector is comprised of the matter variables. Nevertheless, other separations of the degrees of freedom are possible [113, 117, 118].

the more compact set of dynamical equations

$$\begin{aligned}\dot{Q}^a &= \frac{\omega(\tau)}{M} G^{ab}(Q) \frac{\partial \mathrm{W}}{\partial Q^b} \ , \\ \dot{q}^\mu &= \omega(\tau) h^{\mu\nu}(Q;q) \frac{\partial \mathrm{W}}{\partial q^\nu} \ ,\end{aligned} \tag{5.5}$$

for a fixed choice of einbein $\omega(\tau)$. Can we find a solution for W? Although it is generally complicated to solve (5.4), we can use the fact that $m^2 \ll M$ to perform a formal perturbative expansion in powers of $1/M$; i.e., we can perform a weak-coupling expansion. As the lowest power of $1/M$ in (5.4) is -1, we make a 'Wentzel-Kramers-Brillouin (WKB)-like' ansatz for Hamilton's characteristic function,

$$\mathrm{W}(Q,q) = M \sum_{n=0}^{\infty} \mathrm{W}_n(Q,q) \frac{1}{M^n} =: M\mathrm{W}_0(Q) + \mathtt{S}(Q;q). \tag{5.6}$$

If we insert (5.6) into (5.4), we can solve for each W_n term perturbatively. In particular, the lowest-order term is a solution to

$$\frac{1}{2} G^{ab}(Q) \frac{\partial \mathrm{W}_0}{\partial Q^a} \frac{\partial \mathrm{W}_0}{\partial Q^b} + V(Q) = 0 \ , \tag{5.7}$$

which is the HJ equation solely for the heavy sector. For this reason, $M\mathrm{W}_0$ may be interpreted as a 'background Hamilton function', which encodes the dynamics of the heavy variables in the absence of the backreaction of the light variables ('no-coupling limit'). We will see that, given a solution $M\mathrm{W}_0$, the dynamics of the higher orders encoded in $\mathtt{S}$ in (5.6) can be understood in terms of the 'background dynamics' defined by $M\mathrm{W}_0$.

5.1.1 The background dynamics

In the no-coupling limit, the dynamics of the heavy variables is dictated by the equations [cf. (5.5)]

$$\dot{Q}^a = \mathcal{N}(\tau) G^{ab} \frac{\partial \mathrm{W}_0}{\partial Q^b} \ , \tag{5.8}$$

where $\mathcal{N}(\tau)$ is the 'background einbein'; i.e., it is a nonvanishing worldline scalar density (with a constant sign). A complete gauge fixing in this limit entails a fixation of $\mathcal{N}(\tau)$. For fixed $\mathcal{N}(\tau) \equiv \mathcal{N}(Q(\tau))$ and $\mathrm{W}_0(Q)$, we assume that it is possible to find a holonomic basis $\left\{\mathbf{B}_1 = \mathcal{N} G^{ab} \partial \mathrm{W}_0 / \partial Q^b, \mathbf{B}_i\right\}, i = 2, \ldots, n$ in the tangent bundle of the heavy-sector configuration space. We also make the simplifying assumption that $\mathbf{B}_1$

is orthogonal to the $\mathbf{B}_i$ vector fields.[4] Then, the normalization of the basis vectors is [cf. (5.7)]

$$\begin{aligned} G_{ab}B_1^a B_1^b &= -2\mathcal{N}^2 V(Q) = \tilde{G}_{11} \ , \\ G_{ab}B_1^a B_i^b &= 0 = \tilde{G}_{1i} \ , \\ G_{ab}B_i^a B_j^b &= \tilde{G}_{ij} \equiv g_{ij} \ . \end{aligned} \tag{5.9}$$

We can subsequently use the integral curves of the basis fields to define new coordinates $x = (x^1, x^i)$ in the heavy-sector configuration space,

$$\begin{aligned} B_1^a &= \mathcal{N} G^{ab} \frac{\partial \mathrm{W}_0}{\partial Q^b} = \frac{\partial Q^a}{\partial x^1} \ , \\ B_i^a &= \frac{\partial Q^a}{\partial x^i} \ . \end{aligned} \tag{5.10}$$

More precisely, this corresponds to a foliation of the heavy-sector configuration space by the level sets of $x^1(Q)$; i.e., $x^1(Q) = s$ is a hypersurface, on which the induced metric has components $g_{ij} = \tilde{G}_{ij}$. The components of its inverse are denoted by g^{ij}. In this way, $x^1(Q)$ plays the role of a background generalized clock.[5] This background clock is more commonly referred to as 'WKB time' [119] because it arises from the WKB-like expansion (5.6).

In what follows, it will be useful to make use of the coordinate transformation (5.10). In particular, we find [cf. (5.7)]

$$\begin{aligned} \frac{\partial \mathrm{W}_0}{\partial x^1} &= \mathcal{N} G^{ab} \frac{\partial \mathrm{W}_0}{\partial Q^a}\frac{\partial \mathrm{W}_0}{\partial Q^b} = -2\mathcal{N} V \ , \\ \frac{\partial \mathrm{W}_0}{\partial x^i} &= B_i^a \frac{\partial \mathrm{W}_0}{\partial Q^a} = 0 \ . \end{aligned} \tag{5.11}$$

Moreover, notice that the determinants of $\mathbf{G}$ and $\tilde{\mathbf{G}}$ are related by $\sqrt{|\tilde{G}|} = \sqrt{|G|} B$, where $B = \det B_A^a$ $(A = 1, \ldots, n)$, and the inverse of B_A^a reads

$$\frac{\partial x^A}{\partial Q^a} = \left(B^{-1}\right)_a^A = \tilde{G}^{AB} G_{ab} B_B^b \ .$$

[4] If $\mathbf{B}_1$ is not orthogonal to $\mathbf{B}_i$, then the components $\tilde{G}_{1i}$ of the metric given in (5.9) will not vanish, and there will be additional terms involving $\tilde{G}_{1i}$ in the subsequent formulae. Nevertheless, the gauge fixing procedure, both at the classical and quantum levels, and our forthcoming conclusions regarding unitarity should not be qualitatively altered by these extra contributions. Moreover, this assumption is also irrelevant to the application of the formalism to the early Universe discussed in Chapter 6.

[5] Notice that the first equation in (5.10) corresponds to the evolution law (5.8).

In this way, we can write the basis vector fields $\partial/\partial Q^a$ in the new basis,[6]

$$
\begin{aligned}
\frac{\partial}{\partial Q^a} &= \left(B^{-1}\right)_a^A \frac{\partial}{\partial x^A} = \tilde{G}^{11} G_{ab} B_1^b \frac{\partial}{\partial x^1} + \tilde{G}^{ij} G_{ab} B_i^b \frac{\partial}{\partial x^j} \\
&= -\frac{1}{2\mathcal{N}V} \frac{\partial \mathrm{W}_0}{\partial Q^a} \frac{\partial}{\partial x^1} + g^{ij} G_{ab} B_i^b \frac{\partial}{\partial x^j} \ .
\end{aligned} \tag{5.12}
$$

5.1.2 WKB time as a classical choice of gauge

As we move away from the no-coupling limit by including higher orders of $1/M$, the HJ equation (5.7) is no longer a suitable description of the dynamics of the heavy variables, as the coupling with the light degrees of freedom is now taken into account. The separation between the background Hamilton function $M\mathrm{W}_0$ and the higher orders encoded in $\mathtt{S}$ in (5.6) can be seen as a canonical transformation, in which the momenta are transformed as follows:

$$
\begin{aligned}
B_A^a P_a = \frac{\partial W}{\partial x^A} &\mapsto \Pi_A = B_A^a P_a - M \frac{\partial \mathrm{W}_0}{\partial x^A} = \frac{\partial \mathtt{S}}{\partial x^A} \ , \ (A = 1, \dots, n) \\
p_\mu = \frac{\partial W}{\partial q^\mu} &\mapsto p_\mu = \frac{\partial \mathtt{S}}{\partial q^\mu} \ .
\end{aligned} \tag{5.13}
$$

If we insert (5.6) into (5.4) and use the coordinates defined in (5.10), we obtain the following equation for $\mathtt{S}(Q; q)$:

$$
\frac{\partial \mathtt{S}}{\partial x^1} + \mathcal{N} C_m + \frac{\mathcal{N}}{M} g^{ij} \frac{\partial \mathtt{S}}{\partial x^i} \frac{\partial \mathtt{S}}{\partial x^j} - \frac{1}{4M\mathcal{N}V} \left(\frac{\partial \mathtt{S}}{\partial x^1} \right)^2 = 0 \ . \tag{5.14}
$$

where we used (5.9) and (5.11). We can solve (5.14) for $\Pi_1 = \partial \mathtt{S}/\partial x^1$ to find

$$
-\Pi_1 := -\frac{\partial \mathtt{S}}{\partial x^1} = -2M\mathcal{N}V \pm 2M\mathcal{N} \sqrt{V \left(V + \frac{1}{M} C_m + \frac{1}{2M^2} g^{ij} \frac{\partial \mathtt{S}}{\partial x^i} \frac{\partial \mathtt{S}}{\partial x^j} \right)} \ . \tag{5.15}
$$

This is an instance of (1.97). Here, the discrete multiplicity σ is given by the choice of positive or negative sign in (5.15). Following the discussion §1.9.2 and §5.1.1, we conclude that (5.15) corresponds to a choice of gauge in which the dynamics of both the heavy variables and the light degrees of freedom is measured with respect to the background clock $x^1(\tau)$. In this way, the (invariant extension of) the right-hand side of (5.15) is the associated physical Hamiltonian. The corresponding fixation of the einbein [cf. (1.63)] is found from the equation $\dot{x}^1 \approx \{x^1, \omega C\} \approx 1$. This corresponds to

[6] In [120], the change of basis (5.12) was also considered in perturbation theory, but the authors of this reference neglected the terms involving $\mathbf{B}_i$.

[cf. (5.5)]

$$\frac{1}{\omega} = \frac{1}{M} G^{ab} \frac{\partial x^1}{\partial Q^a} P_b = \frac{1}{M} \tilde{G}^{11} \frac{\partial \mathrm{W}}{\partial x^1} = \frac{1}{\mathcal{N}} - \frac{\Pi_1}{2M\mathcal{N}^2 V} \ , \tag{5.16}$$

where we used (5.11). We can rewrite (5.16) as

$$\omega = \frac{\mathcal{N}}{1 - \frac{\Pi_1}{2M\mathcal{N}V}} \ . \tag{5.17}$$

5.1.3 Perturbation theory

We can expand the physical Hamiltonian (5.15) and the gauge-fixed einbein (5.17) in powers of $1/M$ to describe the dynamics of the light variables q^μ, p_μ, as well as the heavy fields x^i, in relation to the background clock $x^1 \equiv \chi$. The expansion of the square root in (5.15) yields

$$\begin{aligned} H_\chi^\sigma = &- 2M\mathcal{N}V + \sigma\Bigg(2M\mathcal{N}|V| + \mathcal{N}\mathfrak{v}C_m \\ &- \frac{\mathcal{N}}{4M|V|}C_m^2 + \frac{\mathcal{N}\mathfrak{v}}{2M} g^{ij}\Pi_i\Pi_j\Bigg) + \mathcal{O}\left(\frac{1}{M^2}\right) \ , \end{aligned} \tag{5.18}$$

where we used (5.13), and we denoted the discrete multiplicity of (5.15) by $\sigma = \pm 1$, whereas $\mathfrak{v} := \mathrm{sgn}(V)$. The choice $\sigma = \mathfrak{v}$ leads to the simplification[7]

$$H_\chi^{\mathfrak{v}} = \mathcal{N}C_m - \frac{\mathcal{N}}{4MV}C_m^2 + \frac{\mathcal{N}}{2M} g^{ij}\Pi_i\Pi_j + \mathcal{O}\left(\frac{1}{M^2}\right) \ . \tag{5.19}$$

Incidentally, this is the solution one obtains by solving (5.14) for $\Pi_1 = \partial \mathrm{S}/\partial x^1$ in an iterative fashion. The iterative solution (5.19) is the classical analogue of the solution found in the BO approach in the quantum theory, as we will examine in §5.2. Indeed, Kiefer and Singh have shown that the term proportional to the square of C_m is obtained as one of the correction terms in the quantum theory in [120]. In §5.2, we will see how extra terms with the time derivatives of C_m and V, which were found in [120], arise in quantum formalism we present. Kiefer and Sigh neglected the term proportional to $g^{ij}\Pi_i\Pi_j$ in [120], but it is worthwhile to emphasize that this term appears, already classically, as a consequence of the weak-coupling expansion of the physical Hamiltonian in the formalism presented here.

It is also important to notice that the terms of order $1/M$ in (5.19) originate from the heavy-sector kinetic term $g^{ij}\Pi_i\Pi_j/(2M) - \Pi_1^2/(4\mathcal{N}^2 MV)$ in (5.14). In [178], similar

[7] Clearly, $\mathfrak{v}$ may vary across the heavy-sector configuration space. Thus, the choice $\sigma = \mathfrak{v}$ is warranted only in regions of the configuration space in which $\mathfrak{v}$ is constant.

terms were obtained and were thought of as "corrections" to the dynamics of the light sector with respect to the notion of time provided by the heavy variables. We consider this interpretation to be slightly misleading because the field equations for the light variables [cf. (5.3)] are not changed in their functional form, only the einbein is fixed when one chooses to describe the dynamics relative to the background clock [cf. (5.17)]. The terms of order $1/M$ in (5.19) follow from the formal weak-coupling expansion of the physical Hamiltonian, but it is not completely accurate to interpret them as corrections solely to the dynamics of light variables, as they involve the heavy fields x^i and Π_i, which are coupled to q^μ, p_μ at this order.[8] In this way, we do not interpret (5.6) as a separation of Hamilton's characteristic function into a function for the heavy sector ($M\mathrm{W}_0$) and another for the light sector ($\mathtt{S}$). Rather, Eq. (5.6) can be seen as canonical transformation [cf. (5.13)]. In the same vein, we note that (5.14) is a HJ equation both for the heavy and light degrees of freedom. As we adopt the gauge in which x^1 is the worldline time coordinate, $\mathtt{S}$ can be seen as Hamilton's principal function (cf. §1.10) associated with the reduced phase space comprised of the (invariant extensions of the) fields q^μ, p_μ and x^i. As these fields are coupled, it is not generally possible to regard $\mathtt{S}$ as dictating the dynamics solely of the light variables.

The expansion of the gauge-fixed einbein (5.17) is also of interest. First, recall from (1.78) that ω is equal to the inverse Faddeev-Popov determinant. Let us then use (5.18) to expand (5.16). The result is

$$\frac{1}{\omega} = \frac{\sigma\mathfrak{v}}{\mathcal{N}} + \frac{\sigma C_m}{2M\mathcal{N}|V|} + \mathcal{O}\left(\frac{1}{M^2}\right) , \tag{5.20}$$

which can be inverted to yield

$$\omega = \sigma\mathfrak{v}\mathcal{N} - \frac{\sigma\mathcal{N}C_m}{2M|V|} + \mathcal{O}\left(\frac{1}{M^2}\right) . \tag{5.21}$$

Equations (5.20) and (5.21) are perturbative expressions for the Faddeev-Popov determinant and the gauge-fixed einbein, respectively, for the complete gauge fixing associated with the background clock x^1. For later reference, we also note that the absolute value of the Faddeev-Popov determinant is

$$\frac{1}{|\omega|} = \frac{1}{|\mathcal{N}|}\left(1 + \frac{C_m}{2MV}\right) + \mathcal{O}\left(\frac{1}{M^2}\right) . \tag{5.22}$$

While the lowest order (no-coupling limit) examined in §5.1.1 yields the dynamics

[8] See [98] for a more extensive and detailed discussion of the weak-coupling expansion of the reduced phase-space field equations.

of the heavy variables in the absence of the light degrees of freedom, we find that the next order (M^0) leads to the dynamics of the q^μ, p_μ variables in a fixed background [i.e., for a fixed trajectory of $Q^a(\tau)$]. This can be seen in two ways. First, Eqs. (5.15) and (5.19) lead to

$$-\frac{\partial \mathtt{S}}{\partial x^1} = \mathcal{N} C_m \left(Q; q, \frac{\partial \mathtt{S}}{\partial q} \right) \tag{5.23}$$

at order M^0. This is simply the time-dependent HJ equation for the light variables in the background defined by the trajectory of the $Q^a(\tau)$. Second, using (5.21), the field equations for q^μ and p_μ [cf. (5.3)] can be written as

$$\begin{aligned} \dot{q}^\mu &= \sigma \mathfrak{v} \mathcal{N}(\tau, x^i(\tau)) \frac{\partial}{\partial p_\mu} C_m(\tau, x^i(\tau); p, q) + \mathcal{O}\left(\frac{1}{M}\right) \ , \\ \dot{p}_\mu &= -\sigma \mathfrak{v} \mathcal{N}(\tau, x^i(\tau)) \frac{\partial}{\partial q^\mu} C_m(\tau, x^i(\tau); p, q) + \mathcal{O}\left(\frac{1}{M}\right) \ . \end{aligned} \tag{5.24}$$

These are the equations for the light variables in a fixed background defined by $(\tau, x^i(\tau))$ and the background einbein $\sigma \mathfrak{v} \mathcal{N}(\tau, x^i(\tau))$. We note that (5.24) is compatible with the lowest-order iterative HJ equation (5.23) for $\sigma = \mathfrak{v}$ [cf. (5.19)]. The inclusion of higher orders of $1/M$ includes corrections to the dynamics of q^μ, p_μ and x^i that originate from the physical Hamiltonian associated with the background clock. These corrections have quantum counterparts which may lead to observable signatures. In the next section, we discuss the quantum theory of mechanical BO systems with diffeomorphism invariance, paying close attention to the definition of the inner product and unitarity. In Chapter 6, we apply the method developed here to a model of the early Universe.

5.2 Quantum theory

5.2.1 The auxiliary and physical Hilbert spaces. Conditional probabilities

The quantum theory can be constructed following the general framework expounded in Chapter 2. As explained there, we begin with a choice of auxiliary Hilbert space equipped with an auxiliary inner product $\langle \cdot | \cdot \rangle$, with respect to which the constraint operator is self-adjoint. Clearly, this is related to a certain choice of factor ordering for the quantum counterpart of (5.2). Let us use the Laplace-Beltrami ordering for both sectors, such that the quantum constraint becomes $\hat{C} := \hat{C}_g + \hat{C}_m$, where[9]

$$\hat{C}_g \Psi := -\frac{1}{2M\sqrt{|Gh|}} \frac{\partial}{\partial Q^a} \left(\sqrt{|Gh|} G^{ab} \frac{\partial \Psi}{\partial Q^b} \right) + MV(Q)\Psi \ , \tag{5.25}$$

[9]For simplicity, we set $c = \hbar = 1$ in this Chapter.

$$\hat{C}_m\Psi := -\frac{1}{2\sqrt{h}}\frac{\partial}{\partial q^\mu}\left(\sqrt{h}h^{\mu\nu}\frac{\partial\Psi}{\partial q^\nu}\right) + V_m(Q;q)\Psi \ . \tag{5.26}$$

Notice that the determinant factors in (5.25) include the determinant $h \equiv \det(h_{\mu\nu})$, due to its parametric dependence on Q, in addition to $G \equiv \det(G_{ab})$. The Laplace-Beltrami ordering guarantees that the quantum constraint retains its form under general coordinate transformations in configuration space [22,23].

The heavy-sector Laplace Beltrami operator is

$$\nabla^2 := \frac{1}{\sqrt{|Gh|}}\frac{\partial}{\partial Q^a}\left(\sqrt{|Gh|}G^{ab}\frac{\partial}{\partial Q^b}\right) \ . \tag{5.27}$$

Using (5.25) and (5.27), the quantum constraint can then be written as

$$\hat{C} = -\frac{1}{2M}\nabla^2 + MV(Q) + \hat{C}_m(Q;\hat{p},q) \ . \tag{5.28}$$

This suggests that we adopt the auxiliary inner product

$$\langle\Psi_{(1)}|\Psi_{(2)}\rangle := \int \mathrm{d}Q\mathrm{d}q \ \sqrt{|Gh|}\,\Psi^*_{(1)}(Q,q)\Psi_{(2)}(Q,q) \ , \tag{5.29}$$

where $\mathrm{d}Q \equiv \prod_a \mathrm{d}Q^a$ and $\mathrm{d}q \equiv \prod_\mu \mathrm{d}q^\mu$. Notice that $\hat{C}$ is symmetric with respect to (5.29), and we assume that it is possible to choose a self-adjoint extension. Moreover, the auxiliary inner product (5.29) is invariant under general coordinate transformations in configuration space.

The definitions of the constraint (5.28) and the auxiliary inner product (5.29) determine the auxiliary Hilbert space. In contrast, the physical Hilbert space is the space of superpositions of the solutions to $\hat{C}\Psi = 0$ that are square-integrable with respect to the physical inner product. Here, instead of the induced inner product (2.11), it is simpler to adopt the definition (2.98), which reads

$$\left(\Psi_{(1)}\middle|\Psi_{(2)}\right) := \sum_\sigma \int \mathrm{d}Q\mathrm{d}q \ \left(\hat{\mu}_\sigma^{\frac{1}{2}}\Psi_{(1)}\right)^* |J|\delta(\chi(Q;q)-s)\hat{\mu}_\sigma^{\frac{1}{2}}\Psi_{(2)} \ , \tag{5.30}$$

where, as in (2.98), $\chi(Q;q)$ is a configuration-space function, $J = \partial(\chi,F)/\partial(Q,q)$ is the Jacobian determinant associated with the transformation $(Q,q) \mapsto (\chi,F)$, and σ are the generalized multiplicity sectors. In analogy to the classical theory, in which the iterative solution of the constraint (5.14) leads to only one multiplicity sector, $\sigma = \mathfrak{v}$ [cf. (5.19)], we will also restrict ourselves to a single multiplicity sector in the quantum theory because we will only solve the quantum constraint iteratively. As a matter of notation (and following the analogy to the classical theory), we denote the single multiplicity sector considered by $\sigma = \mathfrak{v}$. Moreover, as we discussed in §2.7 [see (2.112)], the inner product (5.30) (restricted to the $\sigma = \mathfrak{v}$ sector) leads to the definition of conditional probabilities,

$$p_\Psi := \frac{1}{(\Psi\,|\Psi)} \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \Psi \right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \Psi \Big|_{\chi=s} . \tag{5.31}$$

To match the classical theory, we are interested in the gauge in which $\chi(Q; q) = x^1(Q)$; i.e., the worldline time coordinate is defined by the background clock (WKB time). In this way, we find that $F = (x^i, q^\mu)$, and (5.31) corresponds to the probability of observing $F = (x^i, q^\mu)$ given that $x^1 = s$. The measure $\hat{\mu}_{\mathfrak{v}}$ should be defined such that (5.30) is conserved with respect to s and positive-definite. We will determine it for the BO system using the weak-coupling expansion of the constraint equation, and we will establish its relation to the classical gauge-fixed einbein (5.21).

5.2.2 The phase-transformed constraint equation

In order to solve $\hat{C}\Psi = 0$, we resort to a weak-coupling expansion in analogy to the classical theory. We make the ansatz

$$\Psi(Q, q) = \exp\left[\mathrm{i} M \mathcal{W}(Q, q)\right] , \tag{5.32}$$

where $\mathcal{W}(Q, q)$ is a complex function. The quantum counterpart of (5.6) is given by the formal expansion

$$\mathcal{W}(Q, q) = \sum_{n=0}^{\infty} \mathcal{W}_n(Q, q) \frac{1}{M^n} =: \mathcal{W}_0(Q) + \frac{1}{M} \mathsf{S}(Q; q). \tag{5.33}$$

It is useful to rewrite (5.32) as

$$\Psi(Q, q) =: \exp\left[\mathrm{i} M \mathcal{W}_0(Q, q)\right] \psi(Q; q) , \tag{5.34}$$

where

$$\psi(Q; q) := \exp\left[\mathrm{i}\mathsf{S}(Q; q)\right] . \tag{5.35}$$

We call (5.34) 'the minimal BO factorization' or 'ansatz'.[10]. Although it is equivalent to (5.32), it is not, a priori, equal to the traditional BO ansatz that is customarily applied in nuclear and molecular physics [121–123] and that has inspired some applications in quantum cosmology [124–126]. In Appendix B, it is shown that the minimal and traditional BO factorizations are equivalent, and the topics of unitarity and backreaction are also discussed.

We also expand the measure $\hat{\mu}_{\mathfrak{v}}$,

$$\hat{\mu}_{\mathfrak{v}} = \sum_{n=0}^{\infty} \frac{1}{M^n} \hat{\mu}_n \left(Q; \hat{p}, q\right) \ , \tag{5.36}$$

and we will determine the two lowest-order coefficients $\hat{\mu}_n$ $(n = 0, 1)$ in what follows.

If we now insert (5.32) into $\hat{C}\Psi = 0$, we find an infinite number of equations (one for each order of $1/M$). We may also work with (5.34) to extract equations for $\mathcal{W}_0(Q, q)$ and $\psi(Q; q)$. The lowest-order equation (order M^2) reads

$$\frac{1}{2} h^{\mu\nu} \frac{\partial \mathcal{W}_0}{\partial q^\mu} \frac{\partial \mathcal{W}_0}{\partial q^\nu} = 0 \ . \tag{5.37}$$

As $\mathbf{h}$ is assumed to be positive-definite, this implies that $\mathcal{W}_0$ does not depend on the light variables; i.e., $\mathcal{W}_0(Q, q) \equiv \mathcal{W}_0(Q)$. The next order (order M) yields the background HJ equation (5.7) for $\mathcal{W}_0$. In this way, we can choose $\mathcal{W}_0$ to be real and identify $\mathcal{W}_0(Q) = \mathrm{W}_0(Q)$, such that the change of coordinates discussed in §5.1.1 can be applied. The subsequent orders yield an equation for $\psi(Q; q)$,

$$\mathrm{i} G^{ab}(Q) \frac{\partial \mathrm{W}_0}{\partial Q^a} \frac{\partial \psi}{\partial Q^b} = \left[\hat{C}_m(Q; \hat{p}, q) - \frac{\mathrm{i}}{2} \nabla^2 \mathrm{W}_0\right] \psi - \frac{1}{2M} \nabla^2 \psi \ . \tag{5.38}$$

For a given $\mathcal{W}_0 = \mathrm{W}_0$, we can regard (5.34) as a phase transformation, just as (5.6) is seen as a canonical transformation in the classical theory [cf. (5.13)]. In this way, Eq. (5.38) is simply the phase-transformed constraint equation.

Let us apply the change of coordinates of §5.1.1 to bring (5.38) to a more useful form. First, the term proportional to $\nabla^2 \mathrm{W}_0$ can be explicitly computed as follows: we

[10] In fact, Eq. (5.34) is a particular case of more general ansätze, e.g., of the form $\{\exp[\mathrm{i}M\mathcal{W}_0] + \exp[-\mathrm{i}M\mathcal{W}_0]\}\psi$. In principle, the selection of a single exponential pre-factor can be a consequence of decoherence [127].

differentiate the first equation in (5.10) with respect to the heavy variables to obtain

$$G^{ac}\frac{\partial^2 \mathrm{W}_0}{\partial Q^b \partial Q^c} = \frac{1}{\mathcal{N}}\frac{\partial B_1^a}{\partial Q^b} - \frac{1}{\mathcal{N}}\frac{\partial}{\partial Q^b}\left(\mathcal{N}G^{ac}\right)\frac{\partial \mathrm{W}_0}{\partial Q^c} \ . \tag{5.39}$$

Using (5.10), (5.27) and (5.39), as well as the fact that $\mathcal{N}$ has a constant sign, we can write

$$\begin{aligned}
\frac{\mathcal{N}}{2}\nabla^2 \mathrm{W}_0 &= \frac{1}{2}\frac{\partial B_1^a}{\partial Q^a} - \frac{1}{2}\frac{\partial}{\partial Q^a}\left(\mathcal{N}G^{ab}\right)\frac{\partial \mathrm{W}_0}{\partial Q^b} + \frac{\mathcal{N}}{2\sqrt{|Gh|}}\frac{\partial \mathrm{W}_0}{\partial Q^a}\frac{\partial}{\partial Q^b}\left(\sqrt{|Gh|}G^{ab}\right)\\
&= \frac{1}{2}\frac{\partial B_1^a}{\partial Q^a} - \frac{G^{ab}}{2}\frac{\partial \mathcal{N}}{\partial Q^a}\frac{\partial \mathrm{W}_0}{\partial Q^b} + \frac{\mathcal{N}G^{ab}}{2\sqrt{|Gh|}}\frac{\partial \mathrm{W}_0}{\partial Q^a}\frac{\partial}{\partial Q^b}\left(\sqrt{|Gh|}\right)\\
&= \frac{1}{2}\frac{\partial B_1^a}{\partial Q^a} - \frac{1}{2\mathcal{N}}\frac{\partial \mathcal{N}}{\partial x^1} + \frac{1}{2\sqrt{|Gh|}}\frac{\partial}{\partial x^1}\left(\sqrt{|Gh|}\right)\\
&= \frac{1}{2}\frac{\partial B_1^a}{\partial Q^a} + \frac{|\mathcal{N}|}{2\sqrt{|Gh|}}\frac{\partial}{\partial x^1}\left(\frac{\sqrt{|Gh|}}{|\mathcal{N}|}\right)
\end{aligned} \tag{5.40}$$

Subsequently, we recall that $\sqrt{|\tilde{G}|} = \sqrt{|G|}B$ and $\tilde{G} = -2\mathcal{N}^2 V g$, where $g = \det(g_{ij})$ [cf. (5.9)]. We also note that the identities

$$\frac{\partial B_B^a}{\partial x^A} = \frac{\partial^2 Q^a}{\partial x^A \partial x^B} = \frac{\partial^2 Q^a}{\partial x^B \partial x^A} = \frac{\partial B_A^a}{\partial x^B} \tag{5.41}$$

imply

$$\left(B^{-1}\right)_a^A \frac{\partial B_A^a}{\partial x^B} = \left(B^{-1}\right)_a^A \frac{\partial B_B^a}{\partial x^A} = \frac{\partial B_B^a}{\partial Q^a} \ . \tag{5.42}$$

Thus, Eq. (5.40) becomes

$$\begin{aligned}
\frac{\mathcal{N}}{2}\nabla^2 \mathrm{W}_0 &= \frac{1}{2}\frac{\partial B_1^a}{\partial Q^a} - \frac{1}{2}\left(B^{-1}\right)_a^A \frac{\partial B_A^a}{\partial x^1} + \frac{|\mathcal{N}|}{2\sqrt{|\tilde{G}h|}}\frac{\partial}{\partial x^1}\left(\frac{\sqrt{|\tilde{G}h|}}{|\mathcal{N}|}\right)\\
&= \frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}} \ .
\end{aligned} \tag{5.43}$$

Finally, we use (5.9), (5.10) and (5.43) to rewrite (5.38) as

$$\begin{aligned} &\mathrm{i}\frac{\partial\psi}{\partial x^1}+\mathrm{i}\left(\frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}}\right)\psi \\ &=\mathcal{N}\hat{C}_m(x;\hat{p},q)\psi-\frac{\mathcal{N}}{2M\sqrt{|\tilde{G}h|}}\frac{\partial}{\partial x^i}\left(\sqrt{|\tilde{G}h|}g^{ij}\frac{\partial\psi}{\partial x^j}\right) \\ &-\frac{\mathcal{N}}{2M\sqrt{|\tilde{G}h|}}\frac{\partial}{\partial x^1}\left(\sqrt{|\tilde{G}h|}\tilde{G}^{11}\frac{\partial\psi}{\partial x^1}\right)\ . \end{aligned} \tag{5.44}$$

This is the quantum counterpart of (5.14). Notice that (5.44) is simply the phase-transformed constraint equation and, as such, it describes the coupled dynamics of the heavy and light sectors. Its solution, $\psi(Q;q)$, is a phase-transformed physical state, and it is not a wave function for the light degrees of freedom only. This is analogous to the remarks posed after (5.19) concerning the classical dynamics. Nevertheless, the quantum dynamics of the light sector can be analyzed with the use of conditional probabilities. We note that the conditional probabilities (5.31) depend solely on $\psi(Q;q)$,

$$p_\Psi := \left.\frac{\left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^*\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}{\int\prod_{i=2}^n\mathrm{d}x^i\prod_{\mu=1}^d\mathrm{d}q^\mu\ \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^*\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}\right|_{x^1=s}\ , \tag{5.45}$$

due to (5.36). In this way, $\tilde{\psi} := \hat{\mu}_{\mathfrak{v}}^{1/2}\psi$ is a conditional wave function. Besides the condition $x^1 = s$, one can, in principle, introduce further conditions, such that

$$p_\Psi(q|Q) := \left.\frac{\left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^*\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}{\int\mathrm{d}q\ \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^*\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}\right|_{x^1=s,x^i=y^i}\ , \tag{5.46}$$

can be interpreted as a probability of observing the light-sector configuration q, given that the heavy sector has been observed at the configuration $x^1 = s, x^i = y^i$ (collectively denoted as Q). This will be useful in §5.2.5, where we discuss the recovery of the quantum dynamics of the light sector in a fixed heavy background, and in Chapter 6, where we apply this formalism to the early Universe.

Our goal is now to solve (5.44) perturbatively in analogy to the iterative solution to (5.14). However, before we analyze the weak-coupling expansion of (5.44), it is worthwhile to discuss the interpretation of terms with imaginary coefficients, such as the logarithmic term in (5.44), as this will be of relevance to the interpretation of the perturbative expansion.

5.2.3 Time-dependent measures and unitarity

Although (5.44) is not a Schrödinger equation, we will see that it leads to an effective Schrödinger evolution in perturbation theory (as was first discussed in [120]). To better understand this effective Schrödinger picture, we must consider how it is related to the definition of the inner product and the concept of unitarity. Let us then analyze the general Schrödinger equation

$$\mathrm{i}\frac{\partial\psi}{\partial x^1} + \mathrm{i}\hat{\Gamma}\psi = \hat{\mathfrak{H}}\psi \ , \tag{5.47}$$

where $\hat{\Gamma}$ is some operator, and $\hat{\mathfrak{H}}$ is a Hamiltonian for the x^i and q^μ degrees of freedom. If both $\hat{\Gamma}$ and $\hat{\mathfrak{H}}$ are self-adjoint with respect to a certain inner product $\langle\cdot|\cdot\rangle$, then the $\mathrm{i}\hat{\Gamma}$ factor would violate unitarity with respect to $\langle\cdot|\cdot\rangle$. Indeed, such terms will be present in the perturbative expansion of (5.44), and they have been interpreted as causes of a violation of unitarity in [120]. However, one can take the position that, instead of using $\langle\cdot|\cdot\rangle$, one should define an inner product $(\cdot|\cdot)$ such that it is conserved by the evolution described by (5.47). In fact, terms with imaginary coefficients such as $\mathrm{i}\hat{\Gamma}$ are indispensable to guarantee unitarity if the measure is time-dependent [128].[11] Conversely, let us then see how the (time-dependent) measure can be defined if the dynamics is dictated by (5.47).

Let us define

$$\begin{aligned}
\langle\psi_1|\psi_2\rangle &:= \int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu f(x,q) \ \psi_1^*(x,q)\psi_2(x,q) \equiv \int \mathrm{d}f \ \psi_1^*\psi_2 \ , \\
(\psi_1|\psi_2) &:= \int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu f(x,q) \ \psi_1^*(x,q)\hat{\mathcal{M}}\psi_2(x,q) \equiv \int \mathrm{d}f \ \psi_1^*\hat{\mathcal{M}}\psi_2 \ ,
\end{aligned} \tag{5.48}$$

where $\hat{\mathcal{M}}$ is an operator to be determined. We assume that it is symmetric with respect to $\langle\cdot|\cdot\rangle$. The symbol $\mathrm{d}f$ in (5.48) is simply a short-hand notation. The conservation of (5.48) (unitarity) is given by the condition $\partial(\psi_1|\psi_2)/\partial x^1 = 0$. From (5.47), we find

$$0 = \mathrm{i}\frac{\partial}{\partial x^1}(\psi_1|\psi_2) = \int \mathrm{d}f \ \psi_1^* \left\{ [\hat{\mathcal{M}}, \hat{\mathfrak{H}}] - \mathrm{i}[\hat{\mathcal{M}}, \hat{\Gamma}]_+ + \frac{\mathrm{i}}{f(x,q)}\frac{\partial}{\partial x^1}\left(f(x,q)\hat{\mathcal{M}}\right) \right\} \psi_2 \ ,$$

where $[\cdot,\cdot]$ denotes a commutator, $[\cdot,\cdot]_+$ is an anticommutator, and we used the assumption that $\hat{\Gamma}$ and $\hat{\mathfrak{H}}$ are (at least) symmetric with respect to $\langle\cdot|\cdot\rangle$. If the above condition is to be satisfied for arbitrary solutions of (5.47), then the operator $\hat{\mathcal{M}}$ must

[11] For example, DeWitt referred to objects of the kind $\partial/\partial x^1 + \partial \log |2Vgh|^{1/4} / \partial x^1$ as 'conservative time derivatives' [128].

be a solution to the equation

$$\frac{\mathrm{i}}{f(x,q)}\frac{\partial}{\partial x^1}\left(f(x,q)\hat{\mathfrak{M}}\right) = \mathrm{i}[\hat{\mathfrak{M}},\hat{\Gamma}]_+ - [\hat{\mathfrak{M}},\hat{\mathfrak{H}}] \ . \tag{5.49}$$

If the solution to (5.49) is a positive-definite operator, then the dynamics dictated by (5.47) is unitary with respect to $(\cdot|\cdot)$. In what follows, we will apply this procedure to the definition of the perturbative measure (5.36) in the expansion of (5.44), and we will see how the perturbative measure corresponds to a quantization of the Faddeev-Popov determinant.

5.2.4 Perturbation theory I

We can now solve (5.44) iteratively. To lowest-order in $1/M$, we obtain

$$\mathrm{i}\frac{\partial\psi}{\partial x^1} + \mathrm{i}\left(\frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}}\right)\psi = \mathcal{N}\hat{C}_m(x;\hat{p},q)\psi + \mathcal{O}\left(\frac{1}{M}\right) \ , \tag{5.50}$$

which is of the form (5.47) with $\hat{\Gamma} = \partial\log|2Vgh|^{1/4}/\partial x^1$ and $\hat{\mathfrak{H}} = \mathcal{N}\hat{C}_m$. As $\hat{C}_m$ is symmetric with respect to $\langle\cdot|\cdot\rangle$ with $f \propto \sqrt{h}$ [cf. (5.48)], it is straightforward to verify that (5.49) is solved by $\hat{\mathfrak{M}} = \hat{1}$ if we choose $f = \sqrt{|2Vgh|}$. We then define the lowest-order measure $\hat{\mu}_0$ in (5.36) as

$$\hat{\mu}_0 \equiv \hat{\mu}_0\left(Q;\hat{p},q\right) := f\hat{\mathfrak{M}} = \sqrt{|2Vgh|} \ , \tag{5.51}$$

such that the physical inner product (5.30) [cf. (5.45)] reads

$$(\Psi_1|\Psi_2) = \int\prod_i \mathrm{d}x^i\prod_\mu \mathrm{d}q^\mu\ \left(|2Vgh|^{\frac{1}{4}}\psi_1\right)^*\left(|2Vgh|^{\frac{1}{4}}\psi_2\right) \ , \tag{5.52}$$

for $x^1 = s$. Equation (5.52) is manifestly positive-definite, and it is conserved (for general values of s) by the dynamics dictated by (5.50) up to order M^0. The measure (5.51) is generally time-dependent; i.e., it depends on the background clock x^1. This is the reason the logarithmic term arises in (5.50). Notice that (5.50) is the quantum counterpart of (5.23), and its solutions are approximations to the phase-transformed solutions of the quantum constraint equation at order M^0.

5.2.5 Light-sector unitarity. Propagation in a fixed background

Although the solutions $\psi(Q;q)$ to (5.50) are not wave functions for the light degrees of freedom only, we can describe the conditional dynamics of the light variables using (5.46). Furthermore, it is also possible to further factorize $\psi(Q;q) = \psi_h(Q)\psi_l(Q;q)$, such that (5.46) reads

$$p_\Psi(q|Q) := \left.\frac{\sqrt{h}\,\psi_l^*\psi_l}{\int \mathrm{d}q\sqrt{h}\;\psi_l^*\psi_l}\right|_{x^1=s,x^i=y^i} + \mathcal{O}\left(\frac{1}{M}\right) \ , \tag{5.53}$$

due to (5.51). We demand that ψ_h be a solution to

$$\mathrm{i}\frac{\partial\psi_h}{\partial x^1} + \mathrm{i}\left(\frac{\partial}{\partial x^1}\log|2Vg|^{\frac{1}{4}}\right)\psi_h = 0 + \mathcal{O}\left(\frac{1}{M}\right) \ ; \tag{5.54}$$

i.e., we impose

$$\psi_h(Q) = |2Vg|^{-\frac{1}{4}}\,\gamma(x^i(Q)) + \mathcal{O}\left(\frac{1}{M}\right) \ , \tag{5.55}$$

where $\gamma(x^i(Q))$ is an arbitrary function. If we further impose $\int\prod_i \mathrm{d}x^i\;\gamma^*(x^i)\gamma(x^i) = 1$, then $\psi_h(Q)$ satisfies

$$\frac{\partial}{\partial x^1}\int\prod_i \mathrm{d}x^i\sqrt{2|Vg|}\;\psi_h^*\psi_h = 0 + \mathcal{O}\left(\frac{1}{M}\right) \ . \tag{5.56}$$

In this way, $\psi_h(Q)$ can be interpreted as a 'marginal wave function' [100, 123] for the heavy variables, the dynamics of which is unitary at order M^0 due to (5.56). The equation for $\psi_l(Q;q)$ is obtained if we insert $\psi(Q;q) = \psi_h(Q)\psi_l(Q;q)$ into (5.50) and use (5.54). The result is

$$\mathrm{i}\frac{\partial\psi_l}{\partial x^1} + \mathrm{i}\left(\frac{\partial}{\partial x^1}\log|h|^{\frac{1}{4}}\right)\psi_l = \mathcal{N}(x)\hat{C}_m(x;\hat{p},q)\psi_l + \mathcal{O}\left(\frac{1}{M}\right) \ . \tag{5.57}$$

This is identical to the usual Schrödinger equation for the light degrees of freedom that propagate in a background defined by fixed values of the heavy variables. In particular, Eq. (5.57) implies that the (conditional) light-sector dynamics associated with the conditional probabilities (5.53) is unitary at order M^0,

$$\frac{\partial}{\partial x^1}\int\prod_\mu \mathrm{d}q^\mu\sqrt{h}\;\psi_l^*\psi_l = 0 + \mathcal{O}\left(\frac{1}{M}\right) \ . \tag{5.58}$$

Thus, the solution Ψ to the constraint equation $\hat{C}\Psi = 0$, has been factorized as

$$\Psi(Q,q) = e^{\mathrm{i}M\mathrm{W}_0(Q)}\psi(Q;q) = e^{\mathrm{i}M\mathrm{W}_0(Q)}\psi_h(Q)\psi_l(Q;q) + \mathcal{O}\left(\frac{1}{M}\right) \ . \tag{5.59}$$

Notice that background clock is defined from the phase W_0, which is generally not the total phase of the 'heavy factor' $\exp(\mathrm{i}M\mathrm{W}_0(Q))\psi_h(Q)$. It is also useful to note that the factorization (5.59) has been used as the traditional BO ansatz (cf. Appendix B) in molecular physics [121].

Finally, we can use (5.53) to compute conditional expectation values of light-sector operators. Given an operator $\hat{O} \equiv \hat{O}(x; \hat{p}, q)$ that is symmetric with respect to the measure $\sqrt{h}\mathrm{d}q$, its conditional expectation value reads

$$\mathrm{E}[O|Q] := \left. \frac{\int \mathrm{d}q\sqrt{h}\ \psi_l^* \hat{O}\psi_l}{\int \mathrm{d}q\sqrt{h}\ \psi_l^*\psi_l} \right|_{x^1=s, x^i=y^i} + \mathcal{O}\left(\frac{1}{M}\right) . \tag{5.60}$$

This leads to the conditional Ehrenfest equation,[12]

$$\frac{\partial}{\partial x^1}\mathrm{E}[O|Q] = \mathrm{E}\left[\frac{\partial \hat{O}}{\partial x^1} + \mathrm{i}\mathcal{N}\left[\hat{C}_m, \hat{O}\right] + \left[\frac{\partial}{\partial x^1}\log|h|^{\frac{1}{4}}, \hat{O}\right] \middle| Q\right] + \mathcal{O}\left(\frac{1}{M}\right) , \tag{5.61}$$

which is to be compared with (5.24). This equation captures the quantum dynamics of the light-sector in a fixed background of the heavy variables.

5.2.6 Perturbation theory II

Let us resume the iterative solution of (5.44) at order $1/M$. We use the lowest-order result (5.50) to replace the higher derivatives in x^1 by factors of $\partial \log|2Vgh|^{1/4}/\partial x^1$ or $\mathcal{N}\hat{C}_m$. The result, after a series of relatively tedious steps, is found to be

$$\begin{aligned} &\mathrm{i}\frac{\partial\psi}{\partial x^1} + \mathrm{i}\hat{\Gamma}\psi = \hat{\mathfrak{H}}\psi = \mathcal{N}\hat{C}_m\psi - \frac{\mathcal{N}}{4MV}\hat{C}_m^2\psi \\ &- \frac{1}{2M\sqrt{2|Vgh|}}\frac{\partial}{\partial x^i}\left(\sqrt{2|Vgh|}\mathcal{N}g^{ij}\frac{\partial\psi}{\partial x^j}\right) + \frac{1}{M}\mathcal{V}\psi + \mathcal{O}\left(\frac{1}{M^2}\right) , \end{aligned} \tag{5.62}$$

which is of the form (5.47) with

$$\begin{aligned} \hat{\Gamma} :=& \frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}} + \frac{1}{2M\sqrt{2|Vgh|}}\frac{\partial}{\partial x^1}\left(\mathfrak{v}\sqrt{\frac{h}{2}\left|\frac{g}{V}\right|}\hat{C}_m\right) \\ &- \frac{1}{4MV}\hat{C}_m\frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}} - \frac{1}{4MV}\left(\frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}}\right)\hat{C}_m , \end{aligned} \tag{5.63}$$

[12] Notice that $\left(\frac{\partial}{\partial x^1}\hat{O}\right)\psi := \frac{\partial}{\partial x^1}\left(\hat{O}\psi\right) - \hat{O}\frac{\partial\psi}{\partial x^1} = \left[\frac{\partial}{\partial x^1}, \hat{O}\right]\psi$ defines the explicit x^1-derivative of the operator.

$$\mathcal{V} := \frac{1}{32\mathcal{N}V|Vgh|}\left(\frac{\partial}{\partial x^1}\sqrt{2|Vgh|}\right)^2 - \frac{1}{2\sqrt{2|Vgh|}}\frac{\partial}{\partial x^1}\left(\frac{1}{4\mathcal{N}V}\frac{\partial}{\partial x^1}\sqrt{2|Vgh|}\right) , \quad (5.64)$$

where $\mathfrak{v} = \mathrm{sgn}(V)$, as before. Equation (5.62) is the quantum counterpart of (5.19). The term $\mathcal{V}/M$ is a quantum correction that arises as a result of the factor ordering in (5.25) and (5.26). We also note that it is, in principle, possible to further factorize $\psi(Q;q) = \psi_h(Q)\psi_l(Q;q)$ as in §5.2.5 in order to discuss unitarity of the (conditional) light-sector dynamics, but we do not pursue this here because (5.62) is sufficient for our purposes (particularly the application in Chapter 6). See, however, the discussion in §B.4.2 and §B.4.3.

It is also important to mention that (5.62) was first derived in [120], but the terms in the second line were not included. Here, they appear as a straightforward consequence of solving (5.44) iteratively.[13] Furthermore, a term similar to the $\mathrm{i}\hat{\Gamma}$ term in (5.62) was regarded as a cause of unitarity violation in [120] because $\psi(Q;q)$ was taken to be the wave function of the light sector equipped with the standard inner product. In contrast, as we have argued above, we note that $\psi(Q;q)$ is simply the phase-transformed solution to the constraint equation, and thus it encodes the dynamics of both heavy and light degrees of freedom. Following the discussion in §5.2.3, we see that (5.62) describes a unitary dynamics with respect to a measure $f\hat{\mathcal{M}}$ that solves (5.49). We now set out find $f\hat{\mathcal{M}}$ and we relate it to the classical Faddeev-Popov determinant.

5.2.7 WKB time as a quantum choice of gauge

Let us define $\hat{\mu}_{\mathfrak{v}} := f\hat{\mathcal{M}}$. We consider the expansion $\hat{\mathcal{M}} := \hat{\mathcal{M}}_0 + \hat{\mathcal{M}}_1/M + \mathcal{O}(1/M^2)$, such that $\hat{\mu}_1 = f\hat{\mathcal{M}}_1$ [cf. (5.36)]. From (5.51), we know that $f = \sqrt{|2Vgh|}$ and $\hat{\mathcal{M}}_0 = \hat{1}$. If we insert this lowest-order result together with (5.63) in (5.49), we obtain an equation for $\hat{\mathcal{M}}_1$,

$$\begin{aligned} &\frac{\mathrm{i}}{\sqrt{|2Vgh|}}\frac{\partial}{\partial x^1}\left(\sqrt{|2Vgh|}\hat{\mathcal{M}}_1\right) \\ &= \mathrm{i}\left[\hat{\mathcal{M}}_1, \frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}}\right]_+ + \frac{\mathrm{i}}{\sqrt{|2Vgh|}}\frac{\partial}{\partial x^1}\left(\mathfrak{v}\sqrt{\frac{h}{2}\left|\frac{g}{V}\right|}\hat{C}_m\right) \\ &- \mathrm{i}\left[\frac{\hat{C}_m}{2V}, \frac{\partial}{\partial x^1}\log|2Vgh|^{\frac{1}{4}}\right]_+ - \left[\hat{\mathcal{M}}_1, \mathcal{N}\hat{C}_m\right] . \end{aligned} \quad (5.65)$$

[13] Recall that we have assumed that $\tilde{G}^{1i} = 0$. If this is not the case, then extra terms with x^i-derivatives should be included in (5.62).

It is straightforward to see that this equation is solved by $\hat{\mathcal{M}}_1 = \hat{C}_m/(2V)$. Thus, we obtain

$$\hat{\mu}_{\mathfrak{v}} := f\hat{\mathcal{M}} = \sqrt{|2Vgh|}\left(1 + \frac{1}{2MV}\hat{C}_m\right) + \mathcal{O}\left(\frac{1}{M^2}\right) . \tag{5.66}$$

It is worthwhile to mention that the author of this thesis has shown in [98] that (5.66) can also be obtained from the Klein-Gordon inner product, but this does not concern us here because the Klein-Gordon inner product is indefinite and we focus on positive-definite products. Incidentally, the measure (5.66) leads to a positive-definite inner product [cf. (5.30)], given that the condition

$$\int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu \sqrt{2|Vg|h}\ \psi^*\psi \gg \frac{1}{M}\int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu \sqrt{\frac{1}{2}\left|\frac{g}{V}\right| h}\ \psi^* \hat{C}_m \psi \tag{5.67}$$

should be fulfilled in perturbation theory and we assume that the eigenvalues of $\hat{C}_m$ are not negative. Moreover, Eq. (5.66) is also similar to inner products that have been analyzed in the study of quantum optics in gravitational fields [129].

Using (5.9) and (5.22), we can rewrite (5.66) in terms of a quantum version of the absolute value of the Faddeev-Popov determinant,

$$\hat{\mu}_{\mathfrak{v}} = \frac{\sqrt{|\tilde{G}h|}}{|\mathcal{N}|}\left(1 + \frac{1}{2MV}\hat{C}_m\right) \equiv \sqrt{|\tilde{G}h|}\,\widehat{\frac{1}{|\omega|}} , \tag{5.68}$$

such that the physical inner product (5.30) (with $\sigma = \mathfrak{v}$) can be written as

$$(\Psi_1|\Psi_2) = \int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu \sqrt{|\tilde{G}h|}\ \Psi_1^* \widehat{\frac{1}{|\omega|}} \Psi_2 \Bigg|_{x^1 = s} . \tag{5.69}$$

In this way, the background clock x^1 (WKB time) corresponds to a quantum choice of gauge. The gauge-fixed dynamics is unitary up to order $1/M$, and it is governed by the effective Schrödinger equation (5.62). Conditional expectation values of observables are given by suitable operator insertions in (5.69) [cf. the conditional probabilities (2.112), (5.31) and (5.45)]. Finally, notice that, due to (5.66), Eq. (5.69) can be written in terms of the conditional wave functions $\tilde{\psi}_{(1,2)} := \hat{\mu}_{\mathfrak{v}}^{1/2}\psi_{(1,2)}$, such that it becomes manifestly positive-definite, $\int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu\ \tilde{\psi}^*_{(1)}\tilde{\psi}_{(2)}$. Thus, the operator $\hat{\mu}_{\mathfrak{v}}$ connects the solutions to $\hat{C}\Psi = 0$ to conditional wave functions.[14]

[14] Recall from footnote 10 that we only consider a single phase pre-factor $\Psi = \exp(\mathrm{i}M\mathrm{W}_0)\psi$. For this reason, different conditional wave functions $\tilde{\psi}_{(1,2)}$ are connected to different states $\Psi_{(1,2)}$ by the same phase transformation.

Chapter 6

Quantum-Gravitational Effects in the Early Universe

With the formalisms of Chapters 2 and 5, we are now in a position to discuss a possible treatment of quantum-gravitational effects in the early Universe based on a relational account of the quantum constraint equation. In §6.1, we give a brief review of the essentials of the classical theory that are necessary for our discussion of the BO approach to quantum theory and its unitarity.[1] We also define the master WDW equation and the associated conditional probabilities. In §6.2, we apply the formalism of Chapter 5 to obtain a unitary, corrected Schrödinger equation for the cosmological perturbations, and the ensuing effects on the primordial power spectra are discussed in §6.3. For convenience, we set $c = \hbar = 1$. Spacetime is four-dimensional with signature $(-, +, +, +)$.[2]

6.1 Cosmological perturbations

As the observable universe is approximately homogeneous and isotropic at large scales, it is reasonable to define the cosmological perturbations on a FLRW background. In addition, as contributions from spatial curvature are flattened to a large degree during the period of inflationary expansion, we focus on a flat FLRW model. We also assume a compact spatial topology for simplicity.

6.1.1 The classical background

The flat FLRW line element reads

$$\mathrm{d}s^2 = -N^2(\tau)\mathrm{d}\tau^2 + a^2(\tau)\mathrm{d}\mathbf{x}^2 \ , \tag{6.1}$$

[1] Further details regarding the theory of cosmological perturbations can be found in [130], while the Hamiltonian theory of perturbations in GR is discussed in [131, 132] and references therein.

[2] This Chapter is based on [62].

and the symmetry-reduced action is [6]

$$S = \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \mathfrak{L}^3 N \left(-\frac{1}{2\kappa} \frac{a\dot{a}^2}{N^2} + \frac{a^3\dot{\phi}^2}{2N^2} - a^3 \mathcal{V}(\phi) \right) \,, \tag{6.2}$$

where $\kappa = 4\pi G/3$, and $\mathfrak{L}$ is an arbitrary length scale. Notice that the cosmological constant has been set to zero, and we define the inflaton as a minimally coupled scalar field $\phi(\tau)$ for simplicity. Following [114,115], it is convenient to perform the redefinitions

$$\begin{aligned} t &\mapsto \mathfrak{L}t \quad && \mathbf{x} \mapsto \mathfrak{L}\mathbf{x} \,, \\ a &\mapsto \frac{a}{\mathfrak{L}} \quad && N \mapsto \frac{N}{\mathfrak{L}} \,, \end{aligned} \tag{6.3}$$

which imply that the spacetime coordinates become dimensionless, whereas the lapse function and scale factor now have dimensions of length. We can then rewrite (6.2) as [cf. (1.40)]

$$\begin{aligned} S &= \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \left(-\frac{1}{2\kappa} \frac{a\dot{a}^2}{N} + \frac{a^3\dot{\phi}^2}{2N} - N a^3 \mathcal{V}(\phi) \right) \\ &= \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \left(p_a \dot{a} + p_\phi \dot{\phi} - NC \right) \,, \end{aligned} \tag{6.4}$$

where the lapse plays the role of the worldline einbein and the initial-value constraint is

$$C = -\frac{\kappa}{2a} p_a^2 + \frac{1}{2a^3} p_\phi^2 + a^3 \mathcal{V}(\phi) \,. \tag{6.5}$$

The de Sitter ('no-roll') limit, which will be sufficient for our analysis, is obtained by setting $\phi =$ const. in the solution to the inflaton field equations,

$$\dot{\phi} \approx \frac{N}{a^3} p_\phi \,, \; \dot{p}_\phi \approx -N a^3 \frac{\partial \mathcal{V}}{\partial \phi} \,. \tag{6.6}$$

This is equivalent to the conditions

$$p_\phi = \frac{\partial \mathcal{V}}{\partial \phi} = 0 \,, \tag{6.7}$$

which imply that the inflaton potential is a constant. In terms of the Hubble parameter H_0 in the de Sitter model [114], we can write

$$\mathcal{V}(\phi) := \frac{H_0^2}{2\kappa} \,. \tag{6.8}$$

Within the no-roll limit, it is straightforward to find the solution to the constraint (6.5),

$$p_a = -\frac{\sigma_0 H_0}{\kappa} a^2 \quad (\sigma_0 = \pm 1) \ . \tag{6.9}$$

Here, the discrete multiplicity sectors are given by $\sigma_0 = 1$ (expanding universe) and $\sigma_0 = -1$ (contracting universe). Using (6.9), the field equation for the scale factor in the proper-time gauge[3] ($N(\tau) = 1$) reads $\dot{a} = \sigma_0 H_0 a(\tau)$, and its solution is the well-known function $a(\tau) = a_0 \exp(\sigma_0 H_0 \tau)$. We also define the conformal time variable for later reference. We denote it by η [not to be confused with the proper time defined in Chapter 1; cf. (1.2)]. In the proper-time gauge, we demand $\dot{\eta} = 1/a(\tau)$, which yields

$$\eta(a) = -\frac{\sigma_0}{H_0 a} \ . \tag{6.10}$$

In terms of the field redefinition

$$a = a_0 \mathrm{e}^{\alpha} \ , \tag{6.11}$$

we can write $\eta = -\sigma_0/(H_0 a_0)\mathrm{e}^{-\alpha}$, which will be convenient in the quantum theory.

6.1.2 Classical perturbations

We now briefly review the aspects of the classical theory of cosmological perturbations that will be useful in the quantum theory to be analyzed in §6.1.3.[4] Perturbations to the FLRW metric are given by the perturbed line element

$$\begin{aligned} \mathrm{d}s^2 = & a^2(\eta) \left\{ -(1-2A)\mathrm{d}\eta^2 + 2(\partial_i B)\mathrm{d}x^i \mathrm{d}\eta \right. \\ & \left. + \left[(1-2\psi)\delta_{ij} + 2\partial_i\partial_j E + h_{ij} \right] \mathrm{d}x^i \mathrm{d}x^j \right\} \ , \end{aligned} \tag{6.12}$$

where the spacetime functions A, B, ψ and E comprise the scalar perturbations of the metric, and the symmetric spatial tensor h_{ij} encodes the tensor perturbations. Notice that (6.12) has been written with respect to a dimensionful conformal time coordinate, as well as a dimensionful scale factor; i.e., we have temporarily reverted the redefinitions (6.3). Besides (6.12), there are also the scalar perturbations of the inflaton, which are denoted by $\varphi(\eta, \mathbf{x})$.

The expansion of the action reads

$$S = S_0 + \delta S + \delta^2 S + \dots \ , \tag{6.13}$$

[3] In this context, the proper-time gauge is called the 'cosmic-time coordinate choice'.
[4] Further details can be found in [114, 115] and the standard references [130–133].

where S_0 is the action for the FLRW background [cf. (6.2)], δS is a term that vanishes if evaluated on a background solution, $\delta^2 S$ is of quadratic order in the perturbations, and the ellipses denote terms of higher orders. In this way, if we define the perturbed metric [cf. (6.12)] around a fixed FLRW solution, the field equations for the perturbative variables on a fixed FLRW background are obtained by varying δS with respect to the perturbations.

The two polarizations $+, \times$ of gravitational waves comprise the physical, independent degrees of freedom among the tensor perturbations, which are invariant under linearized diffeomorphisms in spacetime. In fact, the lowest-order dynamics of the perturbations is most conveniently described by such invariants, often called 'master gauge-invariant variables' [114]. Another linearized-diffeomorphism invariant is the Mukhanov-Sasaki variable [114, 130]

$$v := a\left\{\varphi + \frac{\dot{\phi}}{\mathcal{H}}\left[A + 2\mathcal{H}(B - \dot{E}) + \frac{\mathrm{d}}{\mathrm{d}\eta}(B - \dot{E})\right]\right\} . \tag{6.14}$$

In (6.14), we have denoted $\cdot \equiv \mathrm{d}/\mathrm{d}\eta$ and $\mathcal{H} = \dot{a}/a$. Let us consider the Fourier transform

$$v(\eta, \mathbf{x}) = \int_{\mathbb{R}^3} \frac{\mathrm{d}^3 k}{(2\pi)^{\frac{3}{2}}} v_{\mathbf{k}}(\eta) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} , \tag{6.15}$$

where $v_{\mathbf{k}}^* = v_{-\mathbf{k}}$. It is also convenient to work with the rescaled Fourier coefficients

$$v_{\mathbf{k}}^{(+,\times)} := \frac{a}{\sqrt{12\kappa}} h_{\mathbf{k}}^{(+,\times)} \tag{6.16}$$

of tensor perturbations. Using (6.15) and (6.16), it is possible to show that $\delta^2 S$ has the simple form [114, 130, 134]

$$\delta^2 S = \int \mathrm{d}\eta \int \mathrm{d}^3 k \left\{ \dot{v}_{\mathbf{k}} \dot{v}_{\mathbf{k}}^* - \omega_{\mathbf{k};\mathrm{S}}^2 |v_{\mathbf{k}}|^2 + \sum_{\lambda=+,\times} \left[\dot{v}_{\mathbf{k}}^{(\lambda)} \left(\dot{v}_{\mathbf{k}}^{(\lambda)}\right)^* - \omega_{\mathbf{k};\mathrm{T}}^2 \left| v_{\mathbf{k}}^{(\lambda)} \right|^2 \right] \right\}, \tag{6.17}$$

where the integration over $\mathbf{k}$ is performed over half of the Fourier space, and we define

$$\omega_{\mathbf{k};\mathrm{S}}^2(\eta) := k^2 - \frac{\ddot{z}}{z} , \ \omega_{\mathbf{k};\mathrm{T}}^2(\eta) := k^2 - \frac{\ddot{a}}{a} , \tag{6.18}$$

with $k = |\mathbf{k}|$, $z := a\dot{\phi}/\mathcal{H}$. Notice that, at the lowest-order, all the Fourier modes of the perturbations evolve independently. In order to work with a more compact notation, we also define

$$v_{\mathbf{k}}^{(\rho)} := \begin{cases} v_{\mathbf{k}} & \text{for } \rho = \mathrm{S} \ , \\ v_{\mathbf{k}}^{(+)} & \text{for } \rho = + \ , \\ v_{\mathbf{k}}^{(\times)} & \text{for } \rho = \times \ , \end{cases} \tag{6.19}$$

and

$$\omega_{\mathbf{k};\rho}^2 := \begin{cases} \omega_{\mathbf{k};\mathrm{S}}^2 & \text{for } \rho = \mathrm{S} \ , \\ \omega_{\mathbf{k};\mathrm{T}}^2 & \text{for } \rho = +, \times \ . \end{cases} \tag{6.20}$$

In a compact spatial topology, the modes are discrete, and we substitute [114, 115]

$$\int \mathrm{d}^3 k \to \frac{1}{\mathfrak{L}^3} \sum_{\mathbf{k}} \ , \tag{6.21}$$

where, as mentioned earlier, $\mathfrak{L}$ is an arbitrary length. We can now repeat the redefinitions (6.3) and, in addition, redefine [114, 115]

$$k \mapsto \frac{1}{\mathfrak{L}} k \ , \ v_{\mathbf{k}}^{(\rho)} \mapsto \mathfrak{L}^2 v_{\mathbf{k}}^{(\rho)} \ . \tag{6.22}$$

In this way, we can use (6.19), (6.20) to rewrite the action (6.17) as

$$\delta^2 S = \int \mathrm{d}\eta \sum_{\mathbf{k}} \sum_{\rho=\mathrm{S},+,\times} \left[\dot{v}_{\mathbf{k}}^{(\rho)} \left(\dot{v}_{\mathbf{k}}^{(\rho)} \right)^* - \omega_{\mathbf{k};\rho}^2 \left| v_{\mathbf{k}}^{(\rho)} \right|^2 \right] \ . \tag{6.23}$$

We subsequently decompose the variables $v_{\mathbf{k}}^{(\rho)}$ in terms of their real and imaginary parts [134],

$$v_{\mathbf{k}}^{(\rho)} = \frac{1}{\sqrt{2}} \left[v_{\mathbf{k};\mathrm{R}}^{(\rho)} + \mathrm{i} v_{\mathbf{k};\mathrm{I}}^{(\rho)} \right] \ , \tag{6.24}$$

such that the action (6.23) leads to the Hamiltonian

$$H := \frac{1}{2} \sum_{\mathbf{k},\rho} \sum_{j=\mathrm{R},\mathrm{I}} \left\{ \left[\pi_{\mathbf{k};j}^{(\rho)} \right]^2 + \omega_{\mathbf{k};\rho}^2 \left[v_{\mathbf{k};j}^{(\rho)} \right]^2 \right\} \ , \tag{6.25}$$

where the canonical momenta of the perturbations are $\pi_{\mathbf{k};j}^{(\rho)} = \dot{v}_{\mathbf{k};j}^{(\rho)}$ ($j = \mathrm{R}, \mathrm{I}$). The Hamiltonian (6.25) will allow us to separately examine the quantum dynamics of each mode (at the lowest order in the perturbations). Lastly, we will use the notation $\mathbf{q} := (\mathbf{k}, j, \rho)$, $v_{\mathbf{q}} := v_{\mathbf{k};j}^{(\rho)}$, $\omega_{\mathbf{q}} := \omega_{\mathbf{k};\rho}$ for brevity.

6.1.3 The master Wheeler-DeWitt equation

The canonical quantization of (6.25) defines the QFT of cosmological perturbations on a curved background given by a classical FLRW model. In the Schrödinger picture, the wave functions $\tilde{\psi}$ correspond to probability amplitudes that evolve according to

$$\mathrm{i}\frac{\partial\tilde{\psi}}{\partial\eta} = \hat{H}\tilde{\psi} \ , \tag{6.26}$$

where the quantum Hamiltonian is

$$\hat{H} := \sum_{\mathbf{q}} \hat{H}_{\mathbf{q}} \ , \tag{6.27}$$

$$\hat{H}_{\mathbf{q}} := \frac{1}{2}\left\{-\frac{\partial^2}{\partial v_{\mathbf{q}}^2} + \omega_{\mathbf{q}}^2 v_{\mathbf{q}}^2\right\} \ . \tag{6.28}$$

As is well-known [134], one can use the Schrödinger equation (6.26) to make the usual predictions regarding the CMB anisotropy spectrum. Nevertheless, we would like to go further and analyze: (1) how quantum fluctuations of the unperturbed FLRW metric (i.e., of the scale factor) may be incorporated; (2) which effects may arise from this quantization of the background.

A first attempt would be to demand that $\tilde{\psi}$ solves not only the Schrödinger equation (6.26) for perturbations, but also a separate quantum constraint for the background, which could be obtained by the standard Dirac quantization of (6.5).[5] This is not, however, the approach we consider. We will follow an alternative route and assume that a single time reparametrization-invariant system encodes the dynamics (and, in particular, interactions) of the background and perturbations. This is achieved by the master WDW equation

$$\left\{\frac{\mathrm{e}^{-3\alpha}}{a_0^3}\left[\frac{\kappa}{2}\frac{\partial^2}{\partial\alpha^2} - \frac{1}{2}\frac{\partial^2}{\partial\phi^2} + a_0^6\mathrm{e}^{6\alpha}\mathcal{V}(\phi)\right] + \frac{\mathrm{e}^{-\alpha}}{a_0}\hat{H}\right\}\Psi(\alpha,\phi,v) = 0 \ , \tag{6.29}$$

which combines the Laplace-Beltrami ordered quantization of the background constraint (6.5) and the quantum Hamiltonian (6.27). Notice that the $v_{\mathbf{q}}$ variables are

[5] In principle, this approach would have to be accompanied by the quantization of linearized constraints, δC, which follow from the term δS of first order in the perturbations that is present in (6.13). See, for example, [133] for an application of these linearized constraints. Up to second order in the perturbations, one could then require $\tilde{\psi}$ to satisfy the zeroth-order constraint, $\hat{C}\tilde{\psi} = 0$, the first-order constraints, $\widehat{\delta C}\tilde{\psi} = 0$, and the second-order Schrödinger equation (6.26). Nevertheless, the master gauge-invariant variables trivialize the δC constraints, and their quantum theory corresponds to the quantization of the reduced phase space of the perturbations, albeit not of the background. Thus one does not need to require $\widehat{\delta C}\tilde{\psi} = 0$ if one quantizes the $v_{\mathbf{q}}$ variables. See [114] for a discussion and further references.

collectively denoted by v, and we have included a factor of $1/a = \mathrm{e}^{-\alpha}/a_0$ [cf. (6.11)] before $\hat{H}$ because the Hamiltonian of perturbations is defined with respect to conformal time, such that it becomes H/a in the proper-time gauge [cf. (6.10)].

In the literature [114, 115, 133], a master WDW equation is commonly solved by means of a weak-coupling expansion, such as the one analyzed in Chapter 5. Indeed, one of the advantages of considering the single master WDW equation is that the weak-coupling expansion of its solutions leads to a systematic derivation of QFT on a curved background [cf. §5.2.5] and also of corrections to the Schrödinger equation (6.26) [cf. §5.2.6]. Moreover, Eq. (6.29) directly encompasses the interaction of a quantum background with the perturbations as a BO system in the sense of Chapter 5 and Appendix B.

It is necessary to understand the relation between the master WDW equation (6.29) and a notion of quantum gauge fixing (in the sense of Chapters 1 and 5), and a comprehensive analysis of the unitarity of the theory is warranted. We believe that the present literature lacks a thorough discussion of these topics, both of which can be tackled with the results of Chapter 5. Indeed, the space of solutions of (6.29) may be endowed with the physical inner product (5.30), where the generalized clock is now a function $\chi(\alpha, \phi; v)$. The conditional probabilities are defined as in (5.31). As the potential in (6.5) is positive due to (6.8) ($\mathfrak{v} = \mathrm{sgn}(a^3\mathcal{V}(\phi)) = 1$), we simply denote $\hat{\mu}_{\mathfrak{v}} \equiv \hat{\mu}$.

In order to concretely discuss the issue of unitarity of the corrected Schrödinger equation, it is sufficient to consider the de Sitter (no-roll) limit. As in the classical theory, we impose $\phi = \phi_0 = \text{const.}$, and this corresponds to further conditioning the probabilities; i.e., we define

$$p_\Psi := \frac{\left(\hat{\mu}^{\frac{1}{2}}\Psi\right)^* \hat{\mu}^{\frac{1}{2}}\Psi\Big|_{\chi=s,\phi=\phi_0}}{\left(\Psi\left|\hat{\mathcal{O}}[P_{\phi_0}|\chi=s]\right|\Psi\right)} \ , \tag{6.30}$$

where $\hat{\mathcal{O}}[P_{\phi_0}|\chi = s]$ is the relational observable defined from the kinematical improper projector

$$\left\langle \phi' \left| \hat{P}_{\phi_0} \right| \phi \right\rangle := \delta(\phi' - \phi)\delta(\phi - \phi_0) \ . \tag{6.31}$$

Following §2.5.6, we can define the matrix element of this observable as

$$\begin{aligned} &\left(\Psi_{(1)}\left|\hat{\mathcal{O}}[P_{\phi_0}|\chi=s]\right|\Psi_{(2)}\right) \\ &:= \int \mathrm{d}\alpha\mathrm{d}\phi\mathrm{d}v \ \left(\hat{\mu}^{\frac{1}{2}}\Psi_{(1)}\right)^* |J|\delta(\phi-\phi_0)\delta(\chi-s)\hat{\mu}^{\frac{1}{2}}\Psi_{(2)} \ , \end{aligned} \tag{6.32}$$

where

$$\mathrm{d}v \equiv \prod_{\mathbf{q}} \mathrm{d}v_{\mathbf{q}} \equiv \prod_{\mathbf{k},\rho,j} \mathrm{d}v_{\mathbf{k};j}^{(\rho)} \ , \tag{6.33}$$

and we have restricted (6.32) to the multiplicity sector $\sigma = \mathfrak{v} = 1$. Furthermore, we also need to impose the supplementary condition $\partial\Psi/\partial\phi = 0$ as the quantum analogue of (6.7). Finally, using (6.8), we can rewrite (6.29) as

$$\left[\frac{\mathrm{e}^{-3\alpha}}{a_0^3}\left(\frac{\kappa}{2}\frac{\partial^2}{\partial\alpha^2} + a_0^6\mathrm{e}^{6\alpha}\frac{H_0^2}{2\kappa}\right) + \frac{\mathrm{e}^{-\alpha}}{a_0}\hat{H}\right]\Psi(\alpha, v) = 0 \ . \tag{6.34}$$

We note that (6.34) has the form of a quantum constraint of a BO system as described in Chapter 5, where the coupling parameter is $\kappa = 1/M$. The heavy-sector is one-dimensional and is comprised solely of the scale factor. We can then use the results of Chapter 5 to establish the unitarity of (6.34) with respect to the physical (gauge-fixed) inner product. This is the topic of the next section. In §6.3, we discuss how the corrections to the Schrödinger equation may be used to compute (potentially observable) effects in the primordial power spectra.

Before we continue, it is worth mentioning a simplification that we adopt in the treatment of $\hat{H}$ in (6.34). In general, the quantization of the frequencies $\omega_{\mathbf{q}}$ in (6.28) may be rather involved because they are complicated functions of the background degrees of freedom and their derivatives [cf. (6.18) and (6.20)]. Therefore, if one attempts to define them as operators in terms of background fields and their conjugate momenta, one would face a complicated factor ordering problem.[6] This issue can be avoided by defining conformal time as a configuration-space function [cf. (6.10)], such that $\omega_{\mathbf{q}}$ could be defined as configuration-space functions of the background degrees of freedom and of η, which is itself a function of the scale factor. This simplification is particularly well-suited for the weak-coupling expansion, and it has also been used in [114–116,135,136]. The de Sitter case becomes especially simple, since the frequencies read [cf. (6.18) and (6.20)]

$$\omega_{\mathbf{q}}^2 \equiv \omega_{\mathbf{k}}^2 := k^2 - \frac{2}{\eta^2(a)} \ , \tag{6.35}$$

for a fixed value of σ_0 in (6.10). In what follows, we thus identify the frequencies in (6.34) with functions of a, such that $\hat{H}$ only depends on this 'heavy' degree of freedom parametrically.

[6]Nonetheless, this ordering ambiguity could provide further corrections to the usual description of QFT on a curved, classical background.

6.2 Weak-coupling expansion. Unitarity

We can use a weak-coupling expansion in powers of κ (which can be seen as the inverse, rescaled Planck mass squared) to find solutions to the constraint (6.34) for the BO system comprised of the scale factor (one-dimensional 'heavy sector') and the perturbations ('light sector'). The light-sector Hamiltonian $\hat{H}$ is of order κ^0. First, it is useful to rewrite (6.34) in the following form:

$$\left(\frac{\kappa}{2}\frac{\partial^2}{\partial\alpha^2} + a_0^6 e^{6\alpha}\frac{H_0^2}{2\kappa} + a_0^2 e^{2\alpha}\hat{H}\right)\Psi(\alpha, v) = 0 \ . \tag{6.36}$$

Equation (6.36) coincides with (5.25) and (5.26) if we formally set $Q^a = \alpha$, $\mathbf{G} = -1$, $V = a^6 H_0^2/2$, $q^\mu = v_{\mathbf{q}}$, $V_m = a^2 \sum_{\mathbf{q}} \omega_q^2 v_{\mathbf{q}}^2/2$, $h^{\mu\nu} = \delta^{\mu\nu} a^2$ (for μ, ν ranging over the $v_{\mathbf{q}}$ variables), and $h = 1$.[7] Following §5.2.2, we then consider the minimal BO ansatz [cf. (5.34)]

$$\Psi(\alpha, v) = \exp\left[\frac{\mathrm{i}}{\kappa}\mathcal{W}(\alpha, v)\right] = e^{\frac{\mathrm{i}}{\kappa}\mathcal{W}_0(\alpha, v)}\psi(\alpha; v) \ , \tag{6.37}$$

which was used in the context of quantum cosmology in [113–116, 120, 135–140] in the form given in (5.32) or in the first equality in (6.37). We find that $\mathcal{W}_0$ only depends on α, and it solves the background HJ equation [cf. §5.2.2 and (6.5)]

$$-\frac{1}{2}\left(\frac{\partial\mathcal{W}_0}{\partial\alpha}\right)^2 + a_0^6 e^{6\alpha}\frac{H_0^2}{2} = 0 \ , \tag{6.38}$$

the solution of which is

$$\mathcal{W}_0(\alpha) = -\frac{\sigma_0 a_0^3 H_0}{3} e^{3\alpha} + \text{const.} \ . \tag{6.39}$$

For convenience, we choose the classically expanding solution with $\sigma_0 = 1$ [cf. (6.9)]. We note that (6.38) corresponds to the constraint $\tilde{C} = -\kappa p_\alpha^2/2 + a^6 H_0^2/(2\kappa)$, which is related to the de Sitter limit of (6.5) by a change of einbein frame, $C = \tilde{C}/a^3$ [cf. (1.41)]. If we choose conformal time [as defined in (6.10)] to be the background clock and if we use the constraint $\tilde{C}$, the background einbein or lapse is determined by the equation

[7] This is a formal identification because the determinant of $h_{\mu\nu} = \delta_{\mu\nu}/a^2$ for μ, ν ranging over the $v_{\mathbf{q}}$ variables is a (divergent) power of the scale factor instead of 1. This power cancels in (5.26) but not in (5.25), such that the result would not agree with (6.36). Nevertheless, the formal identification used here simply corresponds to adopting the Laplace-Beltrami ordering solely in the heavy sector, while the light-sector Hamiltonian is simply $\hat{C}_m = a^2\hat{H}$ [cf. (6.27)]. As h is a spectator variable in the derivation of (5.62), this formal identification is allowed and yields the correct result, as can be verified by a direct computation, which was performed in [62].

[cf. (6.5)]

$$1 \approx \mathcal{N}\{\eta, \tilde{C}\} = -\mathcal{N}\frac{\partial \mathcal{W}_0}{\partial \alpha}\frac{\partial \eta}{\partial \alpha} = a^2\mathcal{N} \ , \tag{6.40}$$

such that $\mathcal{N} = 1/a^2$.[8] The subsequent orders in perturbation theory are found by following §5.2.6. At order κ, we find that the phase-transformed wave function $\psi(\alpha; v)$ is a solution to the corrected Schrödinger equation

$$\mathrm{i}\frac{\partial \psi}{\partial \eta} + \mathrm{i}\hat{\Gamma}\psi = \hat{H}\psi - \frac{\kappa H_0^2 \eta^4}{2}\hat{H}^2\psi + \kappa\mathcal{V}\psi + \mathcal{O}\left(\kappa^2\right) \ , \tag{6.41}$$

where we used (5.62) with $\mathcal{N} = 1/a^2$, $V = a^6 H_0^2/2$, $h = 1$, and $\hat{C}_m = a^2\hat{H}$, as well as (6.10). Furthermore, since the heavy-sector configuration space is one-dimensional in this case, there is no contribution from the terms involving the x^i degrees of freedom in (5.62), and we have formally set $g = 1, g^{ij} = 0$. The term $\kappa\mathcal{V}$ is given in (5.64) and, in this case, it is only a function of conformal time. Therefore, we can absorb $\kappa\mathcal{V}$ into an order-κ η-dependent phase redefinition of ψ. This is allowed because, as we will see, the physical inner product is insensitive to phase transformations of ψ, as it should be. Finally, $\hat{\Gamma}$ is given in (5.63) and, in the present case, it reduces to

$$\hat{\Gamma} = \frac{\partial}{\partial \eta}\log|H_0^2\eta^3|^{-\frac{1}{2}} + \frac{\kappa}{2}H_0^2|\eta|^3\frac{\partial}{\partial \eta}\left(|\eta|\hat{H}\right) - \kappa H_0^2\eta^4\hat{H}\frac{\partial}{\partial \eta}\log|H_0^2\eta^3|^{-\frac{1}{2}} \ . \tag{6.42}$$

We can use (6.42) together with $\hat{H}^2\psi = \mathrm{i}\hat{H}\partial\psi/\partial\eta + \mathrm{i}\hat{H}\hat{\Gamma}\psi + \mathcal{O}(\kappa)$ to bring (6.41) to a form in which the unitarity of the evolution is manifest. First, we multiply both sides of (6.41) by $|H_0^2\eta^3|^{-1/2}$ to obtain

$$\begin{aligned} &\mathrm{i}\frac{\partial}{\partial \eta}\left(|H_0^2\eta^3|^{-\frac{1}{2}}\psi\right) + \frac{\mathrm{i}\kappa}{2}H_0|\eta|^{\frac{3}{2}}\left[\frac{\partial}{\partial \eta}\left(\eta\hat{H}\right)\right]\psi + \frac{\mathrm{i}\kappa}{2}H_0|\eta|^{\frac{3}{2}}|\eta|\hat{H}\frac{\partial \psi}{\partial \eta} \\ &- \frac{\mathrm{i}\kappa}{2}H_0\left(\frac{\partial}{\partial \eta}\log|\eta|^{-\frac{3}{2}}\right)|\eta|\hat{H}\psi = \hat{H}\left(|H_0^2\eta^3|^{-\frac{1}{2}}\psi\right) + \mathcal{O}\left(\kappa^2\right) \ , \end{aligned}$$

where, as discussed above, we discarded the $\kappa\mathcal{V}$ term. Subsequently, we use the Leibniz rule to find

$$\mathrm{i}\frac{\partial}{\partial \eta}\left[\left(1 + \frac{\kappa H_0^2\eta^4}{2}\hat{H}\right)|H_0^2\eta^3|^{-\frac{1}{2}}\psi\right] = \hat{H}\left(|H_0^2\eta^3|^{-\frac{1}{2}}\psi\right) + \mathcal{O}\left(\kappa^2\right) \ . \tag{6.43}$$

[8] Due to the relation $C = \tilde{C}/a^3$ [cf. (1.41)], the change of einbein frame (1.3) implies that the background lapse associated with C is $a^3\mathcal{N} = a$, which is the usual value for the lapse in the conformal time coordinate [cf. derivation of (6.10)].

Notice that

$$\hat{\mu} := |H_0^2\eta^3|^{-1}\left(1+\kappa H_0^2\eta^4\hat{H}\right)+\mathcal{O}\left(\kappa^2\right) \tag{6.44}$$

is an instance of (5.66), and thus it corresponds to a quantum version of the absolute value of the Faddeev-Popov determinant. Its inverse is $\hat{\mu}^{-1} = \left(1-\kappa H_0^2\eta^4\hat{H}\right)|H_0^2\eta^3| + \mathcal{O}(\kappa^2)$. If we define $\tilde{\psi} := \hat{\mu}^{1/2}\psi$, then (6.43) becomes the Schrödinger equation

$$\mathrm{i}\frac{\partial\tilde{\psi}}{\partial\eta} = \hat{H}_{\text{eff}}\tilde{\psi}\ , \tag{6.45}$$

where the effective (or corrected) Hamiltonian at order κ is

$$\hat{H}_{\text{eff}} := \hat{H} - \kappa\frac{H_0^2\eta^4}{2}\hat{H}^2 + \mathcal{O}(\kappa^2)\ , \tag{6.46}$$

and it governs the dynamics of cosmological perturbations. Evidently, Eq. (6.46) may be found by directly applying the weak-coupling expansion to (6.36) instead of using the general results of Chapter 5. This was shown in [62].

We note that the matrix element (6.32) can now be written as

$$(\Psi_1|\Psi_2)_{\text{dS}} \equiv \left(\Psi_{(1)}\left|\hat{\mathcal{O}}[P_{\phi_0}|\chi=s]\right|\Psi_{(2)}\right) := \int \mathrm{d}v\ \tilde{\psi}^*_{(1)}\tilde{\psi}_{(2)}\ , \tag{6.47}$$

where $\tilde{\psi}_{(1,2)} = \hat{\mu}^{1/2}\psi_{(1,2)} = \hat{\mu}^{1/2}\exp(-\mathrm{i}\mathcal{W}_0/\kappa)\Psi_{(1,2)}$ is evaluated at $\eta = s$ and $\phi = \phi_0$. Below, we consider arbitrary values of s, and we simply identify s with the variable η. The constant ϕ_0 will be omitted. The quadratic form (6.47) may be regarded as the physical inner product in the de Sitter limit. Similarly, the conditional probabilities (6.30) become

$$p_\Psi := \frac{|\tilde{\psi}|^2}{(\Psi|\Psi)_{\text{dS}}}\ , \tag{6.48}$$

where $\tilde{\psi}$ plays the role of a conditional wave function. Thus, the evolution dictated by the Schrödinger equation (6.45) is manifestly unitarity (up to order κ) with respect to the physical inner product (6.47), and this guarantees the conservation of the conditional probabilities (6.48). More precisely, we conclude that $\hat{H}_{\text{eff}}$ is symmetric with respect to (6.47) [cf. (6.27) and (6.28)], and it is formally self-adjoint if the weak-coupling expansion is well-defined and adequate boundary conditions are chosen for $\tilde{\psi}_{(1,2)}$. Notice that (6.47) is insensitive to (possibly η-dependent) phase transformations of $\psi_{(1,2)} = \exp(-\mathrm{i}\mathcal{W}_0/\kappa)\Psi_{(1,2)}$ or of $\tilde{\psi}_{(1,2)} = \hat{\mu}^{1/2}\psi_{(1,2)}$, as mentioned above. Furthermore, since the heavy sector is one-dimensional here, the inner product (6.47) establishes the unitarity of the light sector regardless of the choice of factorization discussed in Appendix B [see (B.30)].

Although we know that the measure (6.44) is related to the Faddeev-Popov determinant via (5.68), it is instructive to verify this explicitly here. First, we rewrite the inner product (6.47) as

$$\begin{aligned}
&\int \mathrm{d}v\ \tilde{\psi}^*_{(1)}\tilde{\psi}_{(2)} = \int \mathrm{d}v\ \psi^*_{(1)}\hat{\mu}\psi_{(2)} \\
&= \int \mathrm{d}v\ \Psi^*_{(1)}|H_0^2\eta^3|^{-1}\left(1+\kappa H_0^2\eta^4\hat{H}\right)\Psi_{(2)} + \mathcal{O}(\kappa^2) \\
&= \int \mathrm{d}v\ \Psi^*_{(1)}|\tilde{G}|^{\frac{1}{2}}a^2\left(1+\kappa H_0^2\eta^4\hat{H}\right)\Psi_{(2)} + \mathcal{O}(\kappa^2)\ ,
\end{aligned} \tag{6.49}$$

where we used $\psi_{(1,2)} = \exp(-\mathrm{i}\mathcal{W}_0/\kappa)\Psi_{(1,2)}$, $\tilde{G} = -2\mathcal{N}^2Vg$ [cf. (5.9)], $\mathcal{N} = 1/a^2$, $V = a^6H_0^2/2$, and $g = 1$. Notice that the last line of (6.49) coincides with (5.69) for $h = 1$ and the measure given in (5.68). Equation (6.49) defines a manifestly positive-definite inner product with a symmetric measure. Second, we note that the classical Faddeev-Popov determinant associated with the choice of conformal time as the background clock and the constraint $\tilde{C}$ is [cf. (1.78) and (6.40)]

$$\frac{1}{\omega} = \{\eta, \tilde{C}\} = \frac{\kappa}{H_0a_0}\left\{\mathrm{e}^{-\alpha}, \frac{p_\alpha^2}{2}\right\} = -\frac{\kappa}{H_0^2a^2}p_\eta\ , \tag{6.50}$$

where p_η is the canonical momentum conjugate to (6.10) (with $\sigma_0 = 1$). Using (6.43), we can then write (6.49) in the alternative form

$$\begin{aligned}
&\int \mathrm{d}v\ \tilde{\psi}^*_{(1)}\tilde{\psi}_{(2)} = \int \mathrm{d}v\ \psi^*_{(1)}\hat{\mu}\psi_{(2)} \\
&= \int \mathrm{d}v\ \psi^*_{(1)}|H_0^2\eta^3|^{-\frac{1}{2}}\left(1+\kappa H_0^2\eta^4\hat{H}\right)|H_0^2\eta^3|^{-\frac{1}{2}}\psi_{(2)} + \mathcal{O}(\kappa^2) \\
&= \int \mathrm{d}v\ \psi^*_{(1)}|H_0^2\eta^3|^{-\frac{1}{2}}\left(1+\mathrm{i}\kappa H_0^2\eta^4\frac{\partial}{\partial\eta}\right)|H_0^2\eta^3|^{-\frac{1}{2}}\psi_{(2)} + \mathcal{O}(\kappa^2) \\
&= \int \mathrm{d}v\ \Psi^*_{(1)}|H_0^2\eta^3|^{-\frac{1}{2}}\mathrm{i}\kappa H_0^2\eta^4\frac{\partial}{\partial\eta}|H_0^2\eta^3|^{-\frac{1}{2}}\Psi_{(2)} + \mathcal{O}(\kappa^2) \\
&= \int \mathrm{d}v\ \Psi^*_{(1)}|\tilde{G}|^{\frac{1}{2}}\left(-\frac{\kappa}{H_0^2a^3}\hat{p}_\eta a\right)\Psi_{(2)} + \mathcal{O}(\kappa^2)\ ,
\end{aligned} \tag{6.51}$$

where the momentum operator conjugate to η is defined as

$$\hat{p}_\eta = -\mathrm{i}|\tilde{G}|^{-\frac{1}{4}}\frac{\partial}{\partial\eta}|\tilde{G}|^{\frac{1}{4}} \tag{6.52}$$

in relation to the metric $\tilde{\mathbf{G}}$ [128]. Thus, the last line of (6.51) is a quantum version of (6.50) with a particular factor ordering. Although the operator inserted in the last line of (6.51) is not generally symmetric with respect to the light-sector measure $\mathrm{d}v$, we note from (6.49) and (6.51) that its quadratic form is positive-definite and equivalent to that of the symmetric operator $\hat{\mu}$ for solutions of the quantum constraint. In this way, the inner product (6.47) is well-defined and conserved with respect to the background clock (conformal time).[9]

We stress that (6.45) has no "unitarity-violating" terms. These terms, which were found and discussed in [114–116, 120], are absorbed into the Faddeev-Popov measure (6.44). The formalism presented here shows that this measure consistently follows from the weak-coupling expansion of the master WDW equation. We thus differ from the previous literature with respect to the definition and interpretation of the inner product and the ensuing unitarity of the evolution of conditional wave functions.[10]

It is also important to note that, at order κ^0, the Schrödinger equation (6.45) coincides with (6.26), and thus QFT in curved spacetime arises from the weak-coupling expansion of the master WDW equation. Although this is well-known from the earlier literature, our formalism makes it clear that the QFT wave function(al) is an instance of a conditional wave function $\tilde{\psi}$ and, therefore, of relative initial data (cf. §2.7.1).

6.3 Corrections to primordial power spectra

We may regard (6.45) as the Schrödinger picture of a QFT on de Sitter space, and the Hamiltonian operator is $\hat{H}_{\text{eff}}$. It is then interesting to examine the corresponding phenomenology: what are the power spectra of perturbations predicted by (6.45)? We now turn to this calculation, and we will see that the spectra coincide with the usual results at the lowest order, whereas the order-κ corrections lead to modifications, the observability of which has to be carefully discussed.

6.3.1 Restriction to a single mode

In the previous literature concerning the BO approach [114–116,135,136,138,140,141], it is common practice to simplify the calculations by restricting oneself to a single Fourier mode (or, more precisely, to a single $v_{\mathbf{q}}$ mode). Here, we also follow this procedure, which is at times called a 'random phase approximation' [138, 140, 141]. Concretely,

[9] To the best of our knowledge, this is a new result. It is important to mention that Barvinsky has discussed the relation between the classical Faddeev-Popov determinant and the physical (gauge-fixed) inner product by means of perturbation theory in powers of $\hbar$ [51], but the relation of the gauge-fixing procedure to the BO approach was not examined. Here [cf. Chapter 5], we show that the BO approach is a particular case of the general framework considered in Chapter 2, and we work with perturbation theory in powers of κ instead of $\hbar$.

[10] Lämmerzahl has discussed a nontrivial definition of the measure in the context of quantum optics in gravitational fields [129].

this involves the ansatz

$$\tilde{\psi}(\alpha; v) = \prod_{\mathbf{q}} \tilde{\psi}_{\mathbf{q}}(\alpha; v_{\mathbf{q}}) \ , \tag{6.53}$$

from which we obtain [cf. (6.27) and (6.45)]

$$\begin{aligned} \hat{H}^2\tilde{\psi} &= \sum_{\mathbf{q}} \hat{H}_{\mathbf{q}}^2\tilde{\psi} + \sum_{\mathbf{q}'\neq\mathbf{q}} \hat{H}_{\mathbf{q}}\hat{H}_{\mathbf{q}'}\tilde{\psi} \\ &= \sum_{\mathbf{q}} \hat{H}_{\mathbf{q}}^2\tilde{\psi} + \tilde{\psi} \sum_{\mathbf{q}'\neq\mathbf{q}} \frac{\hat{H}_{\mathbf{q}}\tilde{\psi}_{\mathbf{q}}}{\tilde{\psi}_{\mathbf{q}}} \frac{\hat{H}_{\mathbf{q}'}\tilde{\psi}_{\mathbf{q}'}}{\tilde{\psi}_{\mathbf{q}'}} \\ &= \sum_{\mathbf{q}} \hat{H}_{\mathbf{q}}^2\tilde{\psi} - \tilde{\psi} \sum_{\mathbf{q}'\neq\mathbf{q}} \frac{\partial_\eta\tilde{\psi}_{\mathbf{q}}}{\tilde{\psi}_{\mathbf{q}}} \frac{\partial_\eta\tilde{\psi}_{\mathbf{q}'}}{\tilde{\psi}_{\mathbf{q}'}} + \mathcal{O}(\kappa) \ . \end{aligned} \tag{6.54}$$

The last term in the right-hand side of (6.54) generally diverges, and one would need to resort to a subtraction scheme, such as the ones considered in [133, 142, 143], in order to regularize (6.54).[11] However, one often assumes that the last term in the right-hand side of (6.54) can be discarded because the terms with η-derivatives add incoherently. It is important to emphasize that, in the absence of a detailed subtraction scheme, this is a formal approximation, which we call the random phase approximation. A complete account of the regularization of (6.34) in the context of the random phase approximation is, to the best of our knowledge, currently lacking.[12] Notwithstanding, it is possible to give a heuristic physical interpretation of this approximation. Clearly, if we neglect the second sum in (6.54), we are discarding interaction terms between the different modes (the different $v_{\mathbf{q}}$ variables). As was argued in [144], this is equivalent to assuming that such interactions are negligible,[13] and that one may concentrate solely on the effects of the quantization of the de Sitter background on the evolution of a given mode. Indeed, the presence of a quantum background is the key physical distinction between the usual QFT in curved spacetime and the master WDW equation.

It is also useful to note that, due to the truncation of the action at quadratic order in the perturbations (6.13), the master WDW equation (6.34) follows from a quantization of the classical theory which is only valid if the higher-order $\mathcal{O}(v^3)$-terms are negligible. Consequently, the Schrödinger equation (6.45) provides a reliable account of the dynamics only in regions of the $v_{\mathbf{q}}$-configuration space where the $\mathcal{O}(v^3)$-corrections can be ignored. In this region, the random phase approximation is reasonable because

[11] Of particular interest is Sec. IV of [142], in which the BO approach is applied to a WDW equation with higher-derivative terms, and the adiabatic subtraction procedure is used. Furthermore, a general overview of the adiabatic subtraction procedure for Schrödinger-picture quantum fields that propagate on FLRW spacetimes is available in [143].

[12] It would be interesting to investigate this in the future.

[13] Somewhat more artificially, one could also consider the case in which only one of $v_{\mathbf{q}}$ fields is classically evolving, such that only this field needs to be quantized.

the second sum in (6.54) includes $\mathcal{O}(v^3)$-terms.

In rest of this Chapter, we make the assumption that it is possible to regularize (6.54) with a subtraction scheme, such that the formal random phase approximation can be applied. In this way, the Schrödinger equation (6.45) reduces to the single-mode equation [cf. (6.28)]

$$\mathrm{i}\frac{\partial\tilde{\psi}_{\mathbf{q}}}{\partial\eta} = \hat{H}_{\mathbf{q}}\tilde{\psi}_{\mathbf{q}} - \kappa\frac{H_0^2\eta^4}{2}\hat{H}_{\mathbf{q}}^2\tilde{\psi}_{\mathbf{q}} \ . \tag{6.55}$$

6.3.2 Relative initial data

Following Chapter 4, we consider that the wave function of the universe should be interpreted as the relative initial data for its quantum evolution. Clearly, in addition to the hypotheses that the weak-coupling expansion and random phase approximation are valid, the choice of relative initial data is a key factor in determining the power spectra. Due to [cf. (6.37) and (6.53)]

$$\Psi(\alpha, v) = \mathrm{e}^{\frac{\mathrm{i}}{\kappa}\mathcal{W}_0(\alpha)}\hat{\mu}^{-\frac{1}{2}}\prod_{\mathbf{q}}\tilde{\psi}_{\mathbf{q}}\left(\eta(\alpha); v_{\mathbf{q}}\right) \ , \tag{6.56}$$

we see that the wave function of the universe $\Psi(\alpha, v)$ is determined by a choice of state for each mode $\tilde{\psi}_{\mathbf{q}}$, which corresponds to a conditional wave function that describes the evolution of perturbations relative to the value of conformal time.[14]

What choice should be made for $\tilde{\psi}_{\mathbf{q}}$? Although one can, in principle, choose general states,[15] it is reasonable to fix $\tilde{\psi}_{\mathbf{q}}$ to coincide with the Bunch-Davies vacuum at the lowest order. Let us then consider

$$\tilde{\psi}_{\mathbf{q}} = \mathcal{N}_{\mathbf{q}}(\alpha)\exp\left\{-\frac{1}{2}\Omega_{\mathbf{q}}(\alpha)v_{\mathbf{q}}^2 - \frac{\kappa}{4}\Gamma_{\mathbf{q}}(\alpha)v_{\mathbf{q}}^4\right\} \ , \tag{6.57}$$

where $\mathfrak{Re}\Omega_{\mathbf{q}}(\alpha)$, $\mathfrak{Re}\Gamma_{\mathbf{q}}(\alpha) > 0$. The goal is to solve for $\mathcal{N}_{\mathbf{q}}(\alpha)$, $\Omega_{\mathbf{q}}(\alpha)$ and $\Gamma_{\mathbf{q}}(\alpha)$ and to choose boundary conditions such that (6.57) reduces to the Bunch-Davies state at order κ^0.

Although we take the $\mathcal{O}(v^3)$-terms to be negligible, such that (6.55) is valid, the inclusion of the quartic term in (6.57) is needed for consistency. Indeed, $\Gamma_{\mathbf{q}}(\alpha)$ will be seen to affect the power spectra,[16] but it does not necessarily lead to non-Gaussianities

[14] Due to the definition (6.10), this conditioning on η is also equivalent to a conditioning on the value of the scale factor. Furthermore, there is a formal conditioning on the value of the scalar field ϕ [cf. (6.32)] due to the way the de Sitter limit was constructed from a more general inflationary model.

[15] See, for example, [116] for a discussion on excited states and their relation to the master WDW equation.

[16] Moreover, the operator $\hat{H}_{\mathbf{q}}^2$ in (6.55) includes a term proportional to $v_{\mathbf{q}}^4$.

in the CMB. The reason for this is that the master WDW equation may have to be replaced by another constraint, which is derived from another truncation of the classical theory, in regions where $\mathcal{O}(v^3)$-terms are not negligible, as was discussed above. A similar remark was given in the semiclassical formalism presented in [145].

The equations for $\mathcal{N}_{\mathbf{q}}(\alpha)$, $\Omega_{\mathbf{q}}(\alpha)$ and $\Gamma_{\mathbf{q}}(\alpha)$ are found by using the ansatz (6.57) in (6.55) and discarding terms of order κ^2. The result is

$$\mathrm{i}\frac{\partial}{\partial\eta}\log\mathcal{N}_{\mathbf{q}} = \frac{\Omega_{\mathbf{q}}}{2} + \frac{\kappa H_0^2\eta^4}{4}\omega_{\mathbf{q}}^2 - \frac{3\kappa H_0^2\eta^4}{8}\Omega_{\mathbf{q}}^2 \,, \tag{6.58}$$

$$\mathrm{i}\frac{\partial\Omega_{\mathbf{q}}}{\partial\eta} = \Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2 - 3\kappa\Gamma_{\mathbf{q}} - \frac{3\kappa H_0^2\eta^4}{2}\Omega_{\mathbf{q}}\left(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2\right) , \tag{6.59}$$

$$\mathrm{i}\frac{\partial\Gamma_{\mathbf{q}}}{\partial\eta} = 4\Omega_{\mathbf{q}}\Gamma_{\mathbf{q}} + \frac{H_0^2\eta^4}{2}(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2)^2 \,. \tag{6.60}$$

6.3.3 Unitarity

It is worthwhile to explicitly confirm the unitarity implied by the inner product (6.47) for the evolution of the relative initial data (6.57). If

$$0 = \frac{\mathrm{i}}{2}\frac{\partial}{\partial\eta}\log\int_{-\infty}^{\infty}\mathrm{d}v_{\mathbf{q}}\ |\tilde{\psi}_{\mathbf{q}}|^2 = \mathrm{i}\mathfrak{Im}\left\langle \mathrm{i}\frac{\partial}{\partial\eta}\right\rangle \tag{6.61}$$

holds, then the norm of $\tilde{\psi}_{\mathbf{q}}$ is conserved. Due to (6.57), we find

$$\left\langle \mathrm{i}\frac{\partial}{\partial\eta}\right\rangle = \left\langle \mathrm{i}\frac{\partial}{\partial\eta}\log\mathcal{N}_{\mathbf{q}} - \frac{\mathrm{i}}{2}\frac{\partial\Omega_{\mathbf{q}}}{\partial\eta}v_{\mathbf{q}}^2 - \frac{\mathrm{i}\kappa}{4}\frac{\partial\Gamma_{\mathbf{q}}}{\partial\eta}v_{\mathbf{q}}^4\right\rangle \,. \tag{6.62}$$

To compute this expectation value, we note that it suffices to perform a set of Gaussian integrals because the non-Gaussian term in (6.57) is proportional to κ, and thus its contribution can be computed in perturbation theory. Using (6.57), (6.58), (6.59) and (6.60) and neglecting terms of order κ^2, we obtain

$$\begin{aligned}
\mathfrak{Im}\left\langle \mathrm{i}\frac{\partial}{\partial\eta}\log\mathcal{N}_{\mathbf{q}}\right\rangle &= \frac{\mathfrak{Im}\Omega_{\mathbf{q}}}{2} - \frac{3\kappa H_0^2\eta^4}{4}(\mathfrak{Re}\Omega_{\mathbf{q}})\mathfrak{Im}\Omega_{\mathbf{q}} \,, \\
\mathfrak{Im}\left\langle -\frac{\mathrm{i}}{2}\frac{\partial\Omega_{\mathbf{q}}}{\partial\eta}v_{\mathbf{q}}^2\right\rangle &= -\frac{\mathfrak{Im}\Omega_{\mathbf{q}}}{2} + \frac{9\kappa H_0^2\eta^4}{8}(\mathfrak{Re}\Omega_{\mathbf{q}})\mathfrak{Im}\Omega_{\mathbf{q}} - \frac{3\kappa H_0^2\eta^4\mathfrak{Im}\Omega_{\mathbf{q}}\left(\omega_{\mathbf{q}}^2 + \mathfrak{Im}\Omega_{\mathbf{q}}^2\right)}{8\mathfrak{Re}\Omega_{\mathbf{q}}} \\
&\quad + \frac{3\kappa(\mathfrak{Re}\Gamma_{\mathbf{q}})\mathfrak{Im}\Omega_{\mathbf{q}}}{4\mathfrak{Re}\Omega_{\mathbf{q}}^2} + \frac{3\kappa\mathfrak{Im}\Gamma_{\mathbf{q}}}{4\mathfrak{Re}\Omega_{\mathbf{q}}} \,, \\
\mathfrak{Im}\left\langle -\frac{\mathrm{i}}{4}\frac{\partial\Gamma_{\mathbf{q}}}{\partial\eta}v_{\mathbf{q}}^4\right\rangle &= -\frac{3\kappa H_0^2\eta^4}{8}(\mathfrak{Re}\Omega_{\mathbf{q}})\mathfrak{Im}\Omega_{\mathbf{q}} + \frac{3\kappa H_0^2\eta^4\mathfrak{Im}\Omega_{\mathbf{q}}\left(\omega_{\mathbf{q}}^2 + \mathfrak{Im}\Omega_{\mathbf{q}}^2\right)}{8\mathfrak{Re}\Omega_{\mathbf{q}}} \\
&\quad - \frac{3\kappa(\mathfrak{Re}\Gamma_{\mathbf{q}})\mathfrak{Im}\Omega_{\mathbf{q}}}{4\mathfrak{Re}\Omega_{\mathbf{q}}^2} - \frac{3\kappa\mathfrak{Im}\Gamma_{\mathbf{q}}}{4\mathfrak{Re}\Omega_{\mathbf{q}}}
\end{aligned}$$

Then, the value of (6.62) is found by adding the three equations above. The result, as expected, is

$$\mathfrak{Im}\left\langle \mathrm{i}\frac{\partial}{\partial\eta}\right\rangle = 0 \ . \tag{6.63}$$

6.3.4 Power spectra I. Definitions

The conditional correlation function [cf. (6.32), (6.47) and (6.48)]

$$\begin{aligned}\langle v_{\mathbf{q}}^2\rangle := \mathrm{E}_\Psi[v_{\mathbf{q}}^2|\eta,\phi_0] &= \frac{\left(\Psi \left|\hat{\mathcal{O}}[v_{\mathbf{q}}^2 P_{\phi_0}|\eta]\right| \Psi\right)}{\left(\Psi \left|\hat{\mathcal{O}}[P_{\phi_0}|\eta]\right| \Psi\right)} \\ &= \frac{\left(\Psi\left|v_{\mathbf{q}}^2\right|\Psi\right)_{\mathrm{dS}}}{(\Psi|\Psi)_{\mathrm{dS}}} \\ &= \frac{\int \mathrm{d}v\ \tilde{\psi}^* v_{\mathbf{q}}^2 \tilde{\psi}}{\int \mathrm{d}v\ \tilde{\psi}^*\tilde{\psi}}\end{aligned} \tag{6.64}$$

reproduces the familiar formula from QFT on curved backgrounds. The power spectrum of the $v_{\mathbf{q}}$ perturbations is then defined in the usual way,

$$\mathcal{P}_v(\mathbf{q}) := \frac{k^3}{2\pi^2}\langle v_{\mathbf{q}}^2\rangle \ . \tag{6.65}$$

Below, we will see that the power spectrum is a function solely of $k = |\mathbf{k}|$, $\mathcal{P}_v(\mathbf{q}) \equiv \mathcal{P}_v(k)$. From (6.53) and (6.57), the conditional correlation function is found to be

$$\langle v_{\mathbf{q}}^2\rangle = \frac{1}{2\mathfrak{Re}\Omega_{\mathbf{q}}} - \frac{3\kappa\mathfrak{Re}\Gamma_{\mathbf{q}}}{4(\mathfrak{Re}\Omega_{\mathbf{q}})^3} \ . \tag{6.66}$$

In order to evaluate the power spectrum (6.65), we will consider the superhorizon limit $\lim_{k\eta\to 0^-}\langle v_{\mathbf{q}}^2\rangle$ because our focus is on large scales. Furthermore, if we expand $\Omega_{\mathbf{q}} = \Omega_{\mathbf{q};0} + \kappa\Omega_{\mathbf{q};1}$ and neglect terms of order κ^2, we can express (6.66) as

$$\langle v_{\mathbf{q}}^2\rangle = \frac{1+\kappa\delta_{\mathbf{q}}}{2\mathfrak{Re}\Omega_{\mathbf{q};0}} \ , \tag{6.67}$$

where we defined the correction term

$$\delta_{\mathbf{q}} = -\frac{\mathfrak{Re}\Omega_{\mathbf{q};1}}{\mathfrak{Re}\Omega_{\mathbf{q};0}} - \frac{3\mathfrak{Re}\Gamma_{\mathbf{q}}}{2(\mathfrak{Re}\Omega_{\mathbf{q};0})^2} \ , \tag{6.68}$$

which encodes the deviation from the usual results of QFT on a fixed background.

The power spectrum of scalar perturbations is usually defined in terms of the comoving curvature perturbations [114, 115]

$$\zeta_{\mathbf{k}} := \sqrt{\frac{3\kappa}{\epsilon}}\frac{v_{\mathbf{k}}^{(\mathrm{S})}}{a} \ , \tag{6.69}$$

which are associated with CMB temperature anisotropies, and are defined on a quasi-de Sitter space characterized by a small but nonzero inflationary slow-roll parameter, $\epsilon = -\dot{H}/H^2$ [with $\cdot \equiv \mathrm{d}/\mathrm{d}\tau$; cf. (6.1)]. Their power spectrum is

$$\mathcal{P}_{\mathrm{S}}(k) := \frac{3\kappa}{\epsilon a^2}\mathcal{P}_v(k) = \frac{3\kappa}{\epsilon a^2}\frac{k^3}{2\pi^2}\left\langle v_{\mathbf{q}}^2\right\rangle \ . \tag{6.70}$$

Similarly, the power spectrum of tensor perturbations is customarily expressed in terms of the rescaled Fourier modes $\sqrt{2}h_{\mathbf{k}}^{(+,\times)}$ [to be compared with (6.16)],

$$\mathcal{P}_{\mathrm{T}}(k) := \sum_{\lambda=+,\times}\frac{24\kappa}{a^2}\mathcal{P}_v(k) = \frac{48\kappa}{a^2}\frac{k^3}{2\pi^2}\left\langle v_{\mathbf{q}}^2\right\rangle \ . \tag{6.71}$$

In general slow-roll models, the correction terms for each spectrum may be different. This was analyzed in [115], where the would-be unitarity-violating terms were simply neglected. In the formalism presented here, we have seen that they can be incorporated into the definition of $\hat{\mu}$ [cf. (6.44)].[17] As we have restricted ourselves to the (quasi-)de Sitter limit, a simplification occurs due to the fact that the frequencies (6.35) coincide, and (6.67) implies that there is a common correction factor,

$$\mathcal{P}_{\mathrm{S,T}}(k) = \mathcal{P}_{\mathrm{S,T;0}}(k)(1+\kappa\delta_{\mathbf{q}}) \ . \tag{6.72}$$

For this reason, the tensor-to-scalar ratio

$$r := \frac{\mathcal{P}_{\mathrm{T}}(k)}{\mathcal{P}_{\mathrm{S}}(k)} \equiv \frac{\mathcal{P}_{\mathrm{T;0}}(k)}{\mathcal{P}_{\mathrm{S;0}}(k)} \tag{6.73}$$

receives no corrections in this limit.

[17] It is important to mention that some of the would-be unitarity-violating terms neglected in [114–116] were, in fact, part of the complex functions $\tilde{\psi}$ and, as such, are not incorporated into $\hat{\mu}$ in our formalism, but they also do not violate unitarity with respect to the inner product (6.47). This difference will also lead to discrepancies in the results discussed in §6.3.6.

6.3.5 Power spectra II. The lowest order

Since the Schrödinger equation (6.45) coincides with the usual QFT Schrödinger equation (6.26) at the lowest order, the power spectra found from (6.67) at order κ^0 must agree with the well-known results. To see that this is indeed the case, we solve the lowest-order of (6.59) by means of the replacement

$$\Omega_{\mathbf{q};0}(\eta) = -\mathrm{i}\frac{\dot{y}_{\mathbf{q}}(\eta)}{y_{\mathbf{q}}(\eta)} \ , \tag{6.74}$$

for which (6.59) becomes

$$\ddot{y}_{\mathbf{q}} + \omega_{\mathbf{q}}^2 y_{\mathbf{q}} = \mathcal{O}(\kappa) \ . \tag{6.75}$$

Due to (6.35), the solution has the well-known form

$$y_{\mathbf{q}}(\eta) \equiv y_{\mathbf{k}}(\eta) = \frac{A}{\sqrt{2k}}\mathrm{e}^{-\mathrm{i}k\eta}\left(1 - \frac{\mathrm{i}}{k\eta}\right) + \frac{B}{\sqrt{2k}}\mathrm{e}^{\mathrm{i}k\eta}\left(1 + \frac{\mathrm{i}}{k\eta}\right) \ . \tag{6.76}$$

As we require $\mathfrak{Re}\Omega_{\mathbf{q};0}(\eta) > 0$, we must impose [cf. (6.74)]

$$B^2 - A^2 = -\mathrm{i}\left[\dot{y}_{\mathbf{k}} y_{\mathbf{k}}^* - \dot{y}_{\mathbf{k}}^* y_{\mathbf{k}}\right] > 0 \ , \tag{6.77}$$

which is satisfied if $A \propto \sinh\vartheta$ and $B \propto \cosh\vartheta$ for $\vartheta \in \mathbb{R}$. If we now truncate (6.57) at the lowest order and demand that it coincides with the Minkowski vacuum when $\eta \to -\infty$ ($a \to 0$), the value of ϑ can be fixed. Indeed, we demand that $\vartheta = 0$ such that

$$\Omega_{\mathbf{k};0}(\eta) \overset{\eta\to-\infty}{\simeq} \frac{\cosh\vartheta\mathrm{e}^{\mathrm{i}k\eta} - \sinh\vartheta\mathrm{e}^{-\mathrm{i}k\eta}}{\cosh\vartheta\mathrm{e}^{\mathrm{i}k\eta} + \sinh\vartheta\mathrm{e}^{-\mathrm{i}k\eta}} k \overset{\vartheta=0}{=} k \ . \tag{6.78}$$

Together with (6.76), this leads us to the usual Bunch-Davies results [114]

$$\Omega_{\mathbf{q};0}(\eta) \equiv \Omega_{k;0}(\eta) = \frac{k^3\eta^2}{1+k^2\eta^2} + \frac{\mathrm{i}}{\eta(1+k^2\eta^2)} \tag{6.79}$$

and

$$\langle v_{\mathbf{q}}^2 \rangle = \frac{1+k^2\eta^2}{2k^3\eta^2} + \mathcal{O}(\kappa) \overset{k\eta\to 0^-}{\simeq} \frac{1}{2k^3\eta^2} + \mathcal{O}(\kappa) \ . \tag{6.80}$$

Using $\kappa = 4\pi G/3$ and (6.10), the power spectra and tensor-to-scalar ratio then read [cf. (6.70) and (6.71)]

$$\mathcal{P}_{\mathrm{S};0}(k) = \frac{3\kappa}{\epsilon a^2}\frac{1}{4\pi^2\eta^2} = \left.\frac{GH_0^2}{\pi\epsilon}\right|_{k=aH_0} , \tag{6.81}$$

$$\mathcal{P}_{\mathrm{T};0}(k) = \frac{24\kappa}{a^2}\frac{1}{4\pi^2\eta^2} = \frac{16GH_0^2}{\pi} , \tag{6.82}$$

$$r = 16\epsilon . \tag{6.83}$$

As the slow-roll parameter ϵ appears in (6.81), and due to the fact that the perturbations freeze at horizon crossing (at least if terms of order κ^2 are neglected), Eq. (6.81) is computed at the instant in which $k = aH_0$.

6.3.6 Power spectra III. Corrections

The inclusion of terms of order κ corresponds to the inclusion of the correction term (6.68) in (6.67). To find this term, we must compute $\Omega_{\mathbf{q};1}$ and $\Gamma_{\mathbf{q}}$. We can solve (6.60) if we substitute $\Omega_{\mathbf{q}} \to \Omega_{\mathbf{q};0}$ [cf. (6.79)] and if we choose the boundary condition $\lim_{\eta\to-\infty}\Gamma_{\mathbf{q}} = 0$, which is consistent with the lowest-order Bunch-Davies solution. The solution then reads[18]

$$\Gamma_{\mathbf{q}}(\eta) = \frac{H_0^2\eta\left(4\mathrm{i}k^2\eta^2 + 4k\eta + \mathrm{i}\right)\mathrm{e}^{4\mathrm{i}\arctan(k\eta)}}{6\left(k^2\eta^2+1\right)^2} - \frac{8H_0^2\eta^4k^3\Gamma(0,-4\mathrm{i}k\eta)\mathrm{e}^{-4\mathrm{i}[k\eta-\arctan(k\eta)]}}{3\left(k^2\eta^2+1\right)^2} . \tag{6.84}$$

This solution vanishes in the infinite past by virtue of

$$\Gamma(0,z) \overset{z\to-\infty}{\simeq} \frac{\mathrm{e}^{-z}}{z} , \tag{6.85}$$

and its late-time behavior can be found from the expansion

$$\Gamma(0,z) = -\gamma_E - \log z + z + \mathcal{O}(z^2) , \tag{6.86}$$

[18] Certain computer algebra software present the solution in terms of the exponential integral function, but we chose to adopt $\Gamma(0,z)$ (the upper incomplete gamma function) that was also used in the formalism of [114].

with the Euler-Mascheroni constant γ_E. We obtain

$$\mathfrak{Re}\Gamma_{\mathbf{q}}(\eta) \overset{\eta\to 0^-}{\simeq} \frac{k^3 H_0^2 \eta^4}{3} \left[-18 + 8\gamma_E + 8\log(4k|\eta|)\right] \,. \tag{6.87}$$

Subsequently, we must compute $\Omega_{\mathbf{q};1}$. Its equation is obtained if we use $\Omega_{\mathbf{q}} = \Omega_{\mathbf{q};0} + \kappa\Omega_{\mathbf{q};1}$ in (6.59) and collect all terms of order κ,

$$\mathrm{i}\frac{\partial\Omega_{\mathbf{q};1}}{\partial\eta} = 2\Omega_{\mathbf{q};0}\Omega_{\mathbf{q};1} - 3\Gamma_{\mathbf{q}} - \frac{3H_0^2\eta^4}{2}\Omega_{\mathbf{q};0}\left(\Omega_{\mathbf{q};0}^2 - \omega_{\mathbf{q}}^2\right) \,.$$

In analogy to the Bunch-Davies vacuum, we will fix the constant of integration by requiring that $\lim_{\eta\to-\infty}\mathfrak{Re}\Omega_{\mathbf{q};1}$ is well-defined (it does not oscillate).[19] The solution is

$$\begin{aligned}\Omega_{\mathbf{q};1}(\eta) = \frac{\mathrm{e}^{2\mathrm{i}\arctan(k\eta)}H_0^2\eta^2}{k\eta+\mathrm{i}} &\left[\frac{10\mathrm{i} + 6k\eta - 3\mathrm{i}k^2\eta^2}{2(k\eta-\mathrm{i})(k\eta+\mathrm{i})}\right. \\ &\left. - \frac{4\Gamma(0,-4\mathrm{i}k\eta)}{(k\eta+\mathrm{i})}\mathrm{e}^{-4\mathrm{i}k\eta} - \frac{2\Gamma(0,-2\mathrm{i}k\eta)}{(k\eta-\mathrm{i})}\mathrm{e}^{-2\mathrm{i}k\eta}\right] \,,\end{aligned} \tag{6.88}$$

due to (6.79) and (6.84). From (6.85), we see that the required boundary condition is satisfied,[20]

$$\lim_{\eta\to-\infty}\mathfrak{Re}\Omega_{\mathbf{q};1}(\eta) = \frac{3H_0^2}{2k^2} \,. \tag{6.89}$$

We can also inspect the late-time limit of (6.88),

$$\mathfrak{Re}\Omega_{\mathbf{q};1}(\eta) \overset{\eta\to 0^-}{\simeq} H_0^2\eta^2\left[5 - 2\gamma_E + 2\log(2k|\eta|) - 4\log(4k|\eta|)\right] \,, \tag{6.90}$$

due to (6.86). With (6.87) and (6.90), as well as (6.80), we can finally compute the correction term (6.68). In the analysis of data concerning the CMB, it is customary to express the results in terms of a pivot (or reference) scale denoted by $k_\star$. For this reason, in order to make (6.68) comparable to observations, we revert the first transformation in (6.22) ($k \to \mathfrak{L}k$) and we choose $\mathfrak{L} = 1/k_\star$.[21] The correction term can then be written

[19] This is analogous to a requirement that was made in formalism of [114].

[20] Incidentally, the reason we fix the boundary condition solely for the real part of $\Omega_{\mathbf{q};1}$ is that its imaginary part does not alter the conditional correlation function (6.64). In fact, one can verify that the imaginary part of (6.88) leads to a large phase in (6.57) in the limit $\eta \to -\infty$, which, nonetheless, does not influence the power spectra.

[21] Notice that k and $k_\star$ are now dimensionful, but the result (6.91) is expressed in terms of their ratio.

as

$$\delta_{\mathbf{q}} \equiv \delta_k(\eta) = H_0^2 \left(\frac{k_\star}{k}\right)^3 \left[4 - 2\gamma_E - 2\log(-2k\eta)\right] , \tag{6.91}$$

and it leads to the corrected power spectra [cf. (6.67), (6.70), (6.71)]

$$\begin{aligned} \mathcal{P}_{\mathrm{S,T}}(k) &= \mathcal{P}_{\mathrm{S,T;0}}(k)\left[1 + \kappa\delta_{\mathbf{q}}\right] \\ &\simeq \mathcal{P}_{\mathrm{S,T;0}}(k)\left\{1 + \kappa H_0^2\left(\frac{k_\star}{k}\right)^3\left[2.85 - 2\log(-2k\eta)\right]\right\} . \end{aligned} \tag{6.92}$$

It is important to emphasize that (6.92) is different from the result presented in [114]. As the constant κ is equal to the inverse, rescaled Planck mass squared used in that reference, the two results can be easily compared. Apart from a difference in numerical factors, we also note that the logarithmic term was absent in the earlier treatment. We now examine the reasons for this discrepancy.

6.3.7 Power spectra IV. Discussion

The disagreement between (6.92) and the earlier literature [114–116, 140] stems from the fact that these preceding works not only discarded the would-be unitarity-violating terms that we have incorporated into the definition of $\hat{\mu}$ in (6.44), but they also neglected the imaginary part of terms of order κ in (6.45) and (6.59), which were also thought to violate unitarity (see also footnote 17). In the present formalism, there is no need to discard these additional terms, as they are simply part of the complex conditional wave functions and do not jeopardize the conservation of the norm of $\tilde{\psi}$. From (6.63), we see that an explicit calculation confirms that the inner product (6.47) is conserved (assuming that the Hamiltonian (6.46) is self-adjoint by an adequate choice of boundary conditions for $\tilde{\psi}$). The inclusion of these additional terms resulted in the different expression (6.92).

The most interesting difference is the logarithmic term. Since the mode k crosses horizon at an instant defined by $aH_0 = k$, the logarithm essentially counts the number of e-folds between horizon crossing and the instant η. Therefore, it grows in conformal time and might invalidate perturbation theory at late times or in the superhorizon limit. Our results regarding the unitarity of the dynamics of a BO system (cf. Chapter 5 and §6.2) clearly depend on whether the perturbative expansion in powers of $\kappa = 1/M$ is well-defined. Before we discuss if and how this can be guaranteed, let us give an approximate estimate of the value of (6.91). We can discard the logarithm if the correction term is computed around horizon crossing, since then $\log(-k\eta) \simeq 0$. The reliability of this evaluation depends on the superhorizon conservation of $\zeta_{\mathbf{k}}$. We obtain

$$\kappa\delta_k \simeq 1.5\,\kappa H_0^2 \left(\frac{k_\star}{k}\right)^3 \,, \tag{6.93}$$

which implies that there is an enhancement of power at large scales and the spectrum acquires a scale dependence. This is essentially the result found in [114], apart from the numerical pre-factor, which was approximately 0.988. There, the upper bound $\kappa H_0^2 \lesssim 1.7 \times 10^{-10}$ was also derived. Using this result, one could also choose the value of η at which the correction term is computed such that $\kappa\delta_k(\eta)$ would not invalidate perturbation theory. Nevertheless, these are heuristic estimations. Can we go beyond them?

It may be that a different choice of relative initial data [cf. (6.57)] can avoid the appearance of terms that grow in conformal time. However, such choice would likely be more complicated than (6.57), and it should have a reasonable justification [such as the analogy to the Bunch-Davies state that guided the construction of (6.57)] instead of being simply engineered. Moreover, it seems reasonable to suppose that a better understanding of the physics behind (6.92) will be gained by applying the present formalism to more general slow-roll models and other realistic accounts of the early Universe. The (quasi-)de Sitter approximation, on which (6.92) is based, may be too simple.

Finally, although the secular growth of the logarithm is worrisome, it is important to note that secular terms frequently appear in perturbative QFT calculations in de Sitter space, for example, in the computation of quantum corrections to correlation functions or to the late-time structure of the Bunch-Davies state [146–148]. A similar logarithm was also present in [144], where the master WDW equation was solved in terms of suitably defined quantum moments. Is there a relation between secular terms found in the literature and the logarithm in (6.92)? This is conceivable because, in the literature [146–150], the logarithmic terms follow from the usual perturbation theory in QFT, whereas the logarithm in (6.92) is a consequence of the weak-coupling expansion, which is akin to a loop expansion (as was explained in [151]).

An interesting question that is left for future work is whether any of the various treatments given to the large time-dependent logarithms in de Sitter space QFT can be adapted to the master WDW equation (6.34). Indeed, the resummation procedures described in the literature might also be applicable in the formalism presented here. In particular, in the framework of the dynamical renormalization group [146,147,149,150], late-time divergences can be subtracted by adequate counterterms that depend on an arbitrary time scale. In this subtraction procedure, the validity of perturbation theory may be improved by the resummation of leading time-dependent logarithms. Thus, it is imaginable that (some of) these schemes could be used in the present formalism in order to guarantee the validity of the perturbative expansion in powers of κ.

Conclusions and Outlook

O.1 Conclusions

Although there are presently various candidate theories of quantum gravitation, each with its merits and shortcomings, two fundamental issues remain unclear. First, is the diffeomorphism symmetry emergent or is it an essential feature of the quantum theory? If it is essential, how should the quantum states be interpreted in a diffeomorphism-invariant way? Can we meaningfully attribute a probabilistic interpretation to them? Second, if there is a physical Hilbert space, how can we define and interpret the operators that act on it? In what sense (if any) can they represent observables?

The search for a (partial) resolution of these issues has spawned numerous interesting proposals, which often combine aspects of quantum field theory, quantum foundations and quantum information science. Regarding the interpretation of the quantum states, some researchers advocate the use of the consistent or decoherent histories formalism to assign probabilities to quantum states also in a diffeomorphism-invariant setting (see, for instance, [152–156]), while others argue that the de Broglie-Bohm theory [26, 27] can meaningfully dissolve the conundrum related to the problem of time in a theory without a preferred time parameter and, perhaps, explain the origin of probabilities for subsystems of the Universe. Rovelli has also suggested a kind of quantum relational dynamics in his 'relational quantum mechanics' [157]. Most notably, the use of the solutions to the quantum constraint in the definition of conditional probabilities has attracted considerable attention in the literature [75, 86–93].

Methods of construction and interpretation of observables have also been actively researched. In particular, one can reasonably define classical observables as diffeomorphism-invariant extensions of geometrical objects [30, 31, 33, 76, 78, 94, 95, 158], which encode the relational dynamics among the different fields of a theory, as Rovelli has emphasized in his "evolving constants of motion" description [17, 96, 97]. The invariant extensions are often also called relational observables [57, 58]. Classically, their interpretation is clear: as they are invariant extensions of the components of tensor fields in certain local coordinates, the relational observables capture the value of a field in terms of generalized clocks and rods; i.e., they yield a prediction for value of field conditioned on the value that is read on the generalized measuring instruments. This is a conditional prediction, and it can be taken to represent the outcome of a measurement. But what are the corresponding quantum observables? And are they relational in any meaningful sense? Indeed, the appropriate procedure of quantization of these observables has remained unsettled [58, 79–81, 94, 95]. In other words, the literature currently lacks a systematic, uncontroversial and model-independent way to define quantum observables in a diffeomorphism-invariant theory.

In this thesis, we have presented a possible formalism for the systematic construction and interpretation of relational observables, both in the classical and quantum theories. We have not solved the measurement problem or the origin of probabilities, but we have suggested a tentative set of postulates in the quantum theory, which bring to the forefront the consequences of diffeomorphism invariance for the probabilistic interpretation as a form of quantum relational dynamics. We have also argued that, under certain circumstances, the dynamics can be understood in terms of conditional probabilities, and the averages of observables correspond to conditional expectation values of geometric objects. This is reasonable because the classical relational observables are, in a sense, conditional quantities. Thus, our work connects the two fundamental issues of probabilities and observables in a diffeomorphism-invariant setting.

We have established the general framework in Chapters 1 and 2, and illustrated the formalism with examples in Chapters 3 and 4. For simplicity and clarity, we have restricted ourselves to mechanical toy models so as to evade problems with regularization and anomalies that might appear in a more general field-theoretical approach, and yet cloud the conceptual issues related to diffeomorphism invariance and the problem of time. The general formalism we have presented is, in principle, model independent and it is applicable to mechanical theories that are integrable, in which the solutions to the classical field equations and to the quantum constraints can be found (with the aid of perturbation theory, if needed). Clearly, this formalism is necessarily provisional and not to be seen as a definitive framework, but we believe it clarifies several conceptual issues at interface of quantum theory and gravitation and, furthermore, it provides a useful set of tools for various toy models, as illustrated in Chapters 3, 4 and 6. These tools may need to be made more rigorous or refined if applied to more realistic (field-theoretical) scenarios.

The method presented here is based on the classical Faddeev-Popov gauge-fixing procedure [20, 21], with which invariant extensions of gauge-fixed quantities (i.e., variables written in a fixed generalized reference frame) are obtained by writing them in an arbitrary frame using integral formulae. We have explained how to perform the corresponding procedure in the canonical (operator-based) quantum theory, and we have compared our proposal with the earlier literature. In particular, we emphasize that a defining feature of our formalism is the operator version of the Faddeev-Popov resolution of the identity, which implies that the identity operator is invariantly extended to the identity in the physical Hilbert space. In contrast, in the earlier method of [53], this was not the case.

The Faddeev-Popov resolution to the identity is tied to a choice of generalized clock that defines a generalized quantum reference frame. We have given an explicit formula for the Faddeev-Popov operator, and we have discussed under what circumstances one can define a physical propagator that defines a unitary quantum evolution in the quantum reference frame. Furthermore, changes of well-defined quantum reference frames can be performed as changes of basis in the physical Hilbert space of the theory. Under certain circumstances, the interpretation of the generalized reference frame can be based on conditional probabilities, which express the time parameter measured by the clock as the condition on which the observations (or more, precisely, probabilistic predictions) of an experimenter in a certain reference frame are based. In this case, we have argued that all the dynamical content of the quantum theory is encoded in conditional wave functions related to the relative initial data of the quantum evolution. Thus, there can be two points of view: (1) the gauge-fixed point of view, which only deals with the conditional wave functions; (2) the manifestly invariant point of view, in which one works with the relational observables.

The method presented here can be regarded as a type of generalization of certain earlier developments [51, 74, 75, 83]. Indeed, we have shown that our formalism recovers the well-known Page-Wootters formalism [75, 86–93] as a particular case, and that it is also related to the 'G-twirl' operations and 'relativization maps' that are often defined when quantum reference frames are discussed in the quantum foundations and quantum information science communities (see, for example, [73–75, 82, 83]). The equivalence between the Page-Wootters approach and the use of a kind of relational observables was first noted in [75] for a particular class of gauge conditions in certain toy models. Our results, which use a definition of quantum observables that is, in principle, different, may be regarded as an extension of [75]. In this way, our formalism, which is based on standard techniques in the treatment of gauge systems, may also be useful in examples of interest to these other communities beyond the context of quantum gravity and cosmology.

It is also worthwhile to emphasize that, due to the method of construction of observables and the ensuing dynamics dictated by physical propagators, one sees that the notion of evolution does not disappear in the quantum theory as is frequently claimed [6, 22, 23]. In this way, the quantum problem of time, which is motivated by the fact that physical states do not depend on an arbitrary choice of worldline time coordinate and seem to be "static", is as illusory as its classical counterpart. Evidently, one must face this conclusion with a bit of skepticism, as the formalism presented here is, as already mentioned, provisional, and there are several other attempts at a solution to the problem of time [22–24]. However, we believe the quantum relational dynamics described here is reasonable.

In particular, we have seen that the formalism is directly useful in cosmology. We have considered the canonical quantum cosmology of minisuperspace models in metric variables. Although this may not be the fundamental variables of quantum gravity, the classical limit can be straightforwardly derived in this approach, which is therefore sufficient for illustrating the general framework developed in Chapters 1 and 2. We have argued that the question of singularity avoidance in cosmology can be related to the quantum relational dynamics by a conditional form of the DeWitt criterion (cf. §4.1), and that the quantum gravitational corrections found from the weak-coupling expansion of the master WDW equation can be straightforwardly embedded in a relational framework.

The calculation of quantum gravitational corrections to the relational dynamics in the early Universe is of direct interest if one is to produce falsifiable predictions, as some of the effects may become observable. For this reason, we also consider the application of the weak-coupling expansion to derive corrections to the primordial power spectra (cf. Chapter 6) one of the central results of this thesis, as it clarifies how the notions of the physical inner product and relational observables may be related to the usual cosmological measurements and observations: all observables are relational, and the usual primordial correlators and other cosmological observables are understood as conditional quantities that are expressed relative to the late-time classical values of the spacetime metric. The corrections found from the weak-coupling expansion take into account the quantum nature of the spacetime background in the early universe, and the fundamental diffeomorphism invariance is encoded in the master WDW equation (6.34).

At this stage, it is useful to note that the calculation of primordial quantum gravitational effects is an active topic of research [114–116, 135, 136, 138–140, 144, 159–162], and that the weak-coupling expansion has been applied in several references in order to obtain corrections to the primordial spectra [114–116, 135, 136, 140]. What is new in our approach is the explicit connection described in Chapter 5 between this expansion and the fundamental relational theory based on the physical inner product and relational observables. We have explicitly shown how the inner product is related to a quantization of the classical Faddeev-Popov determinant, leading to a clear relation between the quantum dynamics and the gauge-fixing procedure that defines a quantum reference frame. To the best of our knowledge, this is a new result. In particular, the closed-form expression for the classical einbein [cf. (5.17)] had not been previously derived. Furthermore, we have shown that the perturbative quantum dynamics is unitary with respect to this inner product. This is important because the question of unitarity in the BO approach has been controversial [114–116, 120, 126, 135, 136, 140, 163]. Our results show that the traditional BO approach (cf. Appendix B) and weak-coupling expansion can be regarded as a particular choice of gauge fixing, and they are an instance of a more general relational framework. Although it is presently unclear whether such a paradigm can describe Nature at the fundamental level, we believe it is worth investigating its the possible observational consequences.

O.2 Outlook

There are several possible avenues of further research. First, as our method generalizes the Page-Wootters formalism, an effort to extend several results that were established in the literature using the Page-Wotters approach would be worthwhile and might lead to novel insights. Second, one can extend the calculation of unitary quantum-gravitational corrections to the primordial spectra to the case of slow-roll inflationary models or more general accounts of the early Universe, which may shed light on the correction terms, particularly the secular logarithm in (6.91). Third, as was mentioned in §6.3.7, it may be possible to adapt some of the resummation techniques from QFT in de Sitter space to ensure the validity of the weak-coupling expansion and improve perturbation theory. This is an important topic because a resummation of the large logarithm in (6.91) could enhance the observability of the corrections by enlarging their overall contribution. Fourth, a better understanding of the random phase approximation [cf. Sec. 6.3.1] is needed. It would be interesting to adopt a certain regularization procedure and verify the exact conditions under which this approximation holds. All of these further developments would facilitate the computation of well-defined quantum-gravitational effects in the early Universe that are hopefully observable.

O.2.1 Relative initial data in field theory

It is important to mention what are the implications of our formalism for the construction of relational observables in the full quantum theory of gravitation. The quantization of diffeomorphism-invariant observables in GR is a very complicated matter because these objects not only generally have involved functional forms but are also possibly nonlocal. However, if the method presented in this thesis could be generalized to field theory, it might be possible to avoid the quantization of complicated invariants. This follows from the equivalence of the two points of view mentioned above: rather than evaluating the arduous observables (invariant point of view), one could work with the conditional probabilities (gauge-fixed point of view), which are frequently simpler to compute. If this proves to be possible, than the eigenstates of self-adjoint relational observables would lead to conditional predictions.

This program would require a cautious regularization of the quantum constraints, and one would need to establish that the quantum theory is indeed not anomalous. These important tasks are outside of the scope of this thesis. If they can be carried out, then a field-theoretic generalization of the framework presented here would, in principle, be feasible. In this case, one would be able to define conditional probabilities and expectation values of geometrical objects (in the gauge-fixed point of view), without the need to evaluate their complicated diffeomorphism-invariant counterparts. The quantum dynamics would be directly encoded in the conditional predictions extracted from the solution to the quantum constraints, which would be regarded in a relational manner as the invariant extension of a certain choice of relative initial data. This is a fascinating topic that could be pursued in the future.

O.2.2 Whence probabilities?

Lastly, we note that the postulates presented in Chapter 5 assume that the Born rule is valid for the induced inner product. However, it is not clear whether this rule should be modified in a diffeomorphism invariant context. Indeed, the measurement problem becomes even more distressing in this context. However, the possibility to define physical propagators as in Chapter 5 suggests that, it might be possible to explain the origin of the Born rule with respect to some (or perhaps many) choice(s) of worldline time coordinate by considering the Schrödinger equation associated with the physical propagator. This could be done in an Everettian context (see, for instance, [164]) or, if one adopts a de Broglie-Bohm perspective, it might even be possible to describe a quantum relaxation process (following [165]) through which the Born rule emerges. We leave these topics for another occasion.

Appendix A

Review of Gauge Systems and Constrained Dynamics

This appendix deals with the theory of constrained Hamiltonian systems. For simplicity, we restrict ourselves to mechanical theories and we review only the basic aspects of the subject that are relevant for the thesis. We mostly follow [6, 33, 34, 48–50], where additional details can be found.

We begin by defining gauge symmetries and reviewing the two Noether theorems in §A.1. We show that the Lagrangian of gauge systems is necessarily singular, which implies that the canonical theory is constrained. The general theory of constrained dynamics is then examined in §A.2. Finally, we present a construction of the so-called reduced phase space of a constrained theory and we discuss its quantization in §A.3.

A.1 Gauge symmetries and singular Lagrangians

We define the classical dynamics via the action functional[1]

$$S[q(\tau)] := \int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \mathcal{L}(q, \dot{q}) \; , \tag{A.1}$$

where the time τ is a real-valued parameter [it is a coordinate on a $(0+1)$-dimensional spacetime]. We assume that the configuration space is a d-dimensional differentiable manifold $\mathcal{Q}$, on which $q(\tau)$ denotes a set of local coordinates for a fixed value of τ. The corresponding velocities are $\dot{q}(\tau) \equiv \mathrm{d}q/\mathrm{d}\tau$. For a given instant $\tau = \tau_0$, we interpret $(q(\tau_0), \dot{q}(\tau_0))$ as local coordinates on the tangent bundle $T\mathcal{Q}$ (sometimes called the velocity phase-space). We will also refer to $q(\tau)$ as fields, as they may correspond to different tensor fields defined on the $(0+1)$-dimensional spacetime. We assume for

[1] For an extension to field theories, fermionic degrees of freedom and higher-derivative theories, see [33, 34] and references therein.

simplicity that the Lagrangian depends only $q(\tau)$ and $\dot{q}(\tau)$, such that it is understood as a function $\mathcal{L} : TQ \to \mathbb{R}$. The Euler derivatives of $\mathcal{L}$ with respect to $q(\tau)$ are defined as

$$\mathcal{L}_a := \frac{\partial \mathcal{L}}{\partial q^a} - \frac{\mathrm{d}}{\mathrm{d}\tau}\frac{\partial \mathcal{L}}{\partial \dot{q}^a} \ , \ (a = 1, \ldots, d) \ . \tag{A.2}$$

If we require that the variation of $S[q(\tau)]$ is stationary, we find from (A.1) the Euler-Lagrange equations $\mathcal{L}_a = 0$.

A.1.1 Noether theorems

The invariance of the action under a set of symmetry transformations has important physical consequences. In the case of 'rigid' symmetries (that do not vary in time), the invariance implies that a set of charges is conserved. In the case of local (gauge) symmetries (that vary in time), one finds that the equations of motion obey a set of 'generalized Bianchi identities' ('Noether identities'). This is the content of the two Noether theorems which we now review. We follow [34] for the proofs.

Let us consider a continuous group of transformations comprised of spacetime coordinate transformations (reparametrizations of τ) and field redefinitions, i.e.,

$$\begin{aligned} \tau \mapsto \tau' &= \tau + \delta\tau(\tau) \ , \\ q(\tau) \mapsto q'(\tau') &= q(\tau) + \delta q(\tau) \ , \end{aligned} \tag{A.3}$$

where δ denotes infinitesimal changes that correspond to transformations close the identity. We consider that these transformations are described in terms of N independent and arbitrary functions $\varepsilon_i(\tau)$ for $i = 1, \ldots, N$, such that[2]

$$\begin{aligned} \delta\tau(\tau) &= T^i(\tau)\varepsilon_i(\tau) \ , \\ \delta q(\tau) &= \sum_{j=0}^{n} Q^i_{(j)}(\tau)\frac{\mathrm{d}^j \varepsilon_i}{\mathrm{d}\tau^j}(\tau) \ , \end{aligned} \tag{A.4}$$

where the functions $Q^i_{(j)}(\tau)$ may functionally depend on the paths $q(\tau)$. Note that it is possible to adopt different linear combinations of the arbitrary functions $\varepsilon_i(\tau)$ without altering the reparametrization and the field redefinitions given in (A.4) if the functions $T^i(\tau)$ and $Q^i_{(j)}(\tau)$ are also suitably redefined. For example, let us consider the simple

[2]The (mechanical) field redefinitions in (A.4) are analogous to the familiar gauge transformations of the vector potential in electromagnetism, $\delta A_\mu = \partial\varepsilon/\partial x^\mu$, or the Lie derivatives of the metric field in general relativity, $\delta g_{\mu\nu} = \varepsilon^\lambda \partial g_{\mu\nu}/\partial x^\lambda + g_{\mu\lambda}\partial\varepsilon^\lambda/\partial x^\nu + g_{\lambda\nu}\partial\varepsilon^\lambda/\partial x^\mu$.

case in which $Q^i_{(j)}(\tau) = 0$ for $j > 1$. We can then perform the redefinitions

$$\begin{aligned} \varepsilon_i(\tau) &=: M_i^I(\tau)\bar{\varepsilon}_I(\tau)\ (I = 1, \ldots, N)\ , \\ \bar{T}^I(\tau) &:= T^i(\tau)M_i^I(\tau)\ , \\ \bar{Q}^I_{(0)}(\tau) &:= Q^i_{(0)}(\tau)M_i^I(\tau) + Q^i_{(1)}(\tau)\frac{\mathrm{d}M_i^I}{\mathrm{d}\tau}(\tau)\ , \\ \bar{Q}^I_{(1)}(\tau) &:= Q^i_{(1)}(\tau)M_i^I(\tau) \end{aligned} \tag{A.5}$$

without altering (A.4). We assume that the matrix with elements $M_i^I(\tau)$ is invertible and it may also functionally depend on the paths $q(\tau)$. It is straightforward to check that the inverse of (A.5) leads back to the original functions $T^i(\tau)$ and $Q^i_{(j)}(\tau)$. If we restrict the arbitrary functions ε to be constants (independent of τ), then the transformations can be seen as elements of an N-dimensional Lie group. In this case, we also restrict the matrix with elements M_i^I to be independent of τ.

The transformations (A.4) correspond to a symmetry if we require that the action (A.1) retains its functional form under (A.3) up to a boundary term, i.e.,

$$\int_{\tau_0'}^{\tau_1'} \mathrm{d}\tau'\ \mathcal{L}\left(q', \frac{\mathrm{d}q'}{\mathrm{d}\tau'}\right) = \int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \mathcal{L}(q, \dot{q}) + F(\tau_1) - F(\tau_0)\ . \tag{A.6}$$

This implies that the Lagrangians differ by the total derivative of some function $F(\tau)$,

$$\frac{\mathrm{d}\tau'}{\mathrm{d}\tau}\mathcal{L}\left(q', \frac{\mathrm{d}q'}{\mathrm{d}\tau'}\right) - \mathcal{L}(q, \dot{q}) = \frac{\mathrm{d}F}{\mathrm{d}\tau}\ , \tag{A.7}$$

or, in infinitesimal form,

$$\frac{\partial \mathcal{L}}{\partial q^a}\delta q^a(\tau) + \frac{\partial \mathcal{L}}{\partial \dot{q}^a}\delta\left(\frac{\mathrm{d}q^a}{\mathrm{d}\tau}\right) + \mathcal{L}\frac{\mathrm{d}\delta\tau}{\mathrm{d}\tau} = \frac{\mathrm{d}F}{\mathrm{d}\tau}\ . \tag{A.8}$$

The following properties are assumed of $F(\tau)$: (1) it can be written in terms of the functions $\varepsilon(\tau)$ and their first n derivatives; (2) $F(\tau) \equiv 0$ if $\varepsilon_i(\tau) \equiv 0$; (3) if ε are constants, then $F(\tau) = \varepsilon_i F_i(\tau)$ up to first order in ε_i.

If we define the same-instant variations

$$\begin{aligned} \bar{\delta}q(\tau) &:= q'(\tau) - q(\tau) = \delta q(\tau) - \dot{q}(\tau)\delta\tau\ , \\ \bar{\delta}\dot{q}(\tau) &:= \dot{q}'(\tau) - \dot{q}(\tau) = \delta\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right) - \ddot{q}(\tau)\delta\tau\ , \end{aligned} \tag{A.9}$$

we can rewrite (A.8) as

$$\frac{\partial \mathcal{L}}{\partial q^a}\bar{\delta} q^a(\tau) + \frac{\partial \mathcal{L}}{\partial \dot{q}^a}\bar{\delta} \dot{q}^a(\tau) + \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\mathcal{L}\delta\tau\right) = \frac{\mathrm{d}F}{\mathrm{d}\tau} \ . \tag{A.10}$$

Due to

$$\delta\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right) = \frac{\mathrm{d}\delta q}{\mathrm{d}\tau} - \frac{\mathrm{d}q}{\mathrm{d}\tau}\frac{\mathrm{d}\delta\tau}{\mathrm{d}\tau} \ , \tag{A.11}$$

one can easily verify that, in contrast to the variation δ, the same-instant variation $\bar{\delta}$ commutes with $\mathrm{d}/\mathrm{d}\tau$. We can then use the Leibniz rule and the definition (A.2) of the Euler derivatives $\mathcal{L}_a$ to obtain

$$\mathcal{L}_a\bar{\delta} q^a(\tau) + \frac{\mathrm{d}Q_{\mathcal{N}}}{\mathrm{d}\tau} = 0 \ , \tag{A.12}$$

where the Noether charge is defined as

$$Q_{\mathcal{N}} = \frac{\partial \mathcal{L}}{\partial \dot{q}^a}\bar{\delta} q^a(\tau) + \mathcal{L}\delta\tau - F(\tau) \ . \tag{A.13}$$

Two important observations can now be made and each will lead to one Noether theorem. First, if the Euler-Lagrange equations $\mathcal{L}_a = 0$ are satisfied, then (A.12) leads to the conservation of the Noether charge. In the special case of a rigid symmetry, for which ε are constants, we can rewrite (A.12) as

$$\mathcal{L}_a\left(\dot{q}^a T^i - Q^{i,a}_{(0)}\right) = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\frac{\partial \mathcal{L}}{\partial \dot{q}^a}\left(Q^{i,a}_{(0)} - \dot{q}^a T^i\right) + \mathcal{L}T^i - F^i\right] \ . \tag{A.14}$$

Equation (A.14) can be summarized as the

First Noether Theorem. *If the action is invariant under an N-dimensional Lie group, then N linearly independent combinations of the Euler derivatives are total time derivatives.*

Second, by integrating (A.12), we obtain

$$\int_{\tau_0}^{\tau_1} \mathrm{d}\tau\ \mathcal{L}_a\bar{\delta} q^a(\tau) = \left.Q_{\mathcal{N}}\right|_{\tau_1} - \left.Q_{\mathcal{N}}\right|_{\tau_0} \ , \tag{A.15}$$

where one considers a set of paths in configuration space that are off shell (i.e., one does not impose $\mathcal{L}_a = 0$). If one also assumes that $\varepsilon(\tau)$ and its first n derivatives vanish at the end points τ_0 and τ_1, then the Noether charge surface term in (A.15) vanishes due to the properties assumed of $F(\tau)$. In this case, equation (A.15) can be rewritten as [cf. (A.4)]

$$\int_{\tau_0}^{\tau_1} \mathrm{d}\tau \; \varepsilon_i(\tau) \left[-\mathcal{L}_a \dot{q}^a T^i + \sum_{j=0}^{n} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}\tau^j} \left(\mathcal{L}_a Q^{i,a}_{(j)} \right) \right] = 0 \; , \tag{A.16}$$

after integrating by parts. Due to the fact that the functions $\varepsilon_i(\tau)$ are arbitrary (up to the chosen boundary conditions), we find from (A.16) the identities

$$-\mathcal{L}_a \dot{q}^a T^i + \sum_{j=0}^{n} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}\tau^j} \left(\mathcal{L}_a Q^{i,a}_{(j)} \right) = 0 \; , \tag{A.17}$$

which are referred to as 'generalized Bianchi identities' [34] or 'Noether identities' [33]. Equation (A.17) can be summarized as the

Second Noether Theorem. *If the action exhibits infinitesimal symmetries that form an infinite continuous group and are described by N arbitrary functions, then one obtains N independent identities of the Euler derivatives.*

In what follows, we consider for simplicity only gauge transformations with $n = 1$, i.e., $Q^i_{(j)}(\tau) = 0$ for $j > 1$. Equation (A.17) then becomes

$$-\mathcal{L}_a \dot{q}^a T^i + \mathcal{L}_a Q^{i,a}_{(0)} - \frac{\mathrm{d}}{\mathrm{d}\tau} \left(\mathcal{L}_a Q^{i,a}_{(1)} \right) = 0 \; . \tag{A.18}$$

A.1.2 Gauge systems are singular

The Noether identities (A.18) imply that the Lagrangian of a gauge system is singular[3], i.e., that $\mathcal{L}$ satisfies

$$\det \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^a \partial \dot{q}^b} = 0 \; . \tag{A.19}$$

Indeed, using (A.2), equation (A.18) can be rewritten as [34]

$$0 = \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^a \partial \dot{q}^l} \ddot{q}^l \dot{q}^a T^i - \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^a \partial \dot{q}^l} \ddot{q}^l \left(Q^{i,a}_{(0)} - \dot{Q}^{i,a}_{(1)} \right) + \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^a \partial \dot{q}^l} \dddot{q}^l Q^{i,a}_{(1)} + \ldots \; , \tag{A.20}$$

[3] As is well-known, the converse does not hold, i.e., not all singular systems exhibit gauge symmetries. In language of the Hamiltonian formulation to be reviewed next, one says that such systems possess second-class constraints only (cf. §A.2.4).

where $\ldots$ stands for terms that do not involve the Hessian $\partial^2\mathcal{L}/\partial\dot{q}^a\partial\dot{q}^l$. As (A.20) must also hold for off-shell paths $q(\tau)$ (i.e., paths that do not satisfy $\mathcal{L}_a = 0$), we may take the derivatives of $q(\tau)$ at each instant as independent variables. In this way, the terms in the right-hand side of (A.20) must vanish separately, and we conclude that $\dot{q}^a T^i$, $Q^{i,a}_{(0)} - \dot{Q}^{i,a}_{(1)}$ and $Q^{i,a}_{(1)}$ are, if non-vanishing, components of null eigenvectors of the Hessian.

A.2 Constrained dynamics

A.2.1 Primary constraints

If one is interested in the canonical quantum theory of gauge systems, one must first understand how to construct a classical Hamiltonian formulation of systems with a singular Lagrangian. The passage to the canonical theory is obtained from the usual Legendre transform. One defines the momenta as

$$p_a := \frac{\partial\mathcal{L}}{\partial\dot{q}^a} \; . \tag{A.21}$$

For regular systems, the Hessian $\partial^2\mathcal{L}/\partial\dot{q}^a\partial\dot{q}^l = \partial p_b/\partial\dot{q}^a$ is invertible and the pairs (q,p) serve as local canonical coordinates on the cotangent bundle $\Gamma = T^*\mathcal{Q}$ (phase space). The time evolution of a phase-space function $f(q,p)$ is generated by the canonical Hamiltonian,

$$H_c(q,p) := p_a\dot{q}^a - \mathcal{L}(q,\dot{q}) \; , \tag{A.22}$$

via the equation of motion

$$\dot{f} = \{f, H_c\} \; , \tag{A.23}$$

where the Poisson bracket of two phase-space functions $f(q,p)$ and $g(q,p)$ is

$$\{f,g\} := \frac{\partial f}{\partial q^a}\frac{\partial g}{\partial p_a} - \frac{\partial f}{\partial p_a}\frac{\partial g}{\partial q^a} \; . \tag{A.24}$$

However, this construction does not hold for singular systems. Due to (A.19), it is not possible to locally invert (A.21) to express all the velocities $\dot{q}$ in terms of the coordinates q and the momenta p. This is a consequence of the fact that the momenta, as defined in (A.21), obey a set of identities[4]

$$\varphi_m\left(q,\frac{\partial\mathcal{L}}{\partial\dot{q}}\right)\equiv 0\ ,\ (m=1,\ldots,M)\ . \tag{A.25}$$

To see that this is true, one can adopt the following procedure. Let the rank of $\partial^2\mathcal{L}/\partial\dot{q}^a\partial\dot{q}^b = \partial p_b/\partial\dot{q}^a$ be $R < d$ and assume for simplicity that it is a constant function of $(q,\dot{q})$. Then, separate the coordinates (after a coordinate transformation, if necessary) into $q=(q^i,q^\mu)$ where $i=1,\ldots,R$ and $\mu=R+1,\ldots,d$. Likewise, $p=(p_j,p_\nu)$, where $j=1,\ldots,R$ and $\nu=R+1,\ldots,d$. This separation is constructed such that the $R\times R$ matrix $\partial p_j/\partial\dot{q}^i$ is invertible and one may locally solve (A.21) for $\dot{q}^i$ to find

$$\dot{q}^i = w^i(q,p_j,\dot{q}^\mu)\ , \tag{A.26}$$

where w^i are some functions of q,p_j and $\dot{q}^\mu$. The velocities $\dot{q}^\mu$ remain unsolved. If we now insert (A.26) into the definition (A.21) of p_ν, we obtain[5]

$$p_\nu = z_\nu(q,\dot{q}^i,\dot{q}^\mu) = z_\nu(q,w^i(q,p_j,\dot{q}^\mu),\dot{q}^\mu) = \tilde{z}_\nu(q,p_j,\dot{q}^\mu)\ , \tag{A.27}$$

where z_ν and $\tilde{z}_\nu$ are some functions. In particular, if we Taylor-expand $\tilde{z}_\nu$ about $\dot{q}^\mu=\dot{q}^\mu_0$,

$$p_\nu = \tilde{z}_\nu(q,p_j,\dot{q}^\mu_0) + \left.\frac{\partial\tilde{z}_\nu}{\partial\dot{q}^{\mu'}}\right|_{\dot{q}^\mu=\dot{q}^\mu_0}(\dot{q}^{\mu'}-\dot{q}^{\mu'}_0)+\ldots\ , \tag{A.28}$$

where $\ldots$ denotes higher powers of $(\dot{q}^{\mu'}-\dot{q}^{\mu'}_0)$, we notice that we must have $\partial\tilde{z}_\nu/\partial\dot{q}^\mu\equiv 0$ for all values of $\dot{q}^\mu$. Otherwise, $\partial\tilde{z}_\nu/\partial\dot{q}^\mu$ has a non-zero rank, which implies that the rank of $\partial p_b/\partial\dot{q}^a$ is larger than R and we arrive at a contradiction. Thus, we find the relations

$$p_\nu = \tilde{z}_\nu(q,p_j)\ , \tag{A.29}$$

which are called primary constraints. The adjective 'primary' is due to the fact that they follow directly from the form of the Lagrangian and the equations of motion $\mathcal{L}_a=0$ are not used in their definition, whereas they are constraints because they do not involve velocities and only restrict the possible values of p_ν.

If we understand the *unconstrained* pairs (q,p) as local canonical coordinates on the cotangent bundle $\Gamma=T^*\mathcal{Q}$, we may consider that the primary constraints define a

[4]We assume for simplicity that the identities (A.25) do not depend explicitly on time τ.
[5]Note that there is no summation over μ in (A.27).

subspace $\Sigma_{(1)}$ in Γ. We designate the term 'primary constraint subspace' to $\Sigma_{(1)}$. If we further suppose the constraints (A.29) define a submanifold that is smoothly embedded in Γ, we refer to $\Sigma_{(1)}$ as the 'primary constraint hypersurface'. As physical motions must satisfy the constraints at all times, the cotangent bundle Γ plays only an auxiliary role in the Hamiltonian formulation of singular systems. For this reason, we refer to Γ as the 'auxiliary phase space'.[6] The 'physical' phase space will be considered in §A.3.

Finally, if we define $M = d - R$ and $m = \nu - R$, we may rewrite (A.29) as

$$\varphi_m(q,p) = p_{m+R} - \tilde{z}_{m+R}(q, p_j) = 0 \ , \ (m = 1, \ldots, M) \ . \tag{A.30}$$

If one substitutes $p_a = \partial\mathcal{L}/\partial\dot{q}^a$, one recovers the identities (A.25) from (A.30). This construction of the primary constraints is, however, often formal or inconvenient. For example, one may wish to rewrite (A.29) such that some symmetry of the physical system under consideration becomes manifest. In fact, as there are many equivalent ways of defining a hypersurface, one can assume that the functions φ_m have a more general form than in (A.30) and that they define the primary constraint subspace implicitly. One may also adopt a redundant description in which the primary constraint hypersurface is described by $M > d-R$ relations. Then, the equations (A.29) or (A.30) are regarded as solutions of the general primary constraints

$$\varphi_m(q,p) = 0 \ , \ (m = 1, \ldots, M \geq d - R) \ , \tag{A.31}$$

which should also reduce to identities [cf. (A.25)] after the substitution $p_a = \partial\mathcal{L}/\partial\dot{q}^a$.

We make the simplifying assumption that no redundant constraints are present, i.e., that $M = d - R$. Moreover, we note that the identities (A.25) are directly related to the null eigenvectors of the Hessian $\partial^2\mathcal{L}/\partial\dot{q}^a\partial\dot{q}^b$. Indeed, the equation

$$0 = \frac{\partial}{\partial\dot{q}^a}\varphi_m\left(q, \frac{\partial\mathcal{L}}{\partial\dot{q}}\right) = \left(\frac{\partial\varphi_m}{\partial p_b}\frac{\partial p_b}{\partial\dot{q}^a}\right)_{p=\partial\mathcal{L}/\partial\dot{q}} \tag{A.32}$$

implies that $V^b_{(m)} = \partial\varphi_m/\partial p_b$, when evaluated at $p_a = \partial\mathcal{L}/\partial\dot{q}^a$, are a set of M vectors annihilated by $\partial p_b/\partial\dot{q}^a = \partial^2\mathcal{L}/\partial\dot{q}^a\partial\dot{q}^b$. Analogously, the equation

$$0 = \frac{\partial}{\partial q^a}\varphi_m\left(q, \frac{\partial\mathcal{L}}{\partial\dot{q}}\right) = \frac{\partial\varphi_m}{\partial q^a} + \left(\frac{\partial\varphi_m}{\partial p_b}\frac{\partial p_b}{\partial q^a}\right)_{p=\partial\mathcal{L}/\partial\dot{q}} \tag{A.33}$$

[6] The auxiliary phase space is also sometimes called the 'kinematical' or 'unconstrained phase space', whereas the unconstrained pairs (q,p) can also be referred to as 'kinematical variables' or 'partial observables' [16]. See also the discussion regarding the notion of observables in §1.7.

implies that $\partial\varphi_m/\partial q^a$ can be determined in terms of a combination of the vectors $V^b_{(m)}$. If we now assume that the $2d\times M$ matrix $\partial\varphi_m/\partial(q^a,p_b)$ has finite elements and is of rank M on the primary constraint hypersurface (known as a 'regularity condition' [33, 34]), then we conclude from (A.33) that $V^b_{(m)}$ are M linearly independent vectors [otherwise the rank of $\partial\varphi_m/\partial(q^a,p_b)$ would be less than M]. The rank-nullity theorem then implies that $V^b_{(m)}$ span the kernel of $\partial p_b/\partial\dot{q}^a$. Consequently, if we can perform the separation $p=(p_j,p_\nu)$ that leads to the explicit solutions (A.29) of the general primary constraints (A.31), then $V^\nu_{(m)} = \partial\varphi_m/\partial p_\nu$ can be seen as an $M\times M$ matrix of rank less than or equal to M. If its rank were less than M, then it would not be possible to locally solve the primary constrains for certain combinations of p_ν, which contradicts the assumption that (A.29) can be found. Thus, if (A.29) can be found, $V^\nu_{(m)}$ is an $M\times M$ matrix with rank M and, thus, it is invertible. In this case, we can rewrite (A.33) as

$$\frac{\partial\tilde{z}_\nu}{\partial q^a} = -V^{(m)}_\nu \frac{\partial\varphi_m}{\partial q^a} \ , \tag{A.34}$$

where $V^{(m)}_\nu := \left[V^\nu_{(m)}\right]^{-1}$ and a summation over m is implied. A similar result can be obtained if we differentiate (A.31) with respect to p_j,

$$\frac{\partial\tilde{z}_\nu}{\partial p_j} = -V^{(m)}_\nu \frac{\partial\varphi_m}{\partial p_j} \ . \tag{A.35}$$

Both (A.34) and (A.35) are useful in the construction of the Hamiltonian for the constrained system.

A.2.2 The total Hamiltonian

A canonical Hamiltonian can now be defined in $\Sigma_{(1)}$ through the usual formula (A.22), where one uses (A.26) and (A.29) as definitions of $\dot{q}^i$ and p_ν. In this way, H_c is understood as a function of the coordinates q and the momenta p_j only. This implies that

$$\frac{\partial H_c}{\partial p_\nu} = 0 \ , \tag{A.36}$$

if p_ν is regarded as an independent variable. One also notes that H_c does not depend on the velocities by virtue of (A.21). In particular, it does not depend on the unsolved velocities $\dot{q}^\mu$ due to (A.21), (A.26) and (A.29), i.e.,

$$\frac{\partial H_c}{\partial \dot{q}^\mu} = \tilde{z}_\mu - \frac{\partial\mathcal{L}}{\partial\dot{q}^\mu} = 0 \ . \tag{A.37}$$

Similarly, one finds

$$\begin{aligned}\frac{\partial H_c}{\partial p_j} &= \dot{q}^j + \frac{\partial \tilde{z}_\nu}{\partial p_j}\dot{q}^\nu \ , \\ \frac{\partial H_c}{\partial q^a} &= -\frac{\partial \mathcal{L}}{\partial q^a} + \frac{\partial \tilde{z}_\nu}{\partial q^a}\dot{q}^\nu = -\dot{p}_a + \frac{\partial \tilde{z}_\nu}{\partial q^a}\dot{q}^\nu \ ,\end{aligned} \tag{A.38}$$

where we used the Euler-Lagrange equations $\mathcal{L}_a = 0$ together with (A.21) in the last equality. The set of $d+R$ equations given in (A.38) is the analogue in $\Sigma_{(1)}$ of the usual Hamilton equations of motion that are defined in Γ for unconstrained theories. Using (A.34) and (A.35), we can rewrite (A.38) in terms of the more general primary constrains φ_m,

$$\begin{aligned}\dot{q}^j &= \frac{\partial H_c}{\partial p_j} + u^m \frac{\partial \varphi_m}{\partial p_j} \ , \\ -\dot{p}_a &= \frac{\partial H_c}{\partial q^a} + u^m \frac{\partial \varphi_m}{\partial q^a} \ ,\end{aligned} \tag{A.39}$$

where we defined $u^m := \dot{q}^\nu V_\nu^{(m)}$, from which we also obtain

$$\dot{q}^\mu = u^m V^\mu_{(m)} = \frac{\partial H_c}{\partial p_\mu} + u^m \frac{\partial \varphi_m}{\partial p_\mu} \tag{A.40}$$

due to (A.36). From (A.39) and (A.40), we conclude that the time evolution of a function $f(q,p)$ defined on the auxiliary phase space Γ is given by the weak equality

$$\dot{f} \approx \{f, H_T\} \ , \tag{A.41}$$

where the Poisson bracket is evaluated on Γ and we defined $H_T := H_c + u^m \varphi_m$, which is called the total Hamiltonian. The equation (A.41) is valid due to the weak equality $\{\cdot, u^m\varphi_m\} \approx u^m\{\cdot, \varphi_m\}$ (i.e., this is an identity that holds on $\Sigma_{(1)}$). Furthermore, whereas the canonical Hamiltonian H_c is only defined on the primary constraint subspace $\Sigma_{(1)}$, the total Hamiltonian H_T can be evaluated in the auxiliary phase space Γ (at least in a neighborhood of $\Sigma_{(1)}$). Thus, H_T is an extension of H_c off the primary constraint hypersurface, and both Hamiltonians coincide when evaluated on $\Sigma_{(1)}$. This is expressed by the weak equality $H_T \approx H_c$.

One can also extend other functions besides the canonical Hamiltonian. A function f_c defined on $\Sigma_{(1)}$ can be extended off the primary constraint subspace in an arbitrary way. Let f be its extension to Γ. Due to the assumed regularity condition on φ_m, their independence and the fact that $V^\nu_{(m)} = \partial\varphi_m/\partial p_\nu$ is invertible, one can (locally) adopt the general primary constraints as coordinates on Γ, such that $f \equiv f(q, p_j, \varphi_m)$. As f is an extension of f_c, we have the condition $f(q, p_j, 0) = f_c(q, p_j)$. Then the following identity holds[7]

$$
\begin{aligned}
f(q, p_j, \varphi_m) &= f_c(q, p_j) + \int_0^1 \mathrm{d}x \, \frac{\mathrm{d}}{\mathrm{d}x} f(q, p_j, x\varphi_m) \\
&= f_c(q, p_j) + \varphi_m \int_0^1 \mathrm{d}x \, \frac{1}{x} \frac{\partial}{\partial \varphi_m} f(q, p_j, x\varphi_m) \\
&=: f_c(q, p_j) + v^m \varphi_m \ ,
\end{aligned}
\tag{A.42}
$$

where the last line defines the function v^m, which is arbitrary due to the arbitrariness of f. Note that v^m might itself depend $\varphi_{m'}$ ($m' = 1, \ldots, M$). We then conclude that $f - f_c = v^m \varphi_m \approx 0$.

A.2.3 The Rosenfeld-Dirac-Bergmann algorithm

The time evolution of functions in the auxiliary phase space dictated by (A.41) is consistent if the primary constraints are preserved in time, i.e.,

$$
\dot{\varphi}_m \approx \{\varphi_m, H_c\} + u^{m'} \{\varphi_m, \varphi_{m'}\} \approx 0 \ . \tag{A.43}
$$

These equations should be solved to give the form of $u^{m'}$. However, it might be the case that some of the equations (A.43) are independent of $u^{m'}$ and that they, in fact, lead to new constraints on the pairs (q, p). The new constraints that are not redundant with respect to the original set of primary constraints are referred to as secondary constraints. The adjective 'secondary' is used to convey the fact that the equations of motion are used in their definition. If secondary constraints are present, one must now ensure that their evolution is consistent by requiring that their time derivative vanishes on the primary constraint subspace. This may lead to new conditions on the $u^{m'}$-functions or to new secondary (sometimes called tertiary) constraints, which must be consistent. The iterative process of requiring consistency of the evolution of primary and secondary constraints (including those that are sometimes called tertiary or that have higher designations) is the Rosenfeld-Dirac-Bergmann algorithm [9, 12, 33, 34, 49]. The procedure stops when the consistency of the evolution of all constraints is obtained. If it is not possible to ensure the consistency of a constraint, then the theory associated with the action (A.1) is inconsistent, a possibility which we discard.

Let there be K secondary constraints at the end. It is useful to denote all primary and secondary constraints with the same notation. Thus, we denote secondary constraints as $\varphi_k(q, p)$ for $k = M + 1, \ldots, M + K$, such that all constraints can be written as $\varphi_l(q, p)$ for $l = 1, \ldots, M + K$. Furthermore, a number of simplifying assumptions

[7]See Theorem 1.1 and Appendix 1.A of [33] for details as well as a global construction of this extension.

can be made. We assume that: (1) the subspace Σ defined by all constraints (i.e., by $\varphi_l = 0$) is a smooth submanifold embedded in the auxiliary phase space Γ; (2) the matrix $\partial\varphi_l/\partial(q^a, p_b)$ has finite elements and is of rank $M+K$ on Σ (regularity condition); (3) the rank of $\{\varphi_l, \varphi_{l'}\}$ is constant on Σ; (4) there are no redundant constraints among $\varphi_l(q,p)$.

What can be said of the form of the functions u^m that are determined in this procedure? They must be solutions of the following inhomogeneous system,

$$\{\varphi_l, H_c\} + u^m\{\varphi_l, \varphi_m\} \approx 0 \ . \tag{A.44}$$

The general solution of (A.44) reads

$$u^m = u^m_{(\text{part})} + \lambda^A u^m_A \ , \tag{A.45}$$

where $u^m_{(\text{part})}$ is a particular solution of (A.44) and u^m_A is a set of linearly independent solutions of the corresponding homogeneous equation $u^m_A\{\varphi_l, \varphi_m\} \approx 0$. Due to the hypothesis that $\{\varphi_l, \varphi_{l'}\}$ has constant rank on the subspace Σ defined by all the constraints, the number of independent solutions u^m_A is constant on Σ. The coefficients λ can be taken to be arbitrary functions on the auxiliary phase space. The total Hamiltonian can now be written as

$$H_T = H_c + u^m\varphi_m = H_c + u^m_{(\text{part})}\varphi_m + \lambda^A u^m_A \varphi_m \ . \tag{A.46}$$

The notation can be simplified if we define $H' := H_c + u^m_{(\text{part})}\varphi_m$ and $\varphi_A := u^m_A\varphi_m$. We thus obtain

$$H_T = H' + \lambda^A \varphi_A \ , \tag{A.47}$$

which dictates the time evolution according to (A.41). After the Rosenfeld-Dirac-Bergmann algorithm is completed and the total Hamiltonian is expressed as in (A.47), we have a constrained canonical theory with $M+K$ constraints φ_l and a number of arbitrary functions λ in the most general case. Moreover, by repeating the derivation of (A.42) for all the constraints (instead of only the primaries), one can extend a function $f|_\Sigma$ defined on Σ to the auxiliary phase space by $f - f|_\Sigma = v^l\varphi_l$.

A.2.4 First-class and second-class functions. The initial value problem

It is also useful to introduce the concepts of first-class and second-class functions. A function f on the auxiliary phase space Γ is said to be first class if it weakly Poisson-commutes with all the constraints, i.e., if it satisfies $\{f, \varphi_l\} = v_l^{l'} \varphi_{l'} \approx 0$ for $l = 1, \ldots, M+K$. If f is not first class, then it is said to be second class. Using the Jacobi identity for Poisson brackets, it is straightforward to see that the Poisson bracket of two first-class functions is also first class [33]. We note that both H' and φ_A defined above are first class due to (A.44) and the homogeneous equation $u_A^m\{\varphi_l, \varphi_m\} \approx 0$. Thus, the total Hamiltonian is first class. This clarifies the role of the constraints as restrictions on the possible initial data of physical motions. Indeed, once the initial conditions $(q(\tau_0), p(\tau_0))$ are chosen at an arbitrary instant of time τ_0 such that $\varphi_l(q(\tau_0), p(\tau_0)) = 0$, then the constraints are satisfied at all times regardless of the choice of arbitrary functions λ due to the fact that H_T is first class.

Let us now assume that it is possible to separate all the constraints φ_l into a set of first-class constraints C_F $(F = 1, \ldots, N_F)$ and a set of second-class constraints χ_S $(S = 1, \ldots, N_S)$ such that $N_F + N_S = M + K$. In principle, this can be achieved by the following iterative procedure (see [33] for details). We start with the matrix $\{\varphi_l, \varphi_{l'}\}$, which is assumed to have constant rank on Σ. If $\det\{\varphi_l, \varphi_{l'}\} \approx 0$, there exists a non-trivial solution to $v^l\{\varphi_l, \varphi_{l'}\} \approx 0$ and $C_1 := v^l \varphi_l$ is first class. Subsequently, we consider the determinant of the matrix of Poisson brackets of all the constraints that are independent from C_1. If this determinant is weakly zero, we can define C_2 and repeat the procedure. The iterations stop when the determinant no longer vanishes weakly, such that the remaining constraints χ_S are second class. As the matrix $\{\varphi_l, \varphi_{l'}\}$ is antisymmetric, the number N_S of second-class constraints must be even. The number N_F of first-class constraints is larger than or equal to the number of arbitrary functions λ, which is the number of first-class primaries. The first-class constraints then obey

$$\{C_F, C_{F'}\} = c_{FF'}^{F''} C_{F''} + \mathcal{O}(\chi^2) \approx 0 \ , \tag{A.48}$$

for some functions $c_{FF'}^{F''}$. As the Poisson bracket of two first-class quantities is also first class, the right-hand side of (A.48) cannot depend on χ_S $(S = 1, \ldots N_S)$, but in general may include quadratic (and higher-order) terms of the second-class constraints.

We can in principle eliminate the second-class constraints from the theory by extending functions $f \mapsto f + v^l \varphi_l$ in a particular way (for a particular choice of v^l). Indeed, the matrix $\chi_{SS'} := \{\chi_S, \chi_{S'}\}$ is by construction invertible on Σ. We denote the inverse by $\chi^{SS'}$. We now define the function

$$f_D(q,p) := f(q,p) - \{f, \chi_S\} \chi^{SS'} \chi_{S'} \ , \tag{A.49}$$

which we refer to as the 'Dirac extension' of $f(q,p)$. It is straightforward to verify that Dirac extensions have the following properties: (1) $\{f_D, \chi_S\} \approx 0$; (2) $\{f_D, C_F\} \approx \{f, C_F\}$; (3) the Poisson bracket of the Dirac extensions of f and g satisfies the weak equality $\{f_D, g_D\} \approx \{f, g\} - \{f, \chi_S\} \chi^{SS'} \{\chi_{S'}, g\} =: \{f, g\}_D$, where $\{\cdot, \cdot\}_D$ is called the 'Dirac bracket' of f and g; (4) if f is a first-class function, then $f_D \approx f$. Consequently, if all (auxiliary) phase-space functions are replaced by their Dirac extensions or, equivalently, all Poisson brackets are replaced by the Dirac brackets, the second-class constraints are effectively eliminated from theory, since all Dirac extensions weakly Poisson-commute with them. If $N_F > 0$, we are thus left with a theory containing solely first-class constraints and arbitrary functions λ. How are these functions related to a gauge symmetry? This is what we examine next. In what follows, we tacitly assume that all functions have been replaced by their Dirac extensions, such that no second-class constraints need to be considered.

A.2.5 Reference frames and the gauge generator

Due to the presence of the arbitrary functions λ in (A.47), the evolution of a function $f(q,p)$ defined on the auxiliary phase space [cf. (A.41)] is not deterministic. For a fixed initial condition $f(q(\tau_0), p(\tau_0))$ specified at a particular instant τ_0, different evolutions are obtained for different choices of λ. We may think of each choice as corresponding to a 'generalized reference frame'. Although the evolution is well-defined once a choice is made, the formalism does not select any preferred frame. Let us consider two choices, $\lambda^A_{(1)}$ and $\lambda^A_{(2)}$, and denote the corresponding evolutions as $f(q_{(1,2)}(\tau), p_{(1,2)}(\tau))$. The difference of the function from one frame to the other at a certain instant of time is given by the same-instant variation $\bar{\delta} f(q(\tau), p(\tau)) := f(q_{(2)}(\tau), p_{(2)}(\tau)) - f(q_{(1)}(\tau), p_{(1)}(\tau))$. Likewise, we denote $\bar{\delta}\lambda^A := \lambda^A_{(2)} - \lambda^A_{(1)}$ and use the symbol $\{\cdot,\cdot\}_{(1,2)}$ for the Poisson bracket taken with respect to the variables in each frame.

As the evolution in each frame is a canonical transformation [generated by $H_T = H' + \lambda^A_{(1,2)}\varphi_A$], we may consider that a change of frame from $\lambda^A_{(1)}$ to $\lambda^A_{(2)}$ is the composition of canonical transformations, namely, the evolution of $f(q_{(1)}(\tau), p_{(1)}(\tau))$ back to $f(q(\tau_0), p(\tau_0))$ and the evolution of this initial value to $f(q_{(2)}(\tau), p_{(2)}(\tau))$ [50]. This motivates us to consider that the change of frame is a canonical transformation, $\bar{\delta} f := \{f, G\}_{(1)}$, where the generator $G \equiv G(q_{(1)}(\tau), p_{(1)}(\tau), \tau)$ must now be constructed.

We begin by noting that the constraints must be satisfied in all frames. Thus, we must have $\{G, \varphi_l\} \approx 0$ ($j = 1, \dots, M+K$), i.e., G must be first class. Furthermore, due to the fact that $\bar{\delta}$ commutes with $\mathrm{d}/\mathrm{d}\tau$ [cf. (A.11)], we have the equality [50]

$$\begin{aligned} &\{\{f,G\}_{(1)}, H_T\}_{(1)} + \left\{f, \frac{\partial G}{\partial \tau}\right\}_{(1)} \approx \frac{\mathrm{d}\bar{\delta} f}{\mathrm{d}\tau} \\ &= \bar{\delta}\frac{\mathrm{d}f}{\mathrm{d}\tau} \approx \{f, H_T\}_{(2)} - \{f, H_T\}_{(1)} + \bar{\delta}\lambda^A \{f, \varphi_A\}_{(1)} \ . \end{aligned} \tag{A.50}$$

Note that we denoted $H_T = H' + \lambda^A_{(1)}\varphi_A$ everywhere in (A.50), and we also used the equality $\bar{\delta}\lambda^A\{f,\varphi_A\}_{(2)} = \bar{\delta}\lambda^A\{f,\varphi_A\}_{(1)}$ for infinitesimal variations $\bar{\delta}\lambda^A$. If we now use

$$\{f,H_T\}_{(2)} - \{f,H_T\}_{(1)} = \bar{\delta}\{f,H_T\} = \{\{f,H_T\}_{(1)},G\}_{(1)} \tag{A.51}$$

together with the Jacobi identity for the Poisson brackets [50], we may rewrite (A.50) as

$$\left\{f, \frac{\partial G}{\partial \tau} + \{G,H_T\}_{(1)} - \bar{\delta}\lambda^A\varphi_A\right\}_{(1)} \approx 0 \ . \tag{A.52}$$

As (A.52) holds for any auxiliary phase-space function $f(q(\tau),p(\tau))$, it is equivalent to the equation

$$\frac{\partial G}{\partial \tau} + \{G,H_T\}_{(1)} - \bar{\delta}\lambda^A\varphi_A = \mathcal{I}(q,p,\tau) \ , \tag{A.53}$$

where $\mathcal{I}(q,p,\tau)$ is a generator of the identity on the constraint hypersurface ('on-shell identity generator'), i.e., it satisfies the conditions [48]

$$\frac{\partial \mathcal{I}}{\partial q^a} = v_a^j\varphi_l + \mathcal{O}(\varphi^2) \ , \ \frac{\partial \mathcal{I}}{\partial p_a} = \tilde{v}^{j,a}\varphi_l + \mathcal{O}(\varphi^2) \ , \ (a = 1,\ldots,d) \ , \tag{A.54}$$

for certain functions v_a^j and $\tilde{v}^{j,a}$, such that $\{f,\mathcal{I}\} \approx 0$ holds for any auxiliary phase-space function $f(q(\tau),p(\tau))$. Note that a linear combination $c^k(\tau)\mathcal{I}_k$ of on-shell identity generators with coefficients $c^k(\tau)$ that only depend on time is still an on-shell identity generator. Let us now use the notation **pfcc** to denote any (arbitrary) linear combination of primary first-class constraints [50], e.g., $\bar{\delta}\lambda^A\varphi_A \equiv \mathbf{pfcc}$. We identify the term 'primary first-class constraint' with the expression 'linear combination of primary first-class constraints'. We also write

$$\{G,H_T\}_{(1)} = \{G,H'\}_{(1)} + \lambda^A_{(1)}\{G,\varphi_A\}_{(1)} + \mathbf{pfcc} \ . \tag{A.55}$$

If we assume that G does not depend explicitly on the choice of $\lambda^A_{(1)}$, then we obtain the following conditions on the generator [48–50],

$$\begin{aligned} &G \text{ is first class} \ , \\ &\frac{\partial G}{\partial \tau} + \{G,H'\} = \mathbf{pfcc} + \mathcal{I}(q,p,\tau) \ , \\ &\{G,\varphi_A\} = \mathbf{pfcc} + \tilde{\mathcal{I}}(q,p,\tau) \ . \end{aligned} \tag{A.56}$$

due to (A.53) and (A.55). In (A.56), we have dropped the subscript from the Poisson bracket, and $\mathcal{I},\tilde{\mathcal{I}}$ are on-shell identity generators. To conform with the first-class condition, we must have $\tilde{\mathcal{I}} \approx 0$. Any auxiliary phase-space function $G(q(\tau), p(\tau), \tau)$ that fulfils the conditions (A.56) is the generator of a symmetry transformation (it maps solutions into solutions [50]) and it can also be interpreted as the generator of a change of generalized reference frames.

As the reference frames are specified by a choice of the arbitrary functions λ, a change of frame is a symmetry that will generally involve arbitrary functions of time and, thus, constitute a gauge transformation. Thus, gauge transformations of fields [cf. (A.4)] can be represented weakly as canonical transformations generated by G in the auxiliary phase space Γ. Let us consider gauge transformations that are solely field redefinitions, i.e., which do not involve time reparametrizations. From (A.4) and (A.9) with $T^i = 0$, we obtain

$$\{q, G\} = \bar{\delta} q(\tau) \equiv \delta q(\tau) = \sum_{j=0}^{n} Q^i_{(j)}(\tau) \frac{\mathrm{d}^j \varepsilon_i}{\mathrm{d}\tau^j} \ . \tag{A.57}$$

This motivates us to make the ansatz $G = \sum_{j=0}^n G^i_{(j)} \mathrm{d}^j \varepsilon_i / \mathrm{d}\tau^j$, where $G^i_{(j)} \equiv G^i_{(j)}(q, p)$ are first-class auxiliary phase-space functions. Note that the arbitrary functions $\varepsilon(\tau)$ are related to the change $\bar{\delta}\lambda^A$ in the functions that determine a reference frame through (A.53). As $\varepsilon_i(\tau)$ and its derivatives are independent variables at a fixed instant, one can use (A.56) to define $G^i_{(j)}$ recursively [48, 50]. We find

$$\{G^i_{(j)}, \varphi_A\} = \textbf{pfcc} + \tilde{\mathcal{I}}^i_{(j)} \ , \ (j = 0, \dots, n) \ , \tag{A.58}$$

as well as

$$\begin{aligned} G^i_{(n)} &= \textbf{pfcc} + \mathcal{I}^i_{(n)} \ , \\ G^i_{(j-1)} &= -\{G^i_{(j)}, H'\} + \textbf{pfcc} + \mathcal{I}^i_{(j-1)} \ , \ (j = 1, \dots, n) \ , \\ \{G^i_{(0)}, H'\} &= \textbf{pfcc} + \mathcal{I}'^{\,i}_{(0)} \ . \end{aligned} \tag{A.59}$$

In this way, we find that $G^i_{(n)}$ is a linear combination of primary first class constraints (up to an on-shell identity generator) and, therefore, $\{G^i_{(n)}, H'\}$ is either a linear combination of primary constraints or a secondary constraint. By following this argument recursively, we conclude from (A.59) that $G^i_{(j)}$ $(j = 0, \dots, n-1)$ are first-class linear combinations of primary and secondary constraints (up to on-shell identity generators). Since the weak equality $\{f, G^i_{(j)} - \mathcal{I}^i_{(j)}\} \approx \{f, G^i_{(j)}\}$ holds for any auxiliary phase-space function and for $j = 0, \dots, n$, we may neglect[8] $\mathcal{I}^i_{(j)}$ and, analogously, $\tilde{\mathcal{I}}^i_{(1)}$, $\mathcal{I}'^{\,i}_{(0)}$.

[8] The specific form of the on-shell identity generators could be relevant for examples involving the calculation of several nested Poisson brackets of G before evaluating the result on the constraint

Furthermore, the number of independent choices for $G^i_{(n)}$ is the same as the number of independent primary first class constraints, which is the number of arbitrary functions λ in the dynamics. Thus, the index i should range over the same set of values as the index A. In general, we can then define $G^i_{(n)} := g^i_{(n),A}\varphi^A$, where $g^i_{(n),A}$ is an invertible matrix, e.g., $g^i_{(n),A} = \delta^i_A$. It is also straightforward to conclude that the minimum value of n for which the recursive algorithm (A.59) is consistent is equal to the number of generations of first-class constraints that arise in the Rosenfeld-Dirac-Bergmann algorithm that are not primary [48]. The corresponding G is then a 'minimal gauge generator' or 'minimal chain'. By summing minimal chains, one can construct non-minimal generators [48]. We will only consider minimal generators, which are then linear combinations of all the independent first-class constraints (that obey the regularity conditions) of the theory. Due to the independence of the arbitrary functions $\varepsilon(\tau)$ and their derivatives for a fixed instant and due to the construction (A.59), we thus find that a minimal gauge generator can be written as

$$G := \sum_{j=0}^{n} G^i_{(j)} \frac{\mathrm{d}^j \varepsilon_i}{\mathrm{d}\tau^j} = v^F C_F \ , \tag{A.60}$$

for some functions v^F, at a fixed instant. For example, our earlier simplifying assumption that $n = 1$ [cf. (A.18)], for which $G = \varepsilon_i(\tau) G^i_{(0)} + \dot{\varepsilon}_i(\tau) G^i_{(1)}$, corresponds to assuming that there is only one generation of secondary first-class constraints if G is minimal.

A.2.6 Gauge orbits and gauge invariance

Given a (minimal) gauge generator G, we may iterate the infinitesimal transformations $\overline{\delta} f = \{f, G\}$ to obtain a finite gauge transformation of the auxiliary phase-space function $f(q(\tau), p(\tau))$. Indeed, by integrating $\overline{\delta} f = \{f, G\}$ on the constraint hypersurface, we obtain a continuous family of gauge-related functions, which may be interpreted as representations of $f(q(\tau), p(\tau))$ in different generalized reference frames. We refer to the family of gauge-related points in the constraint hypersurface as a 'gauge orbit' [33]. A finite gauge transformation corresponds to a 'finite displacement' along the gauge orbit.[9]

Gauge orbits are weakly equal to the integral curves of the vector field $X_G := \{\cdot, G\}$ associated with a (minimal) gauge generator. From (A.60), we find $X_G \approx v^F\{\cdot, C_F\} =: v^F X_F$ at a fixed instant. Due to the assumed independence and regularity conditions on

hypersurface. This will not be considered here.

[9]We only consider finite gauge transformations that are continuously connected to the on-shell identity transformation ('small-gauge transformations'). There may be finite transformations that are not continuously connected to the identity ('large-gauge transformations'), but these will not be analyzed here [33].

the constraints, the vectors X_F are linearly independent and their integral curves can be considered as independent gauge orbits (at a fixed instant). Moreover, from (A.48) and the Jacobi identity for the Poisson brackets, we find that the vectors X_F obey the Frobenius integrability condition, i.e., $[X_F, X_{F'}]f = \{f, c^{F''}_{FF'} C_{F''} + \mathcal{O}(\chi^2)\} \approx c^{F''}_{FF'} X_{F''} f$ for any auxiliary phase-space function f. This implies that their gauge orbits can be used to foliate the constraint hypersurface, i.e., it is possible to find local coordinates (ξ, t) on Σ such that the integral curves of X_F are described by $\xi^r = \text{const.}$ ($r = 1, \ldots, R := 2d - M - K - N_F$), whereas t^F ($F = 1, \ldots, N_F$) are the parameters along the integral curves.

As before, due to the independence and regularity conditions satisfied by the constraints, we may adopt φ_l as coordinates on Γ. We notice that both the first-class C_F and second-class χ_S constraints are collectively denoted by φ_l. In this way, we can locally extend the coordinate system (ξ, t) on Σ to a system $z = (\xi, t, \varphi)$ on the auxiliary phase space. More precisely, we extend (ξ, t) to functions in the auxiliary phase space as follows,

$$\xi^r \mapsto \xi'^r = \xi^r_D + \{\xi^r_D, t^F_D\} C_F \ , \ t^F \mapsto t^F_D \ , \tag{A.61}$$

where ξ^r_D and t^F_D are the Dirac extensions of ξ^r and t^F with respect to the second-class constraints χ_S [cf. (A.49)]. As t^F are the curve parameters, we must have $\{t^F_D, C_{F'}\} = X_{F'} t^F_D \approx \delta^F_{F'}$. Then (A.61) implies that $\{\xi'^r, t^F_D\} \approx 0$. Moreover, as ξ are constant along the gauge orbits of X_F, we obtain $X_F \xi'^r = \{\xi'^r, C_F\} \approx 0$. Thus, ξ'^r are first class by construction. For simplicity, we drop the D subscript of t^F_D and the prime superscript of ξ'^r in what follows. The z coordinates are then defined as $z^r := \xi^r$, $z^{R+F} := t^F$, $z^{R+N_F+F} := C_F$, $z^{R+2N_F+S} = \chi_S$. As these coordinates are generally not canonical, the Poisson brackets (A.24) become

$$\{f, g\} = \omega^{\beta\gamma} \frac{\partial f}{\partial z^\beta} \frac{\partial g}{\partial z^\gamma} \ , \tag{A.62}$$

where f, g are tacitly understood as Dirac extensions of a pair of auxiliary phase-space functions with respect to the χ_S constraints. The coefficients $\omega^{\beta\gamma} = \{z^\beta, z^\gamma\}$ are the components of an invertible antisymmetric tensor that only equals $\mathrm{diag}(\hat{0}, \hat{1}, -\hat{1}, \hat{0})$ if the coordinates are canonical. In particular, we have

$$\omega^{R+N_F+F, R+2N_F+S} = \{C_F, \chi_S\} \approx 0 \ . \tag{A.63}$$

By construction, we also obtain

$$\begin{aligned} \omega^{r,R+N_F+F} &= \{\xi^r, C_F\} \approx 0 \ , \ \omega^{r,R+2N_F+S} = \{\xi^r, \chi_S\} \approx 0 \ , \\ \omega^{R+F,R+N_F+F'} &= \{t^F, C_{F'}\} \approx \delta^F_{F'} \ , \ \omega^{R+F,R+2N_F+S} = \{t^F, \chi_S\} \approx 0 \ , \\ \omega^{r,R+F} &= \{\xi^r, t^F\} \approx 0 \ . \end{aligned} \tag{A.64}$$

These components will be useful for the definition of the symplectic form in the physical phase space in §A.3. It is also useful to note the relation

$$X_F = \{\cdot, C_F\} = \omega^{\beta\gamma} \frac{\partial C_F}{\partial z^\gamma} \frac{\partial}{\partial z^\beta} \approx \frac{\partial}{\partial t^F} \ , \tag{A.65}$$

which is a consequence of (A.62), (A.63) and (A.64). Equation (A.65) implies that X_F is tangent to the constraint hypersurface Σ.[10]

The first relation in (A.64) implies that $\{\xi, G\} \approx 0$ at a fixed instant due to (A.60). More generally, we can introduce the following definition.

Definition A.1 (Gauge invariance)**.** A function f defined on the auxiliary phase space is said to be 'gauge invariant' if it weakly Poisson-commutes with every gauge generator, i.e., if $\{f, C_F\} \approx 0$ at every instant, which leads to $\bar{\delta} f = \{f, G\} \approx 0$. Consequently, the functional form of f does not change under a general gauge transformation.

Remark A.1. Gauge-invariant quantities are also customarily referred to as 'Dirac observables'. This terminology is a priori unrelated to the definition of the physical observables of a gauge theory (cf. the discussion in §1.7) and it is not to be confused with the Dirac extensions defined in (A.49).

Remark A.2. From (A.60), (A.62) and (A.64), we conclude that the restriction of a first-class (and, therefore, gauge-invariant) quantity to the constraint hypersurface can be written as a function solely of ξ coordinates.

As the total Hamiltonian is first class, it follows from (A.47) and Remark A.2 that

$$H_T = H'(\xi, \varphi) + \lambda^A \varphi_A =: H_0(\xi) + H_1^l(\xi)\varphi_l + \lambda^A \varphi_A + \mathcal{O}(\varphi^2) \ , \tag{A.66}$$

where, in constrast to λ, the H_1 functions are determined (not arbitrary). The evolution

[10] In general, a vector field X is tangent to Σ if $X\varphi_l \approx 0$ $(l = 1, \ldots, M+K)$. The vector fields $X_S := \{\cdot, \chi_S\}$ associated with the second-class constraints are not tangent to Σ because $X_S \varphi_l = \{\varphi_l, \chi_S\}$ does not vanish weakly for at least one value of l.

of the z coordinates is then easily computed from (A.62), (A.63) and (A.64). We find

$$
\begin{aligned}
\dot{\xi}^r &= \{\xi^r, H_T\} = \omega^{\beta\gamma}\frac{\partial \xi^r}{\partial z^\beta}\frac{\partial H_T}{\partial z^\gamma} = \omega^{r,r'}\frac{\partial H_T}{\partial \xi^{r'}} \approx \omega^{r,r'}\frac{\partial H_0}{\partial \xi^{r'}} \ , \\
\dot{t}^F &= \{t^F, H_T\} = \omega^{\beta\gamma}\frac{\partial t^F}{\partial z^\beta}\frac{\partial H_T}{\partial z^\gamma} \approx \delta^F_l H^l_1 + \delta^F_A \lambda^A \ , \\
\dot{\varphi}_l &= \{\varphi_l, H_T\} \approx 0 \ .
\end{aligned}
\tag{A.67}
$$

The last equality holds by construction, due to the Rosenfeld-Dirac-Bergmann algorithm (cf. §A.2.3).

A.2.7 Gauge fixing and invariant extensions

The presence of first-class constraints and arbitrary functions λ in the total Hamiltonian (A.47) are distinguishing marks of a gauge symmetry. Depending on the physical question being asked, it may be useful to impose extra constraints that fix λ and remove the arbitrariness of the evolution dictated by (A.41). This procedure is called 'gauge fixing' (or 'gauge fixation') and the extra constraints are referred to as 'gauge conditions' (or 'gauges' for brevity). As is also discussed in Chapter 1, the choice of gauge conditions can be seen as a choice of the generalized reference frame relative to which the dynamics (A.41) is analyzed.

In principle, one may choose conditions χ that depend explicitly on time, on the local coordinates on the auxiliary phase space Γ as well as on the arbitrary functions λ, and on a number of their time derivatives, i.e.,

$$
\chi(q, \dot{q}, \dots, p, \dot{p}, \dots, \lambda, \dot{\lambda}, \dots, \tau) = 0 \ . \tag{A.68}
$$

In particular, gauge conditions $\chi(q, p, \tau)$ that only depend on time and on the local canonical coordinates on Γ are referred to as 'canonical gauge conditions' (or 'canonical gauges' for brevity). In what follows, we tacitly focus on canonical gauges for simplicity. We also assume that all the chosen gauge conditions are independent, i.e., that there are no redundant constraints among the (A.68).

In order for a set of gauge conditions to be admissible, it must satisfy two consistency requirements [33]. First, the conditions need to be accessible: if we start from an arbitrary reference frame, i.e., an arbitrary set of local coordinates on Γ and arbitrary functions λ, it must be possible to reach a set that satisfies (A.68) by a finite gauge transformation determined by a well-defined choice of the functions $\varepsilon(\tau)$. Second, the only gauge transformation that leaves (A.68) invariant is the (on-shell) identity transformation. In this case, we say that the conditions (A.68) form a complete gauge fixing.

Once a canonical gauge is fixed, the functions λ are determined by requiring that the gauge is preserved by the dynamics, i.e., $\dot{\chi} = \partial\chi/\partial\tau + \{\chi, H_T\} \approx 0$ [cf. (A.73) and (A.74)]. How many (independent) conditions are necessary to form a complete gauge fixing? At first, one might suppose that the number of gauge conditions should be equal to the number of arbitrary functions λ to be fixed, which is the number of primary first-class constraints. However, in this case, the consistency conditions

$$0 \approx \{\chi, G\} = \sum_{j=0}^{n} \frac{\mathrm{d}^j \varepsilon_i}{\mathrm{d}\tau^j} \left\{\chi, G^i_{(j)}\right\} \tag{A.69}$$

generally lead to a set of differential equations for the $\varepsilon(\tau)$ functions, but do not determine their initial values. Different choices of the initial values may lead to gauge transformations that are different from the identity and that preserve the chosen gauge conditions. In this way, one needs to impose further gauge conditions to fix the initial values of $\varepsilon(\tau)$ [49]. Thus, the number of gauge conditions must be sufficient to fix the values of $\varepsilon(\tau)$ and their first n time derivatives at every instant of time. As was discussed in the previous section (§A.2.5), the number of these values is equal to the number of independent (primary and secondary) first-class constraints in the theory (for a minimal generator). Therefore, the number of independent gauge conditions must be equal to N_F [33].

Given the (canonical) gauge conditions χ_F ($F = 1, \ldots, N_F$), equation (A.69) will reduce to the on-shell identity if the only solution is $\mathrm{d}^j\varepsilon_i/\mathrm{d}\tau^j = 0$ ($j = 0, \ldots, n$) at every instant. This is fulfilled if the determinant of $\{\chi_F, G^i_{(j)}\}$ is non-vanishing. For a minimal generator, we obtain the equivalent requirement

$$\det\{\chi_F, C_{F'}\} \neq 0 \ , \tag{A.70}$$

due to (A.56). Due to (A.65), equation (A.70) is equivalent to

$$0 \neq \det X_{F'}\chi_F \approx \det \frac{\partial \chi_F}{\partial t^{F'}} \ . \tag{A.71}$$

The determinant in (A.70) and (A.71) is called the 'Faddeev-Popov determinant' [20, 21]. It is worthwhile to mention that it may be impossible to choose gauge conditions such that (A.70) is satisfied globally in the auxiliary phase space Γ, and one may have to admit the possibility that (A.70) or (A.71) is fulfilled only locally, i.e., only in a certain region of Γ. This problem is referred to as the 'Gribov obstruction' or 'Gribov problem' [33]. Due to this obstruction, one sees that the gauge choices (choices of generalized reference frames) are generally only of an approximate nature.

Let $\Gamma|_\chi$ denote the subspace of Γ defined by the canonical gauge conditions and let $\Sigma|_\chi$ represent the intersection of $\Gamma|_\chi$ with the constraint hypersurface Σ. Once a set of gauge conditions is fixed, we interpret the restriction $f|_\chi$ of an auxiliary phase-space function f to $\Sigma|_\chi$ as the description of f in a particular reference frame and we refer to $f|_\chi$ as a 'gauge-fixed quantity' or a 'gauge-fixed function'.

Let us now adopt the local coordinate system $z = (\xi, t, \varphi)$, for which the Poisson brackets are given in (A.62). We can then write an auxiliary phase-space function as $f \equiv f(\xi, t, \varphi)$ and the canonical gauge conditions read $\chi(\xi(\tau), t(\tau), \varphi(\tau), \tau)$. As a set of admissible gauges χ defines a single reference frame, it must select a single point in each gauge orbit. Thus, the conditions $\chi(\xi(\tau), t(\tau), \varphi(\tau) = 0, \tau) = 0$ must have a solution for the t coordinates, i.e., they must imply

$$t^F = t^F_\chi(\xi(\tau), \tau) \ , \ (F = 1, \ldots, N_F) \ , \tag{A.72}$$

in a region where (A.71) holds. Here, t_χ is some function for which $\chi(\xi(\tau), t_\chi, \varphi(\tau) = 0, \tau)$ is identically zero. To see that the solution (A.72) fixes the arbitrary functions λ in the dynamics, we use (A.67) to obtain

$$\delta^F_l H^l_1 + \delta^F_A \lambda^A \approx \dot{t}^F = \dot{t}^F_\chi \ . \tag{A.73}$$

Moreover, by requiring that $\chi(\xi, t_\chi, \varphi, \tau) \equiv 0$ is preserved by the evolution ($\dot{\chi} \approx 0$), we find

$$\dot{t}^F_\chi \approx \left[\left(\frac{\partial \chi}{\partial t}\right)^{-1}\right]^{F,F'} \left(-\frac{\partial \chi_{F'}}{\partial \tau} - \frac{\partial \chi_{F'}}{\partial \xi^r}\dot{\xi}^r\right) \ . \tag{A.74}$$

Equations (A.73) and (A.74) imply that the functions λ are now determined in terms of the functions H_1 and t_χ or, equivalently, H_1 and χ.

Given an auxiliary phase-space function $f(\xi(\tau), t(\tau), \varphi(\tau), \tau)$, the corresponding gauge-fixed quantity is $f|_\chi \equiv f(\xi(\tau), t_\chi, \varphi(\tau) = 0, \tau)$. Due to (A.72), one sees that gauge-fixed quantities only depend on ξ and τ and are, therefore, gauge invariant. More precisely, we can define the function

$$\mathcal{O}[f|\chi](\xi(\tau), t(\tau), \tau) := f(\xi(\tau), t_\chi, \varphi(\tau) = 0, \tau) \equiv f|_\chi \ , \tag{A.75}$$

which is constant along the gauge orbits. The function $\mathcal{O}[f|\chi]$ may be seen as a particular extension of $f|_\chi$ off of $\Sigma|_\chi$, one that is the same in every reference frame. We refer to $\mathcal{O}[f|\chi]$ as the 'invariant extension of f in the gauge χ'. Although it is defined as a function on the constraint hypersurface Σ, one can extend $\mathcal{O}[f|\chi]$ to the auxiliary phase space in the usual way, $\mathcal{O}[f|\chi] \mapsto \mathcal{O}[f|\chi] + v^l \varphi_l$, given a choice of v^l.

The following simple fact must, however, be emphasized. The functional relation between the invariant extension $\mathcal{O}[f|\chi]$ and its "seed" function f (when both are understood as auxiliary phase-space functions) in general depends on the chosen gauge conditions χ [33, 76]. This motivates us to introduce the following notion, which plays a key role in the definition of observables analyzed in §1.7.

Definition A.2 (Gauge (in)dependence)**.** A function defined on the auxiliary phase space is said to be 'gauge dependent' if its physical interpretation depends on a choice of canonical gauge conditions. Gauge dependent functions are, therefore, relational quantities, as they are to be interpreted with respect to a certain reference frame. Functions that are not gauge dependent are said to be 'gauge independent'.

Remark A.3. Due to (A.75), one may take the terms 'relational', 'gauge dependent' and 'gauge-fixed' as synonyms.

We stress that the two definitions A.1 and A.2 are distinct. In particular, a function may be gauge invariant but not gauge independent: its physical interpretation may refer to a choice of gauge, even though its functional form may not change under a general gauge transformation. In general, invariant extensions are simultaneously gauge-invariant and gauge-dependent (relational) quantities. The relevance of gauge-dependent functions depends on the ontology and the definition of observables of the theory.

It is frequently more useful to write $\mathcal{O}[f|\chi]$ in terms of the function f written in an arbitrary frame, i.e., for an arbitrary value of the t coordinates. This can be achieved by the formula

$$\mathcal{O}[f|\chi] = \int \mathrm{d}t \, \left|\det \frac{\partial \chi_F}{\partial t^{F'}}\right| \prod_{F=1}^{N_F} \delta(\chi_F(\xi, t, \varphi = 0, \tau)) f(\xi, t, \varphi = 0) \ , \tag{A.76}$$

where we have omitted the τ-arguments of each function for simplicity and we adopted the shorthand notation $\mathrm{d}t \equiv \prod_{F'=1}^{N_F} \mathrm{d}t^{F'}$ for the measure of integration over the values of $t^{F'}$ at a fixed instant. The delta functions of χ_F serve to fix the gauge, whereas the Jacobian factor $\left|\det \partial\chi_F/\partial t^{F'}\right|$ is included in order to change the variables from t to χ, which is permissible in regions where (A.71) is satisfied. One can then integrate (A.76) to recover (A.75). From (A.75) and (A.76), we see that invariant extensions have the following general properties: (1) they are defined on the constraint hypersurface Σ but can be extended to the auxiliary phase space Γ; (2) they can be written in terms of an arbitrary gauge but coincide with $f|_\chi$ once restricted to $\Sigma|_\chi$; (3) they are gauge invariant.

As the Jacobian factor in (A.76) is also a function of the (ξ, t) coordinates, we can replace it by its gauge-fixed value due to the delta functions, i.e.,

$$\left|\det \frac{\partial \chi_F}{\partial t^{F'}}\right| (\xi(\tau), t(\tau), \varphi(\tau) = 0, \tau) \mapsto \Delta_\chi := \left|\det \frac{\partial \chi_F}{\partial t^{F'}}\right| (\xi(\tau), t_\chi, \varphi(\tau) = 0, \tau) \ . \quad \text{(A.77)}$$

The quantity Δ_χ can be seen as an invariant extension of the Faddeev-Popov determinant given in (A.70) and (A.71). Whenever there is no risk of confusion, we will simply refer to Δ_χ as the Faddeev-Popov determinant. Note that Δ_χ also satisfies the identity

$$\Delta_\chi^{-1} = \int \mathrm{d}t \ \prod_{F=1}^{N_F} \delta(\chi_F(\xi, t, \varphi = 0, \tau)) = \left|\det \frac{\partial \chi_F}{\partial t^{F'}}\right|^{-1} (\xi, t_\chi, \varphi = 0, \tau) \ , \quad \text{(A.78)}$$

in regions where the gauge is admissible, i.e., where (A.70) and (A.71) are fulfilled. Note that we have once again omitted the τ-arguments of each function in (A.78). Equation (A.78) can also be taken as the definition of Δ_χ in terms of an average of the gauge-fixing delta functions taken over the gauge orbits. Due to (A.78), we can rewrite (A.76) as

$$\begin{aligned} \mathcal{O}[f|\chi] &= \Delta_\chi \int \mathrm{d}t \ \prod_{F=1}^{N_F} \delta(\chi_F(\xi, t, \varphi = 0, \tau)) f(\xi, t, \varphi = 0) \\ &= \frac{\int \mathrm{d}t \ \prod_{F=1}^{N_F} \delta(\chi_F(\xi, t, \varphi = 0)) f(\xi, t, \varphi = 0, \tau)}{\int \mathrm{d}t \ \prod_{F=1}^{N_F} \delta(\chi_F(\xi, t, \varphi = 0))} \ . \end{aligned} \quad \text{(A.79)}$$

From (A.76) or (A.79), we see that the invariant extension of the identity function is still the identity, i.e., $\mathcal{O}[1|\chi] \equiv 1$, as it should be. Equations (A.76) and (A.79) make it clear that invariant extensions can be obtained by writing gauge-fixed functions in an arbitrary gauge by means of an average taken over the gauge orbits. This motivates us to consider the more general objects

$$\mathcal{O}_\omega(\xi(\tau), \tau) := \int \mathrm{d}t \ \omega(\xi(\tau), t(\tau), \varphi(\tau) = 0, \tau) \ , \quad \text{(A.80)}$$

which are averages of functions $\omega(\xi(\tau), t(\tau), \varphi(\tau), \tau)$ over the gauge orbits. One sees that (A.79) is a particular case of (A.80). Equation (A.80) yields an invariant if the following equality is satisfied at each instant,

$$X_F \mathcal{O}_\omega = \int \mathrm{d}t \ \{\omega, C_F\} \approx \int \mathrm{d}t \ \frac{\partial \omega}{\partial t^F} = 0 \ . \quad \text{(A.81)}$$

Evidently, the validity of (A.81) depends on the region of the gauge orbits over which one integrates and on the boundary conditions of ω for different values of t^F. Both (A.79) and (A.81) are considered in the analysis of Chapter 1.

A.3 The reduced phase space and its quantization

As was mentioned in §A.2, the cotangent bundle $\Gamma = T^*\mathcal{Q}$ plays an auxiliary role in the Hamiltonian theory of constrained systems because all physical trajectories must be defined on the constraint hypersurface Σ. Consequently, one might expect that Σ could play the role of a 'physical' phase space. However, this is not true because the constraint hypersurface does not inherit a well-defined Poisson-bracket structure [33]. This can be easily seen if we adopt the local coordinates $z = (\xi, t, \varphi)$ in Γ. The components $\omega_{\beta\gamma}$ of the symplectic form in Γ are defined by $\omega_{\beta\gamma}\omega^{\gamma\eta} = \delta_\beta^\eta$, where $\omega^{\gamma\eta}$ defines the Poisson brackets according to (A.62). The induced two-form on Σ then has the components $\omega_{\bar\beta\bar\gamma}$, where the indices $\bar\beta, \bar\gamma$ are restricted to run over the values of the coordinates ξ, t only. If this induced two-form were invertible, one would be able to define a Poisson-bracket structure from its inverse. However, by using (A.63), (A.64) and (A.65) together with the antisymmetry of $\omega_{\beta\gamma}$, we find that $\omega_{\bar\beta\bar\gamma}X_F^{\bar\gamma} = \omega_{\bar\beta\bar\gamma}\omega^{\bar\gamma,R+N_F+F} \approx \omega_{\bar\beta\gamma}\omega^{\gamma,R+N_F+F} = \delta_{\bar\beta}^{R+N_F+F} = 0$. In this way, X_F are null eigenvectors of the induced two-form on Σ, which is thus not invertible (see [33] for further details).

Nevertheless, the fact that the constraint hypersurface can be foliated by the integral curves of X_F suggests that we may take the quotient of Σ by the orbits of X_F. As is well-known [33], this quotient space has a well-defined Poisson-bracket structure and, therefore, it serves as the 'physical' phase space of a constrained theory. We will denote it by Γ_{phys} and assume that it is a C^∞-manifold. As it is a quotient space, the physical phase space is also frequently called the 'reduced phase space' [33].

The Poisson-bracket structure on Γ_{phys} can be derived from the auxiliary phase-space brackets $\omega^{r,r'} = \{\xi^r, \xi^{r'}\}$. Indeed, ξ can be interpreted as local coordinates on the quotient space. Furthermore, although ξ and $\omega^{r,r'}$ were defined as functions on the auxiliary phase space, due to the fact that ξ and $\omega^{r,r'}$ are first class, we know from Remark A.2 (page 207) that the restriction of $\omega^{r,r'}$ to the constraint hypersurface is a function only of the ξ coordinates and, therefore, the Poisson bracket $\{f,g\}_{\Gamma_{\text{phys}}} := \omega^{r,r'}|_\Sigma \partial f/\partial\xi^r \partial g/\partial\xi^{r'}$ is well-defined for any pair of functions on Γ_{phys}. The induced two-form on Γ_{phys} is then simply given by the components $\omega_{r,r'}|_\Sigma$, since $\omega_{r,r'}\omega^{r',r''} = \omega_{r\gamma}\omega^{\gamma r''} = \delta_r^{r''}$ due to (A.64).

A.3.1 Dynamics of reference frames in the reduced phase space

The reduced phase space is obtained by identifying all points along the gauge orbits of X_F. Due to (A.60), this corresponds to considering that, at a given instant, all admissible choices of reference frames correspond to same physical state. In other words, a point in Γ_{phys} corresponds to an equivalence class of reference frames. Furthermore, functions $f(\xi)$ on the reduced phase space are by construction gauge invariant. Does one lose information about the dynamics when restricting oneself to Γ_{phys}? Are the different 'points of view' associated with each generalized reference frame lost when passing to the reduced phase space? The answer is no.

As we have seen in §A.2.7, the choice of gauge conditions, which determines the reference frame, is in general only admissible locally in the auxiliary phase space due to the Gribov obstruction. In regions of Γ where (A.70) holds, we may invariantly extend functions. As we assume that the second-class constraints were previously effectively eliminated by working with Dirac extensions [cf. (A.49)], the invariant extensions $\mathcal{O}[f|\chi]$ thus weakly Poisson-commute with both the first-class and the second-class constraints and are, therefore, first class. From Remark A.2 (page 207), we then conclude that $\mathcal{O}[f|\chi]$ can be expressed as functions solely of the ξ coordinates. In this way, invariant extensions of functions in a certain gauge are functions in the reduced phase space. This holds at a fixed moment of time. But what about the dynamics?

By taking the total time derivative of (A.75), we obtain

$$\dot{\mathcal{O}}[f|\chi] = \left(\frac{\partial f}{\partial \tau} + \frac{\partial f}{\partial \xi^r}\dot{\xi}^r + \frac{\partial f}{\partial t^F}\dot{t}^F_\chi\right)_{t=t_\chi,\varphi=0} . \tag{A.82}$$

Due to (A.65), (A.66), (A.67) and (A.73), equation (A.82) becomes

$$\begin{aligned} \dot{\mathcal{O}}[f|\chi] &= \left[\frac{\partial f}{\partial \tau} + \omega^{r,r'}\frac{\partial f}{\partial \xi^r}\frac{\partial H_0}{\partial \xi^{r'}} + \{f, C_F\}(\delta^F_l H^l_1 + \delta^F_A \lambda^A)\right]_{t=t_\chi,\varphi=0} \\ &= \left.\frac{\partial f}{\partial \tau}\right|_{t=t_\chi,\varphi=0} + \{f, H_0 + H^l_1\varphi_l + \lambda^A\varphi_A\}_{t=t_\chi,\varphi=0} \\ &= \left.\frac{\partial f}{\partial \tau}\right|_{t=t_\chi,\varphi=0} + \{f, H_T\}_{t=t_\chi,\varphi=0} \\ &= \mathcal{O}\left[\frac{\partial f}{\partial \tau} + \{f, H_T\}\middle|\,\chi\right] , \end{aligned} \tag{A.83}$$

where the functions λ are fixed by (A.73) and (A.74). Equation (A.83) shows that the time evolution of the invariant extension of a function with respect to a certain gauge corresponds to the invariant extension of the function's time evolution with respect to the same gauge. In this way, the (deterministic) gauge-fixed equations of motion can be represented in the reduced phase space. Thus, all the dynamical information related to a certain choice of reference frame (gauge condition) can be, in principle, encoded in reduced phase-space functions in a gauge-invariant way, i.e., without constraints. This is the reason the reduced phase space can be regarded as the physical phase space.

One can also describe the evolution of reduced phase-space functions using the Poisson bracket structure in Γ_{phys} as follows. For each instant of time, let $Q(\tau) = (q(\tau), p(\tau))$ be a set of local canonical coordinates on the auxiliary phase-space Γ. We assume that for each point of Γ, there is a neighborhood W in which the coordinate transformation $Q(\tau) \equiv Q(\xi(\tau), t(\tau), \varphi(\tau))$ is well defined.[11] If we further assume that a set of gauge conditions χ is admissible in W [cf. (A.70) and (A.71)], we can define the gauge-fixed functions [cf. (A.75)]

$$\mathcal{O}[Q|\chi] = Q(\xi(\tau), t_\chi, \varphi(\tau) = 0) \equiv Q|_\chi \ , \tag{A.84}$$

which represent (a portion of) the physical trajectories in a particular reference frame. The physical trajectories are labeled by the physical initial values $\mathcal{O}[Q|\chi]|_{\tau=0}$, which are compatible with the constraints (cf. A.2.4); i.e., they weakly Poisson-commute with the constraint functions when seen as functions in the auxiliary phase space. We then assume that the family of tangent vectors X_{phys} to the physical trajectories (labeled by the physical initial values) defines a smooth vector field in a region of Γ_{phys}. We refer to this vector field as the 'physical' or 'reduced' Hamiltonian vector field. Furthermore, any function H_{phys} that satisfies

$$X_{\text{phys}} = \{\cdot, H_{\text{phys}}\}_{\Gamma_{\text{phys}}} \tag{A.85}$$

is referred to as the 'physical' or 'reduced' Hamiltonian, and it describes the gauge-fixed physical evolution. Note that its definition may be valid only locally in Γ_{phys} due to the Gribov obstruction. Physical Hamiltonians may be defined even in the case in which there is no non-trivial canonical Hamiltonian and $H' \equiv 0$ (cf. §1.9.2).

A.3.2 Limitations of the reduced phase-space description

The formalism presented in the previous sections of this appendix is, in principle, a complete account of the classical canonical formulation of constrained (and, in particular, gauge) systems. The next step is to analyze the quantum theory.

Nevertheless, there is a series of limitations to the practical applicability of the formalism presented here, in particular concerning the concept of the reduced phase space Γ_{phys}. It may be difficult or even impossible to explicitly construct Γ_{phys}, since this requires the construction of a complete set of gauge-invariant functions ξ, which are solutions to $\{\xi, C_F\} \approx 0$. In practical field-theoretic applications (such as in GR), the task of defining the ξ coordinates is rather involved. One might attempt to find a complete set of invariants by using invariant extensions $\mathcal{O}[f|\chi]$, but this method is subject to the Gribov obstruction. Moreover, it may be that no set of functions ξ can serve as canonical coordinates on Γ_{phys} for which the Poisson brackets acquire their canonical form. Due to these and other difficulties, it may be preferable to develop

[11]More precisely, let (U, ϕ_Q) with $\phi_Q : U \subset \Gamma \to \tilde{U} \subset \mathbb{R}^{2d}$ and (V, ϕ_z) with $\phi_z : V \subset \Gamma \to \tilde{V} \subset \mathbb{R}^{2d}$ be the coordinate charts associated with each coordinate system. We then assume that $W := U \cap V \neq \emptyset$ and that $\phi_z \circ \phi_Q^{-1}$ is a diffeomorphism, such that the two charts are smoothly compatible.

other methods of analysis, such as the study of the Becchi-Rouet-Stora-Tyutin (BRST) cohomology, in which case one enlarges the (auxiliary) phase space (instead of reducing it) by including extra degrees of freedom related to the so-called 'ghosts' (see [33] for further details).

For the applications in this thesis, however, the analysis of gauge systems based on the reduced phase space is both sufficient and illuminating, since it clarifies the definition and physical meaning of the (relational) observables of a gauge theory (cf. the discussion on the definition of observables presented in §1.7; see also **Conclusions and Outlook** for a discussion on possible further developments). Furthermore, as the relation between reduced phase-space functions and the local canonical coordinates on the auxiliary phase-space [cf. (A.84)] is of importance in the analysis of Chapter 1 and, indeed, throughout the thesis, it will be useful to develop a quantum theory that not only encompasses the reduced phase-space dynamics but also the description in the auxiliary phase space. This will be the topic of §A.3.4. In §A.3.3, we construct the Hamilton-Jacobi formalism of the classical theory as a first step towards quantization.

A.3.3 Hamilton-Jacobi formalism

As before, we assume that the second-class constraints have already been eliminated from the theory [e.g., by using the Dirac extensions (A.49)] and that it is possible to find canonical coordinates denoted by (q^a, p_a) for $a = 1, \ldots d - N_S/2$ with respect to which the only remaining constraints C_F $(F = 1, \ldots, N_F)$ are first class. The Hamilton-Jacobi canonical transformation is obtained from the generating function $\mathcal{F} = \mathrm{S}(q, P, \tau) - Q^a P_a$, where (Q, P) are the new canonical coordinates. The Lagrangians for each set of canonical pairs are related by $p_a\dot{q}^a - H_T = P_a\dot{Q}^a - K_T + \mathrm{d}\mathcal{F}/\mathrm{d}\tau$, where H_T is the total Hamiltonian for an arbitrary choice of the functions λ. The new total Hamiltonian K_T is required to vanish identically. In this way, we obtain the usual unconstrained Hamilton-Jacobi equations

$$\begin{aligned} p_a = \frac{\partial \mathrm{S}}{\partial q^a}\ ,\ Q^a = \frac{\partial \mathrm{S}}{\partial P_a}\ , \\ 0 = \frac{\partial \mathrm{S}}{\partial \tau} + H_T\left(q, \frac{\partial \mathrm{S}}{\partial q}\right)\ . \end{aligned} \tag{A.86}$$

The first two equations can, in principle, be inverted to yield $q \equiv q(Q, P)$ and $p \equiv p(Q, P)$. If we now take into account the fact that the momenta p are constrained by $C_F(q, p)$, we obtain the additional requirements

$$C_F\left(q, \frac{\partial \mathrm{S}}{\partial q}\right) = 0\ ,\ (F = 1, \ldots, N_F)\ , \tag{A.87}$$

which may be seen as constraints on the new momenta P. In the particular case in which the first-class constraints are abelian, i.e., in which the functions $c_{FF'}^{F''}$ in (A.48) are identically zero, we may define the first N_F new momenta such that $C_F(q,p) = P_F$ without loss of generality.[12] In this case, equation (A.87) implies that $P_F = 0$. Let us denote the remaining new momenta as $k_i := P_{N_F+i}$ $(i = 1, \ldots, d - N_S/2 - N_F)$. The restriction of Hamilton's principal function to the first-class constraint hypersurface, $S(q,k,\tau) := \mathrm{S}(q,P,\tau)|_{P_F=0}$, no longer depends on P_F, and the conjugate variables $t^F := Q^F$ may be seen as the parameters along the gauge orbits. Moreover, the k_i momenta and their conjugate coordinates $x^i := Q^{N_F+i}$ Poisson-commute with the constraints P_F by construction. Thus, they form a set of $2d - 2N_F - N_S = 2d - M - K - N_F = R$ conjugate pairs of gauge-invariant functions that can be used to define canonical coordinates on the reduced phase space [i.e., we may adopt $\xi := (x,k)$] [33]. An analogous construction can be made in the quantum theory, where solutions of the quantum constraint equations can be used to define a basis in the so-called 'physical' or 'reduced' Hilbert space.

A.3.4 Quantum theory

The quantization of gauge systems is a rich subject. There are many approaches, each with its advantages and shortcomings. We will focus solely on the canonical (operator-based) quantum theory and will not discuss path integrals. For a detailed account of path integrals for constrained and gauge systems, the reader is referred to [33] and references therein.

Let us assume that the reduced phase space Γ_{phys} can be constructed, i.e., that the limitations discussed in §A.3.2 can be overcome. Then, the quantum theory could be obtained by promoting the complete set of gauge-invariant functions ξ to operators $\hat{\xi}$ acting on a Hilbert space $\mathcal{H}_{\text{phys}}$ equipped with an inner product $(\cdot|\cdot)$. The $\hat{\xi}$ operators should be symmetric with respect to $(\cdot|\cdot)$, i.e., for any pair of states in the domain of $\hat{\xi}$, we should obtain $(\psi_{(1)}|\hat{\xi}\psi_{(2)}) = (\hat{\xi}\psi_{(1)}|\psi_{(2)})$. Furthermore, one assumes that it is possible to find self-adjoint extensions of $\hat{\xi}$. We refer to $\mathcal{H}_{\text{phys}}$ as the 'physical' or 'reduced' Hilbert space. This construction of the quantum theory may suffer from severe factor-ordering ambiguities if the classical coordinates ξ are not canonical, in which case the quantization of the Poisson bracket structure $\{\cdot,\cdot\}_{\Gamma_{\text{phys}}}$ may not be straightforward. It may also be complicated to promote $H'(\xi, \varphi = 0)$ [cf. (A.66)] or H_{phys} [cf. (A.85)] to self-adjoint (extensions of symmetric) operators due to ordering ambiguities.

Furthermore, a direct quantization of ξ may leave unclear or unexplored the relation

[12]Given a set of constraints C_F that satisfies (A.48), it is possible to locally adopt an equivalent description of the constraint hypersurface such that the constraint functions are abelian. This can be achieved by suitable local redefinitions of the constraint functions or of the canonical coordinates on Γ. See [33] for details.

of the quantum dynamics (e.g., of correlation functions of $\hat{\xi}$) to the auxiliary variables (q,p) in Γ [cf. (A.84)]. If one adopts a definition of observables in which (q,p) play a certain (relational) role (cf. discussion on the definition of observables in §1.7, one would like to express the dynamics of physical correlation functions also in terms of (q,p). For this reason, it is useful to develop a quantum theory that not only surpasses some of the difficulties found in a direct quantization of the ξ coordinates, but also encompasses both the auxiliary and reduced phase-space descriptions. This is, in principle, achieved by the so-called 'Dirac quantization' scheme.

Dirac quantization proceeds in analogy to the construction of the classical canonical theory, in which one first considers constraints in an auxiliary phase space and subsequently one constructs a reduced phase space. In the corresponding quantum theory, one starts with an auxiliary Hilbert space and a definition of gauge orbits and afterwards one considers the definition of a physical (or reduced) Hilbert space of gauge-invariant states. As explained above (see also Chapter 2), the construction of the auxiliary Hilbert space may not be merely one of convenience, but it may also be relevant for the interpretation of conditional probability amplitudes, depending on the ontology and the definition of observables of the theory.

Before Dirac-quantizing the theory, it is useful (although not necessary [33]) to eliminate the second-class constraints at the classical level [e.g., by using the Dirac extensions (A.49)]. As in the Hamilton-Jacobi formalism (cf. §A.3.3), we thus assume that one can define canonical coordinates (q^a, p_a) for $a = 1, \ldots d - N_S/2$ that are subject only to first-class constraints C_F $(F = 1, \ldots, N_F)$. The auxiliary Hilbert space $\mathcal{H}$ can then be obtained via the usual canonical quantization procedure for the variables (q^a, p_a). One considers the operators $(\hat{q}, \hat{p})$, which satisfy the same-instant commutation relations $[\hat{q}^a, \hat{p}_b] = \mathrm{i}\hbar\delta^a_b$ $(a, b = 1, \ldots d - N_S/2)$ and which are self-adjoint (extensions of symmetric) operators, given a definition of the auxiliary inner product $\langle\cdot|\cdot\rangle$ in $\mathcal{H}$.

States in $\mathcal{H}$ are referred to as 'auxiliary' or 'kinematical' states. Given an auxiliary state $|\psi\rangle$, we define its evolution through the Schrödinger equation [cf. (A.86)]

$$\mathrm{i}\hbar\frac{\partial}{\partial\tau}|\psi\rangle = \hat{H}_T|\psi\rangle \ , \tag{A.88}$$

where $\hat{H}_T := H'(\hat{q},\hat{p}) + \lambda^A\varphi_A(\hat{q},\hat{p})$ and we assume that: (1) both $H'(\hat{q},\hat{p})$ and $\varphi_A(\hat{q},\hat{p})$ are self-adjoint operators with a particular choice of factor ordering; (2) the coefficients λ are chosen to be arbitrary c-numbers rather than operators in order to avoid ordering ambiguities.

The operators $\varphi_A(\hat{q},\hat{p})$ are the quantum analogues of the primary first-class constraints. In fact, we assume that all classical first-class constraints can be promoted to operators $\hat{C}_F \equiv C_F(\hat{q},\hat{p})$ that are self-adjoint with respect to the auxiliary inner product $\langle\cdot|\cdot\rangle$ with a certain factor ordering. It must be stressed, however, that the first-class condition is not always preserved in the quantum theory. Indeed, it may be that the Poisson brackets (A.48) acquire quantum corrections, i.e., that one finds $[\hat{C}_F, \hat{C}_{F'}] = \hat{c}^{F''}_{FF'}\hat{C}_{F''} + \hbar^2 \hat{d}_{FF'}$. Here, $\hat{c}^{F''}_{FF'}$ is a quantization of the classical functions $c^{F''}_{FF'}$, whereas the operator $\hat{d}_{FF'}$ is independent from $\hat{C}_F$ ($F = 1, \ldots, N_F$) and has no classical counterpart. This operator is called an anomaly and it breaks the gauge symmetry of the theory [33]. A similar operator may appear in the commutator of $H'(\hat{q}, \hat{p})$ with $\hat{C}_F$ ($F = 1, \ldots, N_F$). In the presence of anomalies, the Dirac quantization procedure is not consistent and one may need to resort to other quantization methods such as BRST theory [33]. We thus assume that no anomalies are present, since the corresponding Dirac quantization is sufficient for the applications considered in this thesis. In this case, we define gauge transformations of auxiliary states as

$$\mathrm{i}\hbar\bar{\delta}\,|\psi\rangle = \hat{G}\,|\psi\rangle \ , \tag{A.89}$$

where the quantum gauge generator is $\hat{G} := \sum_{j=0}^{n} \hat{G}^i_{(j)} \mathrm{d}^j\varepsilon_i/\mathrm{d}\tau^j|_{\tau=\tau_0} \equiv v^F \hat{C}_F$ [cf. (A.60)]. We assume that the arbitrary functions ε and their derivatives are chosen to be c-numbers rather than operators, which are evaluated at a fixed instant $\tau = \tau_0$. Note that (A.88) and (A.89) define the Schrödinger picture of the auxiliary quantum dynamics and of gauge transformations, respectively. Provided there are no anomalies and (A.88) and (A.89) are integrable, one can then pass to the Heisenberg picture in the usual way.

From (A.89), we note that gauge-invariant states $|\Psi\rangle$ must be annihilated by the quantum gauge generator at every instant of time, i.e., $\hat{G}\,|\Psi\rangle = 0$. This then implies that the quantum first-class constraints need to be fulfilled

$$\hat{C}_F\,|\Psi\rangle = 0 \ . \tag{A.90}$$

Equation (A.90) is the quantum analogue of the definition of the classical first-class constraint hypersurface. States that are annihilated by the constraints at every instant of time are said to be ‘on shell’. Thus, gauge-invariant states are on shell. Due to the definition of the quantum gauge generator, the converse is also true: on-shell states are gauge invariant.

Given a set of linearly independent gauge-invariant states denoted by $|k\rangle$, we can define on-shell operators as

$$\hat{\mathcal{O}} := \sum_{k',k} \mathcal{O}(k',k)\,|k'\rangle\,\langle k| \ , \tag{A.91}$$

for some choice of function $\mathcal{O}(k',k)$. The summation in (A.91) is formal and may be replaced by an integration if the k labels are continuous. These operators correspond to linear transformations of the on-shell states. It is straightforward to verify that (A.91) defines a gauge-invariant operator, i.e., one that satisfies $[\hat{\mathcal{O}}, \hat{C}_F] = 0$. In fact, on-shell operators satisfy the stronger condition $\hat{\mathcal{O}}\hat{C}_F = \hat{C}_F\hat{\mathcal{O}} = \hat{0}$. If the set of $|k\rangle$ states is complete, i.e., if any gauge-invariant (on-shell) state can be written as a linear combination of the $|k\rangle$ states, then it is sufficient to consider only gauge-invariant operators that are on-shell, i.e., of the form given in (A.91). In Chapter 2, we extensively discuss how classical invariant extensions of the form (A.79) can be promoted to on-shell operators of the form (A.91) in the quantum theory (for the particular case of theories that are invariant under local time translations).

In contrast to the auxiliary Hilbert space $\mathcal{H}$ of kinematical states $|\psi\rangle$, we can define the physical or reduced Hilbert space $\mathcal{H}_{\text{phys}}$ as the space of gauge-invariant states that are square-integrable with respect to a choice of 'physical' inner product $(\cdot|\cdot)$. Given a complete set of linearly independent on-shell states $|k\rangle$, their physical inner product can be defined by regularizing their auxiliary inner product with the insertion of a certain operator $\hat{\mu}$, i.e., $(k'|k) := \langle k'|\hat{\mu}|k\rangle$. The 'measure' $\hat{\mu}$ is an operator in the auxiliary Hilbert space and it should be chosen such that: (1) $(k'|k)$ is positive definite and gauge invariant; (2) there exist superpositions $|\Psi_{(i)}\rangle$ of $|k\rangle$ that have finite norm and overlap, i.e., $|(\Psi_{(i)}|\Psi_{(j)})|^2 < \infty$, where i and j are labels on the possibly different superpositions. More precisely, the gauge-invariance of $(k'|k)$ entails that $\hat{C}_F$ should be realized as a self-adjoint zero operator, i.e., $(k'|\hat{C}_F k) = (\hat{C}_F k'|k) = 0$ for $F = 1, \ldots, N_F$.

If $\langle k'|k\rangle$ satisfies the two conditions above, then one may choose $\hat{\mu}$ to be the identity in the auxiliary Hilbert space, i.e., $\hat{\mu} = \hat{1}$. In general, however, it is necessary to regularize the inner product of gauge invariant states to guarantee that both conditions are fulfilled. Let us assume that $\hat{\mu}$ has been fixed and that the complete set of linearly independent states $|k\rangle$ have been orthonormalized such that $(k'|k) = \delta(k', k)$, where $\delta(\cdot, \cdot)$ stands for a Kronecker or Dirac delta depending on whether the k labels are discrete or continuous. In this case, we consider $|k\rangle$ to define a basis in the physical Hilbert space and the on-shell operators (A.91) can be interpreted as quantizations of certain reduced phase-space functions. For this reason, the Dirac quantization programme is a type of reduced phase-space quantization. Evidently, the results of the Dirac quantization of a theory may differ from those obtained by a direct quantization of the reduced phase-space coordinates ξ, for example, due to factor-ordering ambiguities. Moreover, as the Dirac quantization starts with the notion of an auxiliary Hilbert space $\mathcal{H}$, it allows one to relate on-shell operators to auxiliary Hilbert space operators, e.g., through the projections $\sum_{k',k} |k'\rangle \langle k'|\hat{A}|k\rangle \langle k|$, where $\hat{A}$ acts on $\mathcal{H}$ and is not gauge invariant [33].

There are two important particular cases in which $\hat{\mu}$ can be fixed. First, if one already knows a complete set of gauge-invariant operators $\hat{\xi}$ that are obtained by the Dirac quantization of well-defined real-valued functions $\xi(q, p)$ defined in the auxiliary phase space, then $\hat{\mu}$ should be chosen such that $\hat{\xi}$ act as self-adjoint operators in the physical Hilbert space $\mathcal{H}_{\text{phys}}$. Second, in analogy to the Hamilton-Jacobi formalism (cf. §A.3.3), if the first-class quantum constraints are abelian, i.e., if $[\hat{C}_F, \hat{C}_{F'}] = 0$ for $F, F' = 1, \ldots, N_F$, then it is possible to find a simultaneous orthonormal basis $|C, k\rangle$ for the constraints in the auxiliary Hilbert space. The indices k now label degeneracies of the constraint spectrum, $\hat{C}_F\,|C, k\rangle = C_F\,|C, k\rangle$ $(F = 1, \ldots, N_F)$. One immediately sees that the gauge-invariant states $|k\rangle := |C = 0, k\rangle$ define an orthonormal basis in the reduced Hilbert space if the physical inner product is defined through the formula [33, 66, 68, 69]

$$\langle C', k'|C, k\rangle =: \delta(C', C)(k'|k) \ , \tag{A.92}$$

which implies $(k'|k) = \delta(k', k)$. This inner product satisfies the above criteria and is well-defined even if the zero is in the continuous part of the constraint spectrum. As is shown in Chapter 2 for the case of local time-translation invariance, the regularization (A.92) corresponds to the insertion $(k'|k) = \langle k'|\hat{\mu}|k\rangle$, where $\hat{\mu}$ is related to any admissible quantum gauge condition, in analogy to the classical formula (A.79). The formalism developed in Chapter 2 can be straightforwardly generalized to any system of abelian quantum constraints.

Once one has defined the physical inner product [e.g., as in (A.92)] and one can construct on-shell operators (A.91) that act on the physical Hilbert space $\mathcal{H}_{\text{phys}}$, it is straightforward to compute physical correlation functions. Let us consider Heisenberg-picture operators $\hat{\mathcal{O}}(\tau)$ that evolve, e.g., with the total Hamiltonian or with another on-shell operator that plays the role of the quantized reduced Hamiltonian [cf. (A.85)]. Then, for any pair of gauge-invariant states $|\Psi_{(1)}\rangle$ and $|\Psi_{(2)}\rangle$, the correlation function of the time-ordered string $\hat{\mathcal{O}} := \mathcal{T}\prod_i \hat{\mathcal{O}}(\tau_i)$ is computed with the physical inner product, i.e., one defines $\langle\hat{\mathcal{O}}\rangle := (\Psi_{(2)}|\hat{\mathcal{O}}|\Psi_{(1)})$.

Appendix B

The Traditional Born-Oppenheimer Approach to the Problem of Time

In this appendix, we offer a critical review of the traditional Born-Oppenheimer (BO) approach to the problem of time, which is to be contrasted with the approach followed in Chapter 5.[1]

B.1 What is the traditional BO approach?

The classical and quantum theories of mechanical systems with local time translation invariance are discussed at length in Chapters 1 and 2, where it is shown that the central object in the Dirac-quantized theory is the quantum constraint (or WDW) equation. As this constraint is a time-independent Schrödinger equation (TISE), one faces the problem of time in the quantum theory. Which time variable (if any) orders the dynamics? How is it defined? While this is the topic of Chapter 2, several (partial) solutions to the problem of time have been proposed in the literature [24].

One of the oldest and most straightforward approaches is the BO approach to the problem of time. It is based on the BO approximation [124, 166–172] used in nuclear and molecular physics to analyze the dynamics of a system of electrons and nuclei [121]. The approximation was established in the work of Born and Oppenheimer [173] and its application to the definition of a time variable from a time-independent equation was discussed in the work of Mott [174, 175].

In its original context, the BO approximation is a combination of a WKB expansion and an adiabatic approximation for a system of electrons and nuclei. Indeed, it is sometimes possible to consider that the nuclei are approximately described by WKB

[1] This appendix is based on [62, 98].

factors in the system's wave function and, therefore, that their dynamics is semiclassical (in an appropriate sense). In addition, one makes an adiabatic approximation, in which the dynamics of the electronic wave function is conditioned on the semiclassical configurations of the nuclei. Concretely, this approximation scheme is controlled by a perturbative expansion (analogous to the weak-coupling expansion discussed in Chapter 5). In their original article [173], Born-Oppenheimer considered that the electrons are much lighter than the nuclei, with a mass m much smaller than the average mass M of the 'heavy' nuclei. In this way, they used $\left(\frac{m}{M}\right)^{\frac{1}{4}}$ as a perturbative parameter to calculate series developments of the relevant physical quantities. At the lowest order in the expansion, the nuclear positions are fixed (classical) parameters, conditioned on which the quantum dynamics of electrons can be described.

The BO approximation can be applied to any system that admits a decomposition of its degrees of freedom into 'heavy variables' (in analogy to the nuclei) and 'light variables' (in analogy to the electrons) [176–178]. The relevance of this procedure to the problem of time rests upon two properties: (1) the perturbative expansion coincides with a WKB expansion in the 'heavy sector'; (2) the quantum dynamics of the 'light sector' is conditioned on the (semiclassical) dynamics of the 'heavy sector'. Due to the first property, a notion of (classical) trajectory for the heavy variables is available at the lowest order, and one may define a 'semiclassical time' parameter (also called 'WKB time' [119]) as the orderer of the dynamics of the heavy variables. Due to the second property, the quantum evolution of the light variables is also governed by the WKB time. Thus, the BO approach avoids the problem of time in the semiclassical regime, in which WKB time 'emerges'.

An early derivation of the semiclassical emergence of time is found in [174, 175], where Mott considered the TISE for a system of α particles and atoms. Mott was able to derive a time-dependent Schrödinger equation (TDSE) for the atoms by assuming that α particles behaved semiclassically and by defining a time parameter from their approximate trajectories. This work has been highly influential and inspired a number of subsequent analyses [176, 177, 179, 180]. Due to the possibility to derive time from a timeless equation in this fashion, some researchers, such as Englert [181], Briggs and Rost [176, 177], and Arce [123], suggest that the TISE should be the fundamental equation that describes the mechanics of closed quantum systems, whereas the TDSE would only hold approximately for the light degrees of freedom.

This idea clearly finds its analogue in the WDW equation of quantum gravity. Indeed, the functional TDSE for matter fields conditioned on a vacuum background was derived from the quantum constraints by Lapchinsky and Rubakov [182] in a way analogous to Mott's work. The analogy to the original scheme of Born and Oppenheimer became clear in [183, 184], where the solutions to the quantum constraints were expanded in powers of the gravitational coupling constant (or, equivalently, the inverse Planck mass), which plays the same role as the perturbative parameter $(m/M)^{1/4}$ in [173]. Perturbation theory holds if this is a weak-coupling expansion (cf. Chapter 5), i.e., if the Planck scale is much larger than other energy scales considered. In this way, the gravitational field usually corresponds to the heavy variables, while matter fields are typically the light degrees of freedom. If one computes terms of higher order in the gravitational coupling constant, one finds corrections to the usual TDSE for matter fields conditioned on a fixed background [120, 137, 151, 185]. The issue of whether these corrections are unitary has been debated in the liteature [120, 163] and is discussed in Chapter 5.

Finally, it is important to note that, if the BO perturbative procedure breaks down, one can either consider that time cannot be defined and the theory is strictly timeless or one can attempt to develop another method of discussing the quantum dynamics. One such method is presented in Chapter 2.

B.2 The semiclassical derivation of time

Let us now critically review the traditional BO approach to the problem of time. The reader is referred to [6, 98, 176–178] for further details. We consider a set of light variables q^μ ($\mu = 1, \ldots, d$) with a typical mass scale m, as well as a set of heavy variables Q^a ($a = 1, \ldots, n$) with a typical scale $M \gg m$. The system is described by the TISE[2]

$$-\frac{\hbar^2}{2M}\sum_{a=1}^{n}\frac{\partial^2\Psi}{\partial(Q^a)^2} + V(Q)\Psi + \hat{H}_{\mathrm{S}}\left(Q; \frac{\partial}{\partial q^\mu}, q_\mu\right)\Psi = E\Psi \ , \tag{B.1}$$

where $\hat{H}_{\mathrm{S}}$ is an operator with a parametric dependence on the heavy variables that furthermore depends on q^μ and their associated momenta. It may be interpreted as the Hamiltonian for the light sector. To solve (B.1), one can make the traditional BO ansatz

$$\Psi(Q, q) = \psi_0(Q)\psi_{\mathrm{BO}}(Q; q) \ , \tag{B.2}$$

which consists of an exact factorization of the total state $\Psi(Q, q)$ [100, 122, 123, 178, 186–188]. The interpretation of each factor, ψ_0 and ψ_{BO}, will be considered in what follows. We can define the BO inner product over the light degrees of freedom [62]

$$\langle\psi_{\mathrm{BO}(1)}|\psi_{\mathrm{BO}(2)}\rangle_{\mathrm{BO}}(Q) := \int \mathrm{d}q \ \psi^*_{\mathrm{BO}(1)}(Q; q)\hat{\mu}_{\mathrm{BO}}\psi_{\mathrm{BO}(2)}(Q; q) \ , \tag{B.3}$$

[2] Evidently, it is possible to consider generalizations of (B.1) (e.g., with a non-trivial configuration space geometry, cf. Chapter 5).

where $\mathrm{d}q \equiv \prod_\mu \mathrm{d}q^\mu$ and $\hat{\mu}_{\mathrm{BO}}$ is a 'measure' to be determined (we assume that $\hat{\mu}_{\mathrm{BO}}$ is symmetric with respect to the flat inner product, i.e., $\hat{\mu}_{\mathrm{BO}}^\dagger = \hat{\mu}_{\mathrm{BO}}$).[3] In certain applications, it may be convenient to write ψ_{BO} in terms of a complete orthonormal system with respect to the BO inner product, i.e., $\psi_{\mathrm{BO}}(Q;q) = \sum_k \chi_k(Q)\psi_k(Q;q)/\psi_0(Q)$, where $\langle\psi_k|\psi'_k\rangle_{\mathrm{BO}} = \delta(k,k')$. In this case, the total state reads $\Psi(Q,q) = \sum_k \chi_k(Q)\psi_k(Q;q)$. We shall not consider this here and we work exclusively with the exact factorization (B.2).

Given the ansatz (B.2), we can solve (B.1) as follows. The first step is to define the 'source' or 'backreaction term' [98, 138, 140, 141, 163]

$$\mathfrak{J}(Q) := \frac{\hbar^2}{2M\psi_0(Q)}\sum_{a=1}^{n}\frac{\partial^2\psi_0}{\partial Q_a^2} - V(Q) + E\ . \tag{B.4}$$

Equation (B.4) is a TISE for the ψ_0 wave function, where $\mathfrak{J}(Q)$ plays the role of another potential term. We will see in what follows how this potential is related to a notion of 'backreaction' of the light degrees of freedom onto the dynamics of the Q variables (cf. Sec. B.3). The second step is to obtain an equation that is to be regarded as an equation for ψ_{BO}. If we use (B.2) and (B.4) in (B.1), the result is

$$\frac{\hbar^2}{M}\sum_{a=1}^{n}\frac{\partial\log\psi_0}{\partial Q^a}\frac{\partial\psi_{\mathrm{BO}}}{\partial Q^a} = \left(\hat{H}_{\mathrm{S}} - \mathfrak{J}\right)\psi_{\mathrm{BO}} - \frac{1}{2M}\sum_{a=1}^{n}\frac{\partial^2\psi_{\mathrm{BO}}}{\partial(Q^a)^2}\ , \tag{B.5}$$

which is usually seen as an equation for ψ_{BO} given a solution for ψ_0. Finally, we assume that $\log\psi_0(Q) = \mathrm{i}M\varphi(Q)/\hbar + \mathcal{O}(M^0)$ and we define the 'phase time' $\partial/\partial t := \sum_{a=1}^{n}\partial\varphi/\partial Q^a\partial/\partial Q^a + \mathcal{O}(1/M)$, such that (B.5) can be written as

$$\mathrm{i}\hbar\frac{\partial\psi_{\mathrm{BO}}}{\partial t} = \left(\hat{H}_{\mathrm{S}}(t) - \mathfrak{J}\right)\psi_{\mathrm{BO}} + \mathcal{O}\left(\frac{1}{M}\right)\ , \tag{B.6}$$

which is a TDSE for ψ_{BO}. A few comments are in order. First, equation (B.6) is only valid when higher order terms in $1/M$ can be neglected, i.e., when a perturbative expansion in the inverse 'heavy mass' is valid. This is clearly a formal procedure and all concrete calculations should involve powers of the small ratio m/M or of some other light mass scale to M, in analogy to the original scheme of Born and Oppenheimer. Second, the time variable in (B.6) was defined from the lowest-order term in $1/M$ of the phase of ψ_0. This lowest-order phase time often has a straightforward meaning: it is the parameter that orders the classical dynamics of the heavy variables. This can

[3] A 'flat measure' ($\hat{\mu}_{\mathrm{BO}} = \hat{1}$) is frequently adopted [124, 126]. However, following the results of Chapter 5, we argue in §B.4.3 that a more general $\hat{\mu}_{\mathrm{BO}}$ is implied by the quantum constraint.

be seen if the expansion in powers of $1/M$ coincides with the standard $\hbar$-expansion for the heavy sector [182–184], which is the case if the total potential in (B.4) scales with M. This yields a semiclassical description of the evolution of the heavy degrees of freedom, in which there is an approximate notion of trajectory that orders the physical configurations of the Q variables. The lowest-order phase time is nothing but this order.[4] Moreover, due to (B.6), one sees that the dynamics of the heavy sector also governs the evolution of the q variables (i.e, Q provide a clock for q).

By considering terms of higher orders in $1/M$ in (B.6), it is possible to compute corrections to the Schrödinger equation [120, 137, 151, 185]. These corrections are sometimes claimed to violate unitarity [114–116, 120], although we will see that the formalism of Chapter 5 resolves this issue. When higher-order corrections are included in (B.6), one may either describe the dynamics with respect to the lowest-order phase time or with respect to a corrected time function that also includes higher orders in $1/M$ of the phase of ψ_0. This corrected phase time can be tentatively interpreted as the orderer of the dynamics of Q when quantum corrections and the backreaction of q are taken into account (see, however, Secs. B.3 and B.4). In the case in which the expansion in powers of $1/M$ coincides with a WKB expansion in the heavy sector, the (corrected) phase time is called WKB time [119].[5]

It is possible to define more general time functions that, for instance, take into account some contributions from the amplitude of ψ_0 [178, 189]. One may also define a time function from the phase of the total state Ψ [190–193].[6] These alternative definitions, however, often lack a clear physical interpretation.

B.3 Backreaction

In what sense is $\mathfrak{J}(Q)$ in (B.4) and (B.6) a backreaction term? Usually [124, 166–168], the backreaction term is associated with the expectation value of the Hamiltonian for the light degrees of freedom taken with respect to the BO inner product (B.3). To see how $\mathfrak{J}(Q)$ is related to this, we first define the general BO average [cf. (B.3)]

$$\langle \hat{O} \rangle_{\mathrm{BO}} := \frac{\langle \psi_{\mathrm{BO}} | \hat{O} | \psi_{\mathrm{BO}} \rangle_{\mathrm{BO}}}{\langle \psi_{\mathrm{BO}} | \psi_{\mathrm{BO}} \rangle_{\mathrm{BO}}} = \frac{\int \mathrm{d}q \ \psi^*_{\mathrm{BO}} \hat{\mu}_{\mathrm{BO}} \hat{O} \psi_{\mathrm{BO}}}{\int \mathrm{d}q \ \psi^*_{\mathrm{BO}} \hat{\mu}_{\mathrm{BO}} \psi_{\mathrm{BO}}} \ , \tag{B.7}$$

[4] More precisely, the lowest-order phase time is the parameter along the approximate trajectories of the Q variables, when these are regarded as parametrized curves in configuration space.

[5] One may also refer to the lowest-order phase time simply as WKB time. This is what was done in Chapter 5.

[6] It is worth mentioning that a notion of quantum trajectories (i.e., at all orders in the semiclassical expansion) is available in the de Broglie-Bohm approach to timeless quantum systems [26, 27]. In this approach, time can also be defined from the phase of the total state Ψ, but we do not consider this here.

which is a function of the Q variables. Operators that are symmetric with respect to the BO inner product (B.3) are denoted as $\hat{O}_{\mathrm{BO}}$; e.g., $\hat{O}_{\mathrm{BO}} := \hat{\mu}_{\mathrm{BO}}^{-1}\hat{O}$ or $\hat{O}_{\mathrm{BO}} := \hat{\mu}_{\mathrm{BO}}^{-\frac{1}{2}}\hat{O}\hat{\mu}_{\mathrm{BO}}^{\frac{1}{2}}$ (with $\hat{O}^\dagger = \hat{O}$). If we take the BO average of (B.5), we find

$$\mathfrak{J}(Q) = \langle \hat{H}_{\mathcal{S}} \rangle_{\mathrm{BO}} - \frac{\hbar^2}{M}\sum_{a=1}^{n} \frac{\partial \log \psi_0}{\partial Q^a} \left\langle \frac{\partial}{\partial Q^a} \right\rangle_{\mathrm{BO}} - \frac{1}{2M}\sum_{a=1}^{n} \left\langle \frac{\partial^2}{\partial (Q^a)^2} \right\rangle_{\mathrm{BO}} . \tag{B.8}$$

It is due to (B.8) that we refer to $\mathfrak{J}(Q)$ as the backreaction term, as $\mathfrak{J}(Q)$ is now seen to be related to the BO average (expectation value) of $\hat{H}_{\mathcal{S}}$, which we assume is symmetric with respect to (B.3). If $\mathfrak{J}(Q) \equiv 0$, we consider that there is no backreaction.

What can be said of the other terms in (B.8)? They lead to 'fluctuation terms' in (B.5), which are terms of the form $(\hat{O}_{\mathrm{BO}} - \langle \hat{O} \rangle_{\mathrm{BO}})/M$. To see this, let us first note that the BO averages $\langle \partial/\partial Q^a \rangle_{\mathrm{BO}}$ play the role of the 'Berry connection' in standard quantum mechanics [194, 195] and, in particular, in applications of the BO approximation to molecular physics [121, 122, 186, 187]. More precisely, we define

$$\left\langle \frac{\partial}{\partial Q^a} \right\rangle_{\mathrm{BO}} (Q) =: V_a(Q) + \mathrm{i} A_a(Q) \; ; \tag{B.9}$$

i.e., V_a and A_a are, respectively, the real and imaginary parts of $\langle \partial/\partial Q^a \rangle_{\mathrm{BO}}$. In usual applications of adiabatic quantum mechanics, one has that $V_a = 0$ and A_a are the components of the Berry connection. Here, however, V_a is so far undetermined and this will be of importance in the analysis of unitarity in the BO approach (cf. Sec. B.4). Subsequently, let us define the objects [98, 124, 126, 166–168, 196]

$$\mathrm{D}_a^{\pm} := \frac{\partial}{\partial Q^a} \pm \left\langle \frac{\partial}{\partial Q^a} \right\rangle_{\mathrm{BO}} , \tag{B.10}$$

which are sometimes referred to as 'covariant derivatives' in the particular case in which $V_a = 0$. If we now insert (B.8) back into (B.4), (B.5) and use the definitions (B.10), we obtain the equations [6, 124, 126, 166–168, 176, 177]

$$-\frac{1}{2M}\sum_{a=1}^{n} \left[\left(\mathrm{D}_a^{+}\right)^2 + \left\langle \left(\mathrm{D}_a^{-}\right)^2 \right\rangle_{\mathrm{BO}} \right] \psi_0 + V\psi_0 = \left(E - \langle \hat{H}_{\mathcal{S}} \rangle_{\mathrm{BO}} \right) \psi_0 , \tag{B.11}$$

$$-\frac{1}{M\psi_0}\sum_{a=1}^{n} \mathrm{D}_a^{+}\psi_0 \mathrm{D}_a^{-}\psi_{\mathrm{BO}} - \frac{1}{2M}\left[\left(\mathrm{D}_a^{-}\right)^2 - \left\langle \left(\mathrm{D}_a^{-}\right)^2 \right\rangle_{\mathrm{BO}} \right] \psi_{\mathrm{BO}} + \left(\hat{H}_{\mathcal{S}} - \langle \hat{H}_{\mathcal{S}} \rangle_{\mathrm{BO}} \right) \psi_{\mathrm{BO}} = 0 , \tag{B.12}$$

in which the fluctuation terms are explicit. It is important to note that (B.11) and (B.12) are equivalent to (B.4) and (B.5), respectively, but the two sets of equations suggest different perspectives regarding the dynamics. Equations (B.4) and (B.5) constitute a linear system for ψ_0 and $\psi_{\rm BO}$ given a choice of $\mathfrak{J}$ as an independent function of Q. In this case, the backreaction term is, in principle, freely specifiable and equation (B.8) restricts the values of the BO averages according to the values of $\mathfrak{J}$. This is equivalent to considering that ψ_0 is arbitrary and that the backreaction term $\mathfrak{J}$ determined by (B.4) is also arbitrary. The BO factorization (B.2) is merely a redefinition of the total state $\Psi(Q, q)$.

Alternatively, one may consider that (B.8) is the definition of $\mathfrak{J}$ and that the BO averages are unrestricted. In this case, equations (B.11) and (B.12) constitute a non-linear system for ψ_0 and $\psi_{\rm BO}$, which is to be solved self-consistently in an iterative fashion. The latter view was adopted in [123,124,126,166–168,171,196,197], where the BO averages in (B.11) and (B.12) were seen as the backreaction from the light degrees of freedom onto the dynamics of the Q variables. In this view, the interpretation of ψ_0 and $\psi_{\rm BO}$ is that they are, respectively, the wave functions of the heavy sector and of the light degrees of freedom. We stress that this alternative interpretation tacitly assumes that each sector evolves unitarily by itself, and we will argue in §B.4.3 that this corresponds to a choice of factorization $\Psi = \psi_0\psi_{\rm BO}$. The BO inner product (B.3) is the inner product for the light sector. The backreaction is also related to the fluctuation terms, which are usually neglected in the adiabatic approximation [this corresponds to neglecting terms of order $1/M$, as can be seen from (B.11) and (B.12); the fluctuation terms correspond to corrections of higher orders in $1/M$].

The possibility to adopt the two perspectives above signals that the concept of backreaction in the traditional BO approach is ambiguous. We briefly analyze the reasons for this and the corresponding consequences in what follows.

B.4 The ambiguity of backreaction and the issue of unitarity

The ambiguity of the notion of backreaction in the BO approach has spawned some debate in the literature. Some authors [198–200] (see also [201]) argue that backreaction terms in the semiclassical scheme followed by the BO approach are arbitrary because they depend on the phase of ψ_0 [via (B.4)], which is itself arbitrary (as was discussed above and as we will see below). On the other hand, it is sometimes claimed that the backreaction term guarantees unitarity of the corrected Schrödinger equation at all orders in $1/M$ [126, 163, 171]. How can this be understood? We argue that the traditional BO approach is equivalent to the formalism of the 'minimal BO ansatz' presented in Chapter 5, which motivates us to critique the connection between unitarity and backreaction.

B.4.1 Factorization ambiguity and its physical meaning

The ambiguity of the backreaction is, in fact, a consequence of the fact that the traditional BO exact factorization (B.2) is ambiguous. As was remarked in [163], the transformations

$$\psi_0(Q) = \mathrm{e}^{\gamma(Q)+\frac{\mathrm{i}}{\hbar}\beta(Q)}\psi_0'(Q)\ ,\ \psi_{\mathrm{BO}}(Q;q) = \mathrm{e}^{-\gamma(Q)-\frac{\mathrm{i}}{\hbar}\beta(Q)}\psi_{\mathrm{BO}}'(Q;q) \tag{B.13}$$

do not alter the total state $\Psi(Q,q)$ if $\gamma(Q)$ and $\beta(Q)$ are real functions of Q. We also assume that they are real analytic functions of $1/M$. In this way, the derivation of (B.6) remains the same regardless of the choice of factors in (B.13).

The transformations (B.13) induce a redefinition of the backreaction term. This can be seen in two ways. First, from the polar decomposition $\psi_0 = R\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\vartheta}$ and (B.13), we see that the amplitude and phase of ψ_0 transform as $R = R'\mathrm{e}^{\gamma}$ and $\vartheta = \vartheta' + \beta$. This implies that the real and imaginary parts of $\mathfrak{J}$ [cf. (B.4)],

$$\begin{aligned} J(Q) &:= \mathfrak{Re}\mathfrak{J}(Q) = \frac{1}{2M}\sum_{a=1}^{n}\left[\frac{\hbar^2}{R}\frac{\partial^2 R}{\partial(Q^a)^2} - \left(\frac{\partial\vartheta}{\partial Q^a}\right)^2\right] - V(Q) + E\ , \\ K(Q) &:= \mathfrak{Im}\mathfrak{J}(Q) = \frac{\hbar}{2M}\sum_{a=1}^{n}\left(\frac{2}{R}\frac{\partial R}{\partial Q^a}\frac{\partial\vartheta}{\partial Q^a} + \frac{\partial^2\vartheta}{\partial(Q^a)^2}\right)\ , \end{aligned} \tag{B.14}$$

are also redefined,

$$\begin{aligned} J &= J' + \frac{1}{2M}\sum_{a=1}^{n}\left[\frac{2\hbar^2}{R'}\frac{\partial R'}{\partial Q^a}\frac{\partial\gamma}{\partial Q^a} + \hbar^2\left(\frac{\partial\gamma}{\partial Q^a}\right)^2 + \hbar^2\frac{\partial^2\gamma}{\partial(Q^a)^2}\right. \\ &\qquad\qquad\left. -2\frac{\partial\vartheta'}{\partial Q^a}\frac{\partial\beta}{\partial Q^a} - \left(\frac{\partial\beta}{\partial Q^a}\right)^2\right]\ , \\ K &= K' + \frac{\hbar}{M}\sum_{a=1}^{n}\left(\frac{\partial\gamma}{\partial Q^a}\frac{\partial\vartheta'}{\partial Q^a} + \frac{1}{R'}\frac{\partial R'}{\partial Q^a}\frac{\partial\beta}{\partial Q^a} + \frac{\partial\gamma}{\partial Q^a}\frac{\partial\beta}{\partial Q^a} + \frac{1}{2}\frac{\partial^2\beta}{\partial(Q^a)^2}\right)\ . \end{aligned} \tag{B.15}$$

The second way to compute the redefinition of the backreaction term is to use (B.8) and to note that the BO averages $\langle\partial/\partial Q^a\rangle_{\mathrm{BO}}$ and $\langle\partial^2/\partial(Q^a)^2\rangle_{\mathrm{BO}}$ also transform under (B.13). Indeed, from (B.9) and (B.13), we find

$$V_a = V_a' - \frac{\partial\gamma}{\partial Q^a}\ ,\ A_a = A_a' - \frac{1}{\hbar}\frac{\partial\beta}{\partial Q^a}\ , \tag{B.16}$$

and (no summation over the index a is implied)

$$\begin{aligned}\mathfrak{Re}\left\langle\frac{\partial^2}{\partial(Q^a)^2}\right\rangle_{\mathrm{BO}} &= \mathfrak{Re}\left\langle\frac{\partial^2}{\partial(Q^a)^2}\right\rangle'_{\mathrm{BO}} - \frac{\partial^2\gamma}{\partial(Q^a)^2} + \left(\frac{\partial\gamma}{\partial Q^a}\right)^2 \\ &\quad - \frac{1}{\hbar^2}\left(\frac{\partial\beta}{\partial Q^a}\right)^2 + \frac{2}{\hbar}\frac{\partial\beta}{\partial Q^a}A'_a - 2\frac{\partial\gamma}{\partial Q^a}V'_a\ , \\ \mathfrak{Im}\left\langle\frac{\partial^2}{\partial(Q^a)^2}\right\rangle_{\mathrm{BO}} &= \mathfrak{Im}\left\langle\frac{\partial^2}{\partial(Q^a)^2}\right\rangle'_{\mathrm{BO}} - \frac{1}{\hbar}\frac{\partial^2\beta}{\partial(Q^a)^2} \\ &\quad + 2\left(\frac{1}{\hbar}\frac{\partial\gamma}{\partial Q^a}\frac{\partial\beta}{\partial Q^a} - \frac{\partial\gamma}{\partial Q^a}A'_a - \frac{1}{\hbar}\frac{\partial\beta}{\partial Q^a}V'_a\right)\ .\end{aligned} \tag{B.17}$$

Equation (B.16) implies that a choice of $\beta(Q)$ is related to a choice of Berry phase. Moreover, Eqs. (B.16) and (B.17) imply that (B.8) retains its form after the redefinitions (B.13) are performed. Using (B.10), we also find

$$\begin{aligned}\mathrm{D}^+_a\psi_0 &= e^{\gamma+\frac{\mathrm{i}}{\hbar}\beta}\frac{\partial\psi'_0}{\partial Q^a} + e^{\gamma+\frac{\mathrm{i}}{\hbar}\beta}\left\langle\frac{\partial}{\partial Q^a}\right\rangle'_{\mathrm{BO}}\psi'_0 = e^{\gamma+\frac{\mathrm{i}}{\hbar}\beta}\mathrm{D}'^{+}_a\psi'_0\ , \\ \mathrm{D}^-_a\psi_{\mathrm{BO}} &= e^{-\gamma-\frac{\mathrm{i}}{\hbar}\beta}\frac{\partial\psi'_{\mathrm{BO}}}{\partial Q^a} - e^{-\gamma-\frac{\mathrm{i}}{\hbar}\beta}\left\langle\frac{\partial}{\partial Q^a}\right\rangle'_{\mathrm{BO}}\psi'_{\mathrm{BO}} = e^{-\gamma-\frac{\mathrm{i}}{\hbar}\beta}\mathrm{D}'^{-}_a\psi'_{\mathrm{BO}}\ ,\end{aligned} \tag{B.18}$$

which implies that (B.11) and (B.12) do not change under the transformations (B.13). Note that $\langle\hat{H}_{\mathrm{S}}\rangle_{\mathrm{BO}}$ also remains unaltered under (B.13). The transformation laws (B.17) can be used together with (B.13) in (B.8) to compute the change in $\mathfrak{J}$.

Equations (B.15), (B.17) and (B.18) show that the backreaction term is ambiguous. That this is a consequence of the arbitrariness of ψ_0 [cf. (B.13)] was discussed in [198, 199]. One may go beyond the scope of the traditional BO approach in search of a well-defined notion of backreaction. For instance, other definitions of backreaction, which use the concepts of decoherence and Wigner functions, are available [198, 202]. In the context of gravitation, where the gravitational field usually plays the role of the heavy degrees of freedom, whereas the matter fields comprise the light sector, further investigations were made in [198, 203, 204] to determine in which circumstances the expectation value of the Hamiltonian $\hat{H}_{\mathrm{S}}$ of matter fields could be used as a source in a semiclassical theory of gravitation. It was concluded that the distribution of $\hat{H}_{\mathrm{S}}$ must have a peak at its average and that quantum corrections to the classical value of the energy-momentum tensor must be small in order for such a semiclassical theory to be well defined.

What is the physical meaning of the factorization ambiguity in the traditional BO approach? As the (semiclassical) time variable is defined from the phase of ψ_0 (cf. discussion in Sec. B.2), we conclude that the redefinition (B.13) (which leads to $\vartheta = \vartheta' + \beta$) amounts to redefining the time variable. This is in line with the reparametrization invariance of the theory. If $\beta(Q) = \beta_0(Q) + \mathcal{O}(1/M)$, then the lowest-order phase time is not altered by this transformation [because we assume that $\vartheta = M\varphi + \mathcal{O}(M^0)$]. It is also worth noting a point that is seldom emphasized in the literature (see the discussion in [62]). In the traditional BO approach, a redefinition of A_a (the Berry connection, if $V_a = 0$) according to (B.16) is tied to a transformation of the (phase) time function. This is relevant if one wishes to use (B.16) to impose a "gauge condition" on A_a, as this condition will also be connected to the choice of time in the BO approach. In other words, the freedom to define the Berry connection is related to freedom of choosing ψ_0, the backreaction term or the time function that parametrizes the dynamics. A choice of ψ_0, $\mathfrak{J}$ or t is equivalent to a choice of the functions $\gamma(Q)$ and $\beta(Q)$ in (B.13).[7] For this reason, the two perspectives regarding the dynamics discussed in §B.3 are equivalent and contain the same arbitrariness. One may consider that ψ_0 and the backreaction are arbitrary, such that the BO factorization is simply a redefinition of the total state $\Psi(Q,q)$, or one may assume that ψ_0 and $\psi_{\rm BO}$ are self-consistent solutions to the nonlinear system of (B.11) and (B.12), where the definition of V_a and A_a are arbitrary [cf. (B.9)].

B.4.2 The traditional and minimal BO factorizations are equivalent

Due to (B.13), one readily notices that we can relate the traditional BO factorization to the minimal BO ansatz given in Chapter 5 [see (5.34)]. Indeed, given the two factorizations, we can use (B.13) as definition of $\gamma(Q)$ and $\beta(Q)$ as follows:

$$\begin{aligned} \psi_0(Q) &= \exp\left[\mathrm{i}M\mathcal{W}_0(Q)\right] \mathrm{e}^{\gamma(Q)+\frac{\mathrm{i}}{\hbar}\beta(Q)} \ , \\ \psi_{\rm BO}(Q;q) &= \psi(Q;q)\,\mathrm{e}^{-\gamma(Q)-\frac{\mathrm{i}}{\hbar}\beta(Q)} \ . \end{aligned} \tag{B.19}$$

This trivially implies that $\Psi = \exp(\mathrm{i}M\mathcal{W}_0)\psi = \psi_0\psi_{\rm BO}$. Furthermore, the equivalence of (B.5) to (5.38) [in the particular case in which the metric of the heavy sector is $G_{ab} = \delta_{ab}$ and $MV(Q) \mapsto V(Q)$] can be established by inserting (B.19) into (B.5) and, subsequently, substituting $\mathfrak{J}$ by the right-hand side of (B.4). For this reason, the two BO ansätze lead to equivalent results. This correspondence is certainly expected, but it motivates us to ask: how does the unitary evolution described in Chapter 5 correspond to a unitary evolution of $\psi_{\rm BO}$? In the literature, there has been some

[7] It is also useful to note that the arbitrariness in the choice of backreaction term $\mathfrak{J}$ is related to the applicability of the weak-coupling expansion (i.e., the expansion in powers of $1/M$) of (B.5). Since the choice of backreaction term corresponds to a choice of ψ_0 [cf. (B.4)] and to a choice of WKB time variable, we conclude that a fixation of $\mathfrak{J}$ determines a 'background' trajectory for the heavy variables [via the integral curves of $\partial/\partial t = \sum_a \partial\varphi/\partial Q^a \partial/\partial Q^a$; cf. (5.10)]. It is with respect to this background trajectory that the weak-coupling expansion is performed, in the sense that the series expansion in $1/M$ (and possibly its convergence) depends on how the heavy variables are separated into a (corrected) phase time and other degrees of freedom, which were denoted by x^i in Chapter 5. Similar remarks were made in [98]. Moreover, Parentani has made a similar observation regarding the choice of backreaction term and its relation to the expansion, emphasizing that the fixation of the backreaction and the background trajectory is a 'background field approximation' [205].

controversy regarding the issue of unitarity in the traditional BO approach [114–116, 120]. Therefore, it is important to understand this issue in detail with respect to the formalism presented in Chapter 5.

B.4.3 Unitarity and conditional probabilities

Let us now examine the issue of unitarity of the equation (B.5). If $\hat{H}_{\mathrm{S}}$ is self-adjoint with respect to the BO inner product (B.3) for some choice of measure $\hat{\mu}_{\mathrm{BO}}$, then the quantum dynamics of ψ_{BO} is manifestly unitary at the lowest order [cf. (B.6)]. The question is whether unitarity can be maintained when corrections of order $1/M$ are included. To understand this, it is important to emphasize that there are two separate issues at play: the unitarity of the evolution of the composite system of heavy and light degrees of freedom, and the unitarity of the evolution solely in the light sector.

If one adopts the view that ψ_0 and the backreaction are arbitrary (cf. §B.3 and §B.4.1), then (B.5) is equivalent to the TISE (B.1) if a choice of ψ_0 is given. Therefore, as already mentioned, the BO factorization is a redefinition of the total state $\Psi(Q, q)$, and we conclude that (B.5) is generally an equation for the coupled system of heavy and light variables instead of an equation solely for the light degrees of freedom. The fact that it coincides with a Schrödinger equation for q^{μ} variables at the lowest order [cf. (B.6)] is a consequence of the factorization procedure. This is analogous to what is shown in Chapter 5, where (5.38) is simply a phase-transformed constraint equation. In this way, one should establish the unitarity (or lack thereof) at the level of the coupled system and, subsequently, analyze the light sector in particular. This is not the usual procedure in the literature, in which one focuses on the second view discussed in §B.3; i.e., one considers the nonlinear system of (B.11) and (B.12). In this case, the arbitrariness of V_a and A_a [cf. (B.9)] is related to the choice of time variable, as we have argued in §B.4.1. We will see that the unitarity (or lack thereof) of the evolution in the light sector follows from a specific choice of V_a.

In this context, it must be stressed that unitarity is to be understood with respect to WKB time. In the customary applications of the BO approximation to problems in molecular and nuclear physics [121–123, 173], an external ("laboratory") time is present and, therefore, whether the theory is unitary (with respect to the external time) is evident from the structure of the total Hamiltonian. Moreover, in these applications, one also does not construct a relational description of time-independent problems, which are described by a TISE. Here, on the contrary, we tackle the TISE (B.1) in a relational way: we define an intrinsic clock from a combination of the degrees of freedom. As we have seen, the intrinsic clock is defined from the heavy variables perturbatively in the BO approach. It is then necessary to ascertain whether the dynamics is unitary relative to the intrinsic clock.

It was established in Chapter 5 that the coupled dynamics of heavy and light degrees of freedom is unitary, and the physical inner product is related to a quantization of the

Faddeev-Popov determinant. The equivalence of the minimal BO formalism presented in Chapter 5 to the traditional BO approach suggests that: (1) the unitarity of the dynamics does not follow simply from the inclusion of the backreaction term, as this term is ambiguous and the minimal BO factorization used in Chapter 5 does not rely explicitly on the concept of backreaction; (2) the BO inner product could be defined in a similar way to the physical (gauge-fixed) inner product used in (5.30), (5.31), (5.45) and (5.69). We will see that this is indeed the case and we will critique the claim that the (arbitrary) backreaction term leads to a unitary dynamics.

To begin with, let us take the results of Chapter 5 to be the most fundamental ones, as they follow from the general formalism presented in Chapters 1 and 2. In particular, the physical inner product (5.30) is clearly related to the gauge symmetry of the total system. Due to the results of §5.2.3, §5.2.4 and §5.2.7, we know that this inner product is conserved (at least up to order $1/M$); i.e., we find

$$\frac{\partial}{\partial t}\left[\int \prod_i \mathrm{d}x^i \prod_\mu \mathrm{d}q^\mu \ \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_1\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_2\right]_{x^1=t} = 0 \tag{B.20}$$

for any two phase-transformed solutions to the quantum constraint equation. A few comments are now in order. First, the equivalent result for the BO inner product would be

$$\frac{\partial}{\partial t}\int \mathrm{d}q \ \psi^*_{\mathrm{BO}(1)}(Q;q)\hat{\mu}_{BO}\psi_{\mathrm{BO}(2)}(Q;q) = 0 \ ; \tag{B.21}$$

i.e., the conservation of the BO inner product (B.3) of any pair of states $\psi_{\mathrm{BO}(1)}$ and $\psi_{\mathrm{BO}(2)}$. Nevertheless, the condition (B.21) is not the one that is used in the literature when the issue of unitarity in the traditional BO approach is analyzed [124,126]. Indeed, the standard approach is to consider only a special case of (B.21), in which one focuses on only one state, $\psi_{\mathrm{BO}(1)} = \psi_{\mathrm{BO}(2)}$. Thus, the unitarity condition becomes

$$\begin{aligned} 0 &= \mathfrak{Re}\left\langle \frac{\partial}{\partial t}\right\rangle_{\mathrm{BO}} + \frac{1}{2}\left\langle \hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial \hat{\mu}_{\mathrm{BO}}}{\partial t}\right\rangle_{\mathrm{BO}} \\ &= \sum_{a=1}^n W^a\left(\mathfrak{Re}\left\langle \frac{\partial}{\partial Q^a}\right\rangle_{\mathrm{BO}} + \frac{1}{2}\left\langle \hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial \hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO}}\right) \\ &= \sum_{a=1}^n W^a\left(V_a + \frac{1}{2}\left\langle \hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial \hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO}}\right) \ , \end{aligned} \tag{B.22}$$

where W^a are the components of the vector $\partial/\partial t$ with respect to the basis spanned by $\partial/\partial Q^a$ and V_a was given in (B.9). In (B.22), we have also used the hypothesis that $\hat{\mu}_{\mathrm{BO}}$ is symmetric with respect to the flat measure and that it commutes with functions that only depend on Q. Furthermore, it is important to mention that the standard proof of unitarity focuses on a flat measure $\hat{\mu}_{\rm BO} \to \hat{1}$, but we do not impose this condition.

The focus on the condition (B.22), which is weaker than (B.21), brings us to the second comment: the unitarity condition obtained in Chapter 5 generally holds for the coupled system of heavy and light degrees of freedom. Indeed, the physical inner product in (B.20) includes an integration over the heavy variables that are different from WKB time (which were denoted by x^i in Chapter 5). In this way, the dynamics of a single sector may generally be non-unitary (as an open system). In spite of this, one can impose unitarity solely in the light sector in terms of the conditional probabilities (5.46), which describe observations of the light sector conditioned on a configuration of the heavy variables. We will argue that this is how the unitarity of the traditional BO approach should be understood; i.e., in analogy to what was done in §5.2.5, we will see that the quantum dynamics of $\psi_{\rm BO}$ can be identified with a conditional evolution, which describes the light sector in relation to a fixed heavy background.

Third, the parameter t in (B.22) is the WKB time, which can either be the lowest-order phase time (as was considered in Chapter 5) or it can defined at each order in the expansion in powers of $1/M$ (corrected phase time), as was discussed after (B.6). If one adopts the corrected phase time, it is still, in principle, possible to define a change of coordinates such as (5.10) in the heavy-sector configuration space. Likewise, one can use the procedure of §5.2.3 to define the measure $\hat{\mu}_{\mathfrak{v}}$, with respect to which the dynamics of $\psi(Q;q)$ in the minimal BO factorization is unitary in relation to the (corrected) phase time. In this way, there is no qualitative modification of the conclusions of Chapter 5. Due to the definition of WKB time, we have $W^a = \sum_{a'=1}^{n} \delta^a_{a'} \partial\varphi/\partial Q^{a'} + \mathcal{O}(1/M)$. If one identifies WKB time with the (corrected) phase time of ψ_0, then $W^a = 1/M \sum_{a'=1}^{n} \delta^a_{a'} \partial\vartheta/\partial Q^{a'}$, since $\vartheta = M\varphi + \mathcal{O}(M^0)$.

Fourth, the proof of (B.22) should amount to verifying that (B.22) is true for any choice of $\psi_{\rm BO}$ that solves (B.5). This is done in Chapter 6 for the particular example of primordial fluctuations over a quasi-de Sitter background. However, the standard proof that is found in the literature [124, 126, 171] makes use of the (frequently tacit) assumption that $V_a|_{\hat{\mu}_{\rm BO}\to\hat{1}} = 0$ or, in other words, that $\langle \partial/\partial Q^a \rangle_{\rm BO}|_{\hat{\mu}_{\rm BO}\to\hat{1}}$ are imaginary and comprise the components of the Berry connection [cf. discussion after (B.9)]. But $V_a|_{\hat{\mu}_{\rm BO}\to\hat{1}} = 0$ is a sufficient condition for (B.22) to be satisfied (in the case in which $\hat{\mu}_{\rm BO} \to \hat{1}$) and, therefore, this assumption makes the standard proof circular. In fact, by assuming that $V_a|_{\hat{\mu}_{\rm BO}\to\hat{1}} = 0$, one is simply making a particular choice of factorization [cf. (B.13) and (B.16)] rather than proving that (B.22) follows from the dynamics dictated by (B.5). According to the discussion in §B.3 and §B.4.1, the dynamics described by (B.5) is equivalent to the one governed by (B.1), which involves all degrees of freedom and not only the light variables.

Let us now see how the unitarity of the traditional BO approach can be understood in relation to (B.20). From the general formalism presented in Chapters 2 and 5, we see that the fundamental quantities that can be predicted in the quantum theory are conditional probabilities. Following (5.46), we conclude that the light sector may be described by the probabilities

$$p_\Psi(q|Q) := \left.\frac{\left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}{\int \mathrm{d}q \, \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi}\right|_Q = \left.\frac{\left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_{\mathrm{BO}}\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_{\mathrm{BO}}}{\int \mathrm{d}q \, \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_{\mathrm{BO}}\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi_{\mathrm{BO}}}\right|_Q , \tag{B.23}$$

which are conditioned on a heavy-sector configuration Q. Notice that: (1) $\hat{\mu}_{\mathfrak{v}}$ is the same as in (B.20); i.e., it is the measure that is determined in §5.2.7 to be related to the Faddeev-Popov determinant; (2) we have used (5.36) and (B.19) to obtain the last equality in (B.23). From (B.23), we see that the conditional probabilities coincide with those determined by the BO inner product (B.3) if we define

$$\hat{\mu}_{\mathrm{BO}} := \mathcal{F}(Q)\hat{\mu}_{\mathfrak{v}}(Q;\hat{p},q) , \tag{B.24}$$

where $\mathcal{F}(Q)$ is an arbitrary positive function of the heavy variables. Due to (5.66), we see that (B.24) satisfies the assumption that it is symmetric with respect to the flat measure.

As the light sector is a subsystem, its unitarity is not guaranteed, in contrast to the unitarity condition (B.20). Nevertheless, we may use (B.19) to define a factorization in which the denominator of (B.23) (the BO norm of ψ_{BO}) is conserved. Indeed, let us define [cf. (B.3), (B.19) and (B.24)]

$$\begin{aligned}\mathcal{G}(Q) &:= \int \mathrm{d}q \, \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}}\psi = \frac{\mathrm{e}^{2\gamma(Q)}}{\mathcal{F}(Q)} \int \mathrm{d}q \, \left(\hat{\mu}_{\mathrm{BO}}^{\frac{1}{2}}\psi_{\mathrm{BO}}\right)^* \hat{\mu}_{\mathrm{BO}}^{\frac{1}{2}}\psi_{\mathrm{BO}} \\ &= \frac{\mathrm{e}^{2\gamma(Q)}}{\mathcal{F}(Q)} \langle\psi_{\mathrm{BO}}|\psi_{\mathrm{BO}}\rangle_{\mathrm{BO}} \ .\end{aligned} \tag{B.25}$$

We obtain $\langle\psi_{\mathrm{BO}}|\psi_{\mathrm{BO}}\rangle_{\mathrm{BO}} = 1$ (for all values of Q and, in particular, for every instant of WKB time) if we demand that[8]

$$\mathrm{e}^{2\gamma(Q)} = \mathcal{F}(Q)\mathcal{G}(Q) = \int \mathrm{d}q \; \psi^* \hat{\mu}_{\mathrm{BO}}\psi \ . \tag{B.26}$$

[8] In particular, the factorization $\psi(Q;q) = \psi_h(Q)\psi_l(Q;q)$ used in §5.2.5 can be seen as a particular case of (B.19). For example, we can define $\psi_h = \exp(\gamma + \mathrm{i}\beta/\hbar)$ and $\psi_l \equiv \psi_{\mathrm{BO}}$, such that $\exp(\mathrm{i}M\mathcal{W}_0)\psi_h\psi_l = \Psi$ [cf. (5.59) and (B.19)]. Just as (B.26) imposes the unitarity condition on the evolution of ψ_{BO}, the function $\psi_h(Q)$ is chosen in §5.2.5 to guarantee the unitarity in the light sector at order M^0 [cf. (5.58)]. In this case, Eq. (5.53) is an instance of (B.23). If, furthermore, $\psi_h(Q)$ is normalizable, it can be interpreted as a marginal wave function for the heavy degrees of freedom [cf. §5.2.5]. The concept of (normalizable) marginal and conditional wave functions has been used in molecular physics and nonrelativistic quantum mechanics [100, 122, 123, 186–188].

This enforces the unitarity of the evolution of ψ_{BO} by a particular choice of factorization [a fixation of $\gamma(Q)$; cf. (B.19)].[9] Using (B.9), (B.13), (B.19) and (B.26), we obtain

$$\begin{aligned}\frac{\partial\gamma}{\partial Q^a} &= \mathfrak{Re}\left\langle\frac{\partial}{\partial Q^a}\right\rangle_{\mathrm{BO};\psi} + \frac{1}{2}\left\langle\hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO};\psi} \\ &= V'_a + \frac{1}{2}\left\langle\hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO};\psi}\ ,\end{aligned} \tag{B.27}$$

where the BO averages are taken with respect to the state ψ. Notice that, due to (B.19) and to (B.24), we may write

$$\begin{aligned}\left\langle\hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO};\psi} &= \int \mathrm{d}q\ \psi^*\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\psi = \int \mathrm{d}q\ \psi^*_{\mathrm{BO}}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\psi_{\mathrm{BO}} \\ &= \left\langle\hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO}}\ .\end{aligned} \tag{B.28}$$

Thus, we can use (B.16), (B.27) and (B.28) to find that the unitarity condition (B.22) is indeed satisfied,

$$V_a = V'_a - \frac{\partial\gamma}{\partial Q^a} = -\frac{1}{2}\left\langle\hat{\mu}_{\mathrm{BO}}^{-1}\frac{\partial\hat{\mu}_{\mathrm{BO}}}{\partial Q^a}\right\rangle_{\mathrm{BO}}\ . \tag{B.29}$$

In particular, we obtain $V_a = 0$ if $\hat{\mu}_{\mathrm{BO}} \to \hat{1}$, as in the standard proof. Finally, due to (B.19) and (B.26), we can write

$$\psi_{\mathrm{BO}}(Q;q) = \frac{\psi(Q;q)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\beta(Q)}}{\sqrt{\int \mathrm{d}q\ \psi^*\hat{\mu}_{\mathrm{BO}}\psi}}\ . \tag{B.30}$$

Equation (B.30) makes it manifest that the choice of $\gamma(Q)$ (factorization) given in (B.26) guarantees that the BO norm of ψ_{BO} is equal to 1 at all instants of WKB time. Notice, however, that this holds only for this particular choice of factorization. In contrast, the unitarity of the physical inner product [cf. (B.20)] depends only on the choice of background clock,[10] and it shows that conditional wave functions evolve unitarily if the inner product is defined in a suitable way that follows from the perturbative expansion of (B.5) [or (5.38)].

[9] Incidentally, notice that one should not fix $\mathcal{F}(Q)$ [instead of $\gamma(Q)$] by requiring that (B.22) is satisfied, as this would lead to a definition of the measure that is dependent on a state [cf. (B.24)] or, alternatively, it would enforce the unitarity condition only for a certain class of states.

[10] Time-dependent transformations of the states in (B.20), such as $\psi(Q;q) = f(x)\psi'(Q;q)$, can be absorbed into a redefinition of the measure $\hat{\mu}_{\mathfrak{v}}$.

Regarding the backreaction term, we note that fixing $\gamma(Q)$ according to (B.26) amounts to a choice of $\mathfrak{J}$, which is otherwise arbitrary [cf. (B.15)] if one takes the perspective that ψ_0 is arbitrary [cf. discussion in §B.3]. Moreover, in the perspective in which ψ_0 and ψ_{BO} are to be found by solving (B.11) and (B.12), we note that equation (B.22) is not a consequence of the equations (B.11) and (B.12). If one takes the BO average of (B.12), the result is trivial ($0 = 0$) and it does not fix the value of V_a. On the contrary, the value of V_a given in (B.29) has to be posited by using the freedom to redefine the BO averages $\langle \partial/\partial Q^a \rangle_{\mathrm{BO}}$ [cf. (B.16)]. Therefore, we conclude that it is not the inclusion of a backreaction terms that yields a unitary dynamics (both for the coupled system and for the light sector, in particular), contrary to what is usually claimed.

It is also worthwhile to mention [163], where the expansion of (B.5) in powers of $1/M$ was considered. There, it was argued that terms that could violate unitarity (in the sense of yielding to a non-zero value of the right-hand side of (B.22)) could be discarded if one performed an appropriate state redefinition according to (B.13).[11] Nevertheless, one must note that certain would-be unitarity violating terms generally depend on q and, therefore, they cannot simply be absorbed into $\psi_0(Q)$ through the transformations (B.13). Regardless of this caveat, the key strategy of [163] is to demand unitarity by choosing $\gamma(Q)$ in perturbation theory. In this way, this corresponds to the procedure of defining the particular factorization (B.26), which leads to a choice of the backreaction term. Rather, in the approach of Chapter 5 (see also Chapter 6), the would-be unitarity-violating terms are incorporated into the definition of the measure $\hat{\mu}_{\mathfrak{v}}$ [cf. §5.2.3 and (5.66)].

Finally, we note that the BO averages correspond to conditional expectation values. Indeed, the average of the operator $\hat{O}_{\mathrm{BO}} := \hat{\mu}_{\mathrm{BO}}^{-\frac{1}{2}} \hat{O}(Q; q, -\mathrm{i}\hbar\partial/\partial q) \hat{\mu}_{\mathrm{BO}}^{\frac{1}{2}}$ reads [cf. (5.46) and (5.60)]

$$\langle \hat{O} \rangle_{\mathrm{BO}} = \frac{\int \mathrm{d}q\ \psi_{\mathrm{BO}}^* \hat{\mu}_{BO} \hat{O}_{\mathrm{BO}} \psi_{\mathrm{BO}}}{\int \mathrm{d}q\ \psi_{\mathrm{BO}}^* \hat{\mu}_{BO} \psi_{\mathrm{BO}}} = \frac{\int \mathrm{d}q\ \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \psi\right)^* \hat{O} \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \psi}{\int \mathrm{d}q\ \left(\hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \psi\right)^* \hat{\mu}_{\mathfrak{v}}^{\frac{1}{2}} \psi} \equiv \mathrm{E}[\hat{O}|Q]. \tag{B.31}$$

It is important to note that the connection between the BO approach and a concept of conditional wave functions was first indicated by Hunter in [100] and afterwards by Arce in [123]. Our formalism differs from the ones presented in [100, 123] due to the fact that the measure $\hat{\mu}_{\mathrm{BO}}$ is, in general, different from $\hat{1}$, and it is associated with the regularization of the inner product of the total states $\Psi(Q; q)$ (solutions to the

[11] It appears that two requirements are made in [163]: (1) ψ_{BO} should be an eigenstate of $\hat{H}_{\mathrm{S}}$; (2) $\mathrm{i}\hbar\partial\psi_{\mathrm{BO}}/\partial t$ should be independent of q. These conditions need not be enforced in the formalism presented in this appendix and in Chapter 5.

constraint equation) via the insertion of the Faddeev-Popov operator (cf. §5.2.7). This association [cf. (5.66) and (B.24)] is new to the best of our knowledge.

From Chapter 5 and Sec. B.4.2, we thus conclude that the BO approach to the problem of time can be seen as a particular case of the relational formalism presented in Chapters 2 and 5 and that it is unitary with respect to a suitably-defined physical (gauge-fixed) inner product. We can use ψ_{BO} to compute conditional expectation values [cf. (B.31)], which encode the dynamics of the light sector in a fixed background defined by heavy degrees of freedom (see also §5.2.5).

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