

Transport
and
Approximate Conservation Laws
in
Low Dimensional Systems



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Abstract

We set up a framework in which controlled lower bounds to conductivities of strongly correlated quantum systems may be calculated perturbatively in situations where the conductivities are infinite in the unperturbed model. This framework is then applied to study the transport properties of almost integrable systems, in general, and heat and spin conductivities in the integrable XXZ Heisenberg spin chain perturbed by various integrability breaking couplings, in particular. Furthermore, we systematically develop a microscopic description of the contribution of spin chains to experimentally measured heat conductivity in spin chain compounds, with an emphasis on the effect of weak disorder.

Kurzzusammenfassung

Wir formulieren eine Störungstheorie mit deren Hilfe Leitfähigkeiten stark korrelierter Quantensysteme, die im ungestörten Fall unendlich sind, berechnet werden können. Wir wenden diese Theorie dann um, allgemein, Transporteigenschaften fast-integrabler Systeme, und speziell, die Wärme- und Spin-Leitfähigkeit in der integrablen XXZ Heisenberg Spinkette mit verschiedenen Störungen, die die Integrabilität brechen, zu studieren an. Zusätzlich entwickeln wir systematisch eine mikroskopische Beschreibung des Spinketten-Beitrags zu in Spinketten-Verbundstoffen experimentell gemessenen Wärmeleitfähigkeit, unter Betonung des Einflusses schwacher Unordnung.

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Introduction

One dimensional models play an increasingly important role in a world where miniaturization spreads and structures are fabricated in which dynamics is restricted to one spatial dimension.

At first sight, models with one spatial dimension may seem structurally much simpler than their three dimensional counterparts. For instance, the problem of a particle in an arbitrary 1D-potential is analytically solvable both classically and quantum mechanically. One might be tempted to guess that one dimensional physics is rather boring. However, many particle systems in 1D show a rich spectrum of unusual phenomena, with a complexity often exceeding that of higher dimensional systems. For example, the Fermi liquid picture, providing an almost ubiquitous description of higher dimensional fermion gases, breaks down for a one dimensional gas of fermions.

Consider one dimensional structures from a practical point of view. A major application that comes into mind is to channel certain degrees of freedom from one end of the microscopic wire to the other, with a huge wealth of possible uses in nanotechnology. Therefore, transport coefficients of one dimensional systems are among the most interesting properties to be studied. Unfortunately, they are also the most challenging to compute.

At this point of the discussion, a special property of many one dimensional models pops up, which turns out to be quite relevant: integrability. Notably, a number of strongly correlated many particle systems in one dimension turn out to be integrable, the XXZ-Heisenberg spin chain. This finding is exceptional; integrability in higher dimensional many particle systems is generically absent as soon as they are interacting.

This observation is relevant in the present discussion for two reasons. First, its integrability allows an analytic treatment of the 1D model and provides exact expressions for physical quantities of interest. Second, integrability comes in hand with an infinite number of conserved currents, which may correlate with – or be identical to – physical currents, which in turn are protected against decay, and thus give rise to singular transport coefficients.

Therefore, we are confronted with the following situation: Simple one dimensional models, which by theoreticians are naturally favored over complicated ones and therefore are studied extensively, allow for an exact eval-

uation of thermodynamic quantities which often match extraordinarily well with experimental data. But as soon as transport is considered – which, as we have argued, is of more interest – the same models give singular answers, in sharp contrast to the real measurements.

Since integrability is such an ubiquitous phenomenon in 1D, it appears to be likely that a real system is not too far away from integrability, or in other words, that it can be described by an integrable model *plus* a weak perturbation which breaks integrability and which may be considered to be small.

The above considerations serve as a motivation to study the question of how transport properties behave under perturbations of systems in which they are singular. Throughout this work, we will assume the deviations from singular behavior to be small, which allows to treat them perturbatively.

The document is arranged as follows. In the first chapter we introduce technical prerequisites for the rest of the work. It shall serve as a pedagogical introduction into two major concepts, the so called Drude weight, a measure of singularness for transport coefficients, and the so called memory matrix formalism, which is a suitable formalism to study the effect of conservation laws on transport. The second chapter is devoted to the derivation of a framework in which lower bounds of conductivities can be calculated perturbatively, and a discussion about the circumstances under which the bounds may become exact. The bounds are expressed in terms of correlation functions which are amenable to practical calculations. In fact, the other part of the work is concerned with the application of that framework to different situations. While the first two chapters are general and do not include any reference to a specific model (in particular there is no dimensional restriction), the following two chapters are devoted to the study of one dimensional spin chains, in particular the XXZ -model, which is integrable. However, integrability is broken by additional couplings, for example next-nearest neighbor or interchain coupling (third chapter) and disorder and/or coupling to phonons (fourth chapter). While the third chapter is of rather theoretical interest, in which the analysis is guided by questions like ‘how does integrability break down’ and ‘how do nonlocal conservation laws affect transport’, the fourth and final chapter is motivated by experimental observations of anomalous contributions to the heat conductivity in spin chain compounds and its aim is an understanding of the microscopic processes leading to these observations.

Chapter 1

Theoretical Foundations

This chapter will introduce several basic notions which are used throughout the following chapters. The material presented is not new and each piece can be found in the literature separately. Here we prepare the material with the following applications in mind and also reveal connections between those pieces of information which would otherwise be time-consuming to extract from the literature.

1.1 Current and Conductivity

Consider the density of an arbitrary physical quantity (e.g. charge, energy, spin, or any other) $\rho(x)$. If the density is locally conserved, the only way the density can change over time is by shifting portions of the quantity from one region to another, i.e. if there exists a finite current density $j(x)$ associated with the density $\rho(x)$. The two are related by a continuity equation,

$$\partial_t \rho(x) + \nabla j(x) = 0. \quad (1.1)$$

In a diffusive system in equilibrium, no current can be present¹. To induce a finite current, it is necessary to drive the system out of equilibrium. Both theoretically and experimentally this is achieved by switching on some symmetry breaking external field $E(x, t)$. The question posed by transport theory is, how does the external field induce movement of the physical quantity $\rho(x)$. More specifically, what is the induced expectation value of the current, $\langle j(x, t) \rangle [E(x, t)]$. In physicist's slang, the system *responds* to an external field by a finite expectation value of some observable (or observables), here the current. Thus the current is a *response* to the external field.

In all but the simplest cases the task to determine the full functional dependence of the current expectation value on an external field with arbitrary

¹For non-diffusive systems this may be different (c.f. persistent currents) and a great part of our considerations is in fact concerned exactly with situations where transport is non-diffusive, see below.

spatial and temporal dependence is far beyond human possibilities from a technical point of view. Therefore, most commonly one restricts oneself to be interested in the simplest of all cases, where the field is homogeneous in space and time, i.e. it is constant, $E(x, t) = E$. Then the current expectation value $\langle j(x, t) \rangle$, (here averaged over a unit cell), is also independent on space, and in most situations as well on time.

While, throughout this document, we will drop the spatial dependence of field and current, the time dependence of the current is of special importance here. Before discussing this subtle and important point, let us first assume that the current does not change over time and introduce the central quantity of this thesis, the dc conductivity. The current depends on the field, $\langle j \rangle = \langle j \rangle(E)$ and one ultimately wants to know how the system responds to small values of the field. One assumes that $\langle j \rangle$ depends smoothly on E . Then one can expand around $E = 0$ and in linear order in the field we can write

$$\langle j \rangle = \sigma_{\text{dc}} E, \quad (1.2)$$

where it is understood that the current density is averaged over the unit cell. This relation defines the dc conductivity σ_{dc} , the transport coefficient which is the main subject of our whole analysis. For small fields thus the response of the current is linear and the theory devoted to the study of this situation is not accidentally referred to as linear response theory. The Kubo formula discussed in the forthcoming sections is the main result of linear response theory applied to transport.

The most common example is where $\langle j \rangle$ is the electrical current and E is the electric field, in which case Eq. (1.2) is a rephrasing of Ohm's law. An other example, which is the most studied case in this work, is where $j = j_Q$ is the heat current, $E = -\nabla T$ is a small temperature gradient. Then $\sigma_{\text{dc}} = \kappa$ is the heat conductivity. For this example, relation (1.2) is referred to as Fourier's law. Also considered is the situation where $j = j_s$ is the spin current, for which one can compute a spin conductivity $\sigma_{\text{dc}} = \sigma_s$.

Turning back our attention to the temporal dependence of the current we next illustrate the different possibilities that may turn up. Picking the most familiar example, consider electric conduction in two different scenarios, in a normal metal and a perfect metal, both at finite temperatures. If one switches on the electric field in a normal metal, as the charge carriers are free to move in space, they are accelerated by the field during an initial period of time and the current increases. But since there are obstacles (nuclei and other electrons) in their way, they regularly will scatter off them, thus effectively losing momentum. After such a collision the charge carriers are again accelerated. As a result, the current can not increase indefinitely, but will saturate at some finite value which is determined by a balance between periods of acceleration and events of scattering. The impurities

and phonons introduce a mechanism for diffusion. Most often one wants to neglect the short initial period of increasing current and is interested in the final, saturated value of the current, i.e. the long time behavior of the response. The normal metal is characterized by a finite conductivity σ_{dc} describing the long time behavior of the current. In the second scenario, the perfect metal, there are no obstacles the charge carriers could scatter off. Therefore the situation in a perfect metal corresponds to a free acceleration of the electrons. Imposing a field on the perfect metal for a longer period, the charge carriers would be accelerated indefinitely, resulting in a current which would increase linearly in time². The long time behavior in this case, therefore, is characterized by an infinite dc conductivity, $\sigma_{\text{dc}} = \infty$. This can be quantified by the so-called Drude weight, which is to be discussed below.

When discussing the conductivity, it is useful to consider a relaxation experiment, in which one prepares the system in a state that shows a pre-defined value of the current expectation value, and lets the system evolve to observe the dynamics of the current. For a normal metal, the following formal procedure leads to a well defined description: At $t = -\infty$ the system is held at thermal equilibrium and no current is present in the system. One then adiabatically switches on the external field which is supposed to reach its final value at $t = 0$, when a finite current expectation value is induced, and 'observes' the system as it relaxes to thermal equilibrium as the field is switched off. For a system in which the current is protected by conservation laws, this procedure is not well defined, as the free acceleration of the charge carriers would formally lead to an infinite current at $t = 0$. In any case, preparing the system in a state carrying a finite amount of the current, if some component of the current is conserved, then it will not relax, i.e. the value of the current does not change over time after the field has been switched off.

1.2 Drude Weight

A common way to calculate the dc conductivity is by restoring the time dependence of the external field, i.e. assuming that it oscillates with frequency ω . This leads to the definition of a frequency dependent conductivity, $\sigma(\omega)$. The real (physical) part of the frequency dependent conductivity is expected to be of the form

$$\text{Re } \sigma(\omega) = \pi D(T) \delta(\omega) + \sigma_{\text{reg}}(\omega), \quad (1.3)$$

²In a real system, at a certain finite value of the current, the system can not maintain the electric field any longer, resulting in a finite current. From the standpoint of an experimentalist, it is the *current* that is 'applied' to the system, and this is possible without voltage drop inside the perfect metal. The two points of view are essentially equivalent. Formally, equation (1.2) is satisfied by means of a product $\infty \cdot 0$, yielding a finite value on the left hand side.

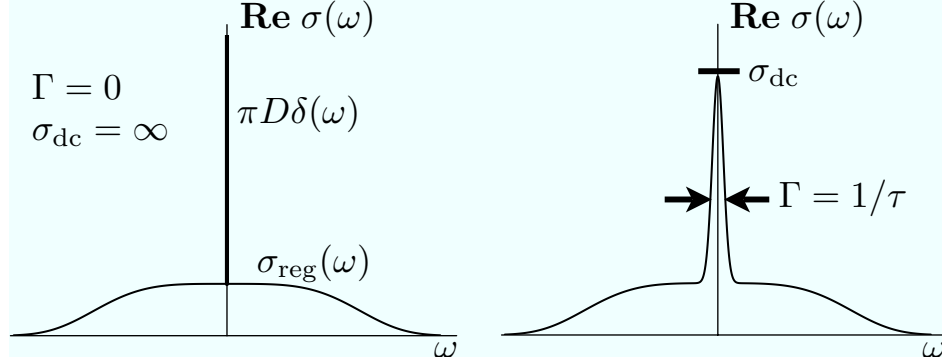


Figure 1.1: Typical conductivities for unperturbed and perturbed cases. For $\Gamma = 0$ a Drude peak shows up in the conductivity, resulting from exact conservation laws. For $\Gamma \neq 0$ the Drude peak broadens and the dc conductivity becomes finite. For small Γ the central peak remains as a distinct feature with a width of the order of Γ and height σ_{dc} . The total weight of the peak is still bound to be equal to πD .

where $\sigma_{\text{reg}}(\omega)$ is the so-called regular part of the conductivity. This relation defines the Drude weight $D(T)$, which is the weight of the singular part of the conductivity at $\omega = 0$ and depends on temperature. In terms of our example from the last chapter, the Drude weight vanishes $D = 0$ for the insulator $\sigma_{\text{dc}} = \sigma_{\text{reg}}(0) = 0$ and the normal metal $\sigma_{\text{dc}} = \sigma_{\text{reg}}(0) > 0$, whereas it is finite $D > 0$ for the superconductor, giving rise to an infinite dc conductivity, $\sigma_{\text{dc}} = \infty$.

To gain a better feeling for the Drude weight, we remind the reader of the Drude theory of metals, in which a simple expression for the frequency dependent conductivity is obtained:

$$\sigma(\omega) = \frac{1}{1/\tau - i\omega} \frac{ne^2}{m}. \quad (1.4)$$

Here the following situation arises. If the scattering rate $\Gamma = 1/\tau$ is finite, there is no singularity present and the dc conductivity is simply $\sigma_{\text{dc}} = \frac{ne^2}{m}\tau$. If, however, for some reason there is nothing the electrons could scatter off, then the regular part of the conductivity would vanish, $\sigma_{\text{reg}}(\omega) = 0$ and a finite Drude weight would show up, $D = \frac{ne^2}{m}$. This is exactly what one should expect from a free, non-interacting gas of electrons in which the electrons are accelerated freely, $J(t) = nev(t) = D \cdot Et$.

Quite generally, the existence of a Drude weight is connected to the presence of a conservation law, here momentum conservation, which protects the current from decaying. Taking into account interactions among the electrons would lead to a finite lifetime of the electron states, causing a redistribu-

tion of momentum between electrons. How complicated the nature of the interactions be, in a translationally invariant model (e.g. a continuum field theory) the conductivity is bound to be infinite and the Drude weight is finite, in spite of the interaction. To obtain a finite value for the conductivity, one needs to introduce some source of scattering. This is the common scenario we will analyze in this thesis: We start from some model in which the current is protected by some conservation law, meaning that the Drude weight is finite, and introduce a perturbation which provides a mechanism to relax the current and thus renders the conductivity finite. As we will show, typically the conductivity is considerably large for small perturbations, as it is in the Drude theory if the scattering rate $\Gamma = 1/\tau$ is small. The general situation is schematically depicted in Fig. 1.1. In the left figure, $\Gamma = 0$, however, in general the current itself does not need to be conserved itself, $[H, J] \neq 0$. This then would lead to a finite regular part, $\sigma_{\text{reg}}(\omega)$. Thinking of a relaxation experiment, some component of the current will relax within microscopic times, while an other component is protected by conservation laws and does not decay over time. The latter one is responsible for the Drude weight. (The small frequency part of the conductivity $\sigma(\omega)$ reflects the long time behavior of the current.) In the right figure some scattering terms have been included in the Hamiltonian which lead to a finite scattering rate Γ . If the perturbation is small, then the conservation laws are violated only weakly and scattering is expected to be weak, meaning that the current relaxes only slowly, leading to a high value of the dc conductivity. This is a motivation to introduce the term *almost conserved current*.

1.3 Problem Setting

After having discussed the Drude weight and its dependence on the scattering rate, we are ready to formulate the general problem setting formally. All further considerations in this chapter are motivated by this problem setting.

Model systems, due to their simplicity, often exhibit symmetries not shared by real materials. For example, the heat conductivity of idealized one-dimensional Heisenberg chains is infinite at arbitrary temperature as the heat current is conserved. However, any additional coupling (e.g. next-nearest neighbor, inter-chain, disorder, phonon, Umklapp, etc.) renders the conductivity finite [1, 2, 3, 4, 5, 6, 7]. If the perturbation is weak, the heat conductivity is, however, large as observed in experiment [8, 9]. For a more general example, consider an arbitrary translationally invariant continuum field theory. Here momentum is conserved which usually implies that the conductivity is infinite for this model. In real materials momentum decays by Umklapp scattering or disorder rendering the conductivity finite. Obviously it is desirable to have a reliable method to calculate transport in

such situations.

We therefore consider systems with the general Hamiltonian

$$H = H_0 + gH_1, \quad (1.5)$$

where for $g = 0$ the relevant heat-, charge- or spin-conductivity is infinite and characterized by a finite Drude weight $D(T) > 0$. As discussed above, H_0 might be an integrable one-dimensional model, a continuum field theory, or just a non-interacting system. The term gH_1 describes a (weak) perturbation which renders the conductivity finite, e.g. due to Umklapp scattering or disorder, see Fig. 1.1. The task is to determine the value of the dc conductivity σ_{dc} as a function of the coupling parameter g in the asymptotic limit $g \rightarrow 0$. The analysis is not straightforward, since a direct perturbation theory for $\sigma(\omega)$ is necessarily singular and thus ill-defined at $\omega = 0$. The natural approach is to aim at a perturbation theory for the *inverse* of the dc conductivity.

On a microscopic level, a small perturbation g shifts the eigenvalues only slightly. We thus may expect that the effect of the perturbation on the Drude peak is to broaden it, while keeping its weight approximately constant. The sharp feature of the right figure in Fig. 1.1 is this broadened 'Drude peak', and its width is of the order of the scattering rate, as may be read off from Eq. (1.4). This reveals a connection between the Drude weight, the dc conductivity and the scattering rate: We can determine the conductivity if we know the other two quantities,

$$\sigma_{\text{dc}} \approx \frac{D}{\Gamma}. \quad (1.6)$$

This relation hints at the possibility to determine σ_{dc} by setting up a perturbation theory for Γ . In one of the following sections we give an expression for the so-called memory matrix, which is a replacement and a generalization of the concept of a scattering rate applying also to situations where a scattering rate Γ can not be defined. In that framework relation (1.6) is replaced by a matrix equation, which, although being more complicated, remains structurally similar to Eq. (1.6). A controlled perturbation theory in g for the memory matrix will then be presented in the next chapter.

What can we expect as the typical behavior of the conductivity under perturbations? According to Fermi's golden rule, the scattering rate Γ is proportional to squares of matrix elements of the perturbation gH_1 , and therefore the general expectation is that the scattering rate Γ is $\propto g^2$. We will find that this expectation is quite robust, and applies also to situations where – for different reasons – one would not expect it to hold. However, we also will find examples where the conductivity is much larger, as $\Gamma \propto g^4$.

1.4 Kubo Formula

The most common method to determine conductivities is to calculate the so-called Kubo formula. In terms of the Kubo formula, the conductivity is given by a current-current correlation function,

$$\sigma(\omega) = -\frac{1}{V\beta} \int_0^\beta d\tau \int_0^\infty dt e^{-i(\omega-i\varepsilon)t} \langle J(-t-i\tau)J(0) \rangle, \quad (1.7)$$

where the limit $\varepsilon \rightarrow 0$ is implied. This is the original expression derived by Kubo, for the derivation of which we refer to the original papers by Kubo [10, 11]. While Kubo has derived this formula with the electrical conductivity in mind, it has been shown a long time ago [12] that the formula can be applied without modification to calculate any conductivity and, in particular, the heat conductivity, just by replacing the electrical current by the heat current in expression (1.7).

The dc conductivity is retained by setting $\omega = 0$ in Eq. (1.7), $\sigma_{\text{dc}} = \sigma(0)$. In practice, the double integral can not be evaluated easily. One gains a more manageable expression by using the fluctuation-dissipation theorem and replacing the current-current correlation function by a retarded response function.³ For a time reversal invariant Hamiltonian one obtains

$$\sigma(\omega) = \frac{i}{\omega} (\chi^T - \chi^R(\omega)), \quad (1.8)$$

$$\chi^R(\omega) = \frac{i}{V} \int_0^\infty dt e^{i\omega t} \langle [J(t), J(0)] \rangle, \quad (1.9)$$

$$\chi^T = \frac{i}{V} \int_0^{-i\beta} dt \langle J(t)J(0) \rangle, \quad (1.10)$$

where $\chi^R(\omega)$ is the retarded current-current response function and χ^T is the isothermal current-current susceptibility. The latter can be expressed as a thermodynamic derivative,

$$\chi^T = \left. \frac{\partial \langle J \rangle}{\partial E} \right|_{T=\text{const.}}. \quad (1.11)$$

These expressions can be derived from the original expression given by Kubo, Eq. (1.7), for example by using Ref. [13] and the calculation is sketched in appendix A.2. In fact, the latter expression for the conductivity, Eq. (1.8), is the one that is more commonly encountered in the literature and is directly derived from linear response. Often these equations are derived for the electric conductivity, and the term proportional to χ^T is referred to as the

³Calculation of the response function – which is defined via a commutator – can be evaluated by means of Matsubara frequency techniques. This often simplifies the problem to the extent that the calculations actually can be carried out.

*diamagnetic term*⁴. In the literature one often encounters the statement that the dc conductivity is obtained by taking the limit $\omega \rightarrow 0$ at the end of the calculation, $\sigma_{\text{dc}} = \lim_{\omega \rightarrow 0} \text{Re } \sigma(\omega)$. This is, however, only true in the absence of a Drude peak, since $\lim_{\omega \rightarrow 0} \sigma(\omega) = \sigma(0)$ only in the absence of singularities at $\omega = 0$. (In this respect, the analysis presented in Mahan's book [14] is misleading and should be enjoyed with a possible additional singularity at $\omega = 0$ in mind.) Before using the limit one thus should check whether a Drude weight is present or not. The recipe to extract the Drude weight from the conductivity may be formulated (see c.f. [15]) as $D = \lim_{\omega \rightarrow 0} \omega \text{Im } \sigma(\omega)$ and inserting Eq. (1.8), we find

$$D = \chi^T - \chi^R(0). \quad (1.12)$$

This leaves us with the expression

$$\sigma_{\text{reg}}(\omega) = \text{Re } \frac{i}{\omega} (\chi^R(0) - \chi^R(\omega)) \quad (1.13)$$

for the regular part. Although there are situations where the regular part diverges in the limit $\omega \rightarrow 0$, we are not interested in this kind of singularities and we shall assume that $\sigma_{\text{reg}}(\omega)$ is smooth at $\omega = 0$, e.g. that the regular part is *regular*. Appendix A.3 is devoted to a closer look on what circumstances can lead to a *singular* regular part of the conductivity.

1.5 Mazur Inequality

Mazur [16] and later Suzuki [17] considered situations where the presence of conservation laws prohibits the decay of certain correlation functions in the long-time limit. In the context of transport theory their result can be applied to systems where the finite-temperature conductivity $\sigma(\omega, T)$ is characterized by a finite Drude weight $D(T) > 0$ at $\omega = 0$, implying non-dissipative transport. As outlined above, a Drude weight can arise only in the presence of conserved quantities which protect the current. Therefore it

⁴Those familiar with the derivation of the electric conductivity and the reasons behind the appearance of the diamagnetic term in this derivation, may wonder, how such a term comes about in the general case. In fact, the diamagnetic term can be traced back to a contribution proportional to the square of the vector potential A^2 to the Hamiltonian, and such a term is present due to the charge conservation induced gauge invariance. Therefore, it is not clear how one possibly could obtain a diamagnetic term *without* a contribution that depends quadratically on the external field. We avoid giving a technical explanation by noting, that in an electron gas the carriers of charge also carry a mass, and therefore it is legitimate to calculate the conductivity associated with the particle (or mass) current subject to a gravitational potential. Such a calculation has to lead to exactly the same expression of the conductivity, including the diamagnetic term. The diamagnetic term is present for any conductivity. Skeptics may find useful the discussion in Ref. [13] and the remarks made in appendix A.2.

is useful to formally take into account all of the conserved quantities present in the system. For this purpose we introduce a basis of conserved quantities⁵, $\{C_i\}$, with $[H, C_i] = 0$, in terms of which Suzuki's expression is formulated. To write a conserved operator in terms of the C_i we need a scalar product, which we chose as the expectation value of the product of operators,

$$\langle AB \rangle = \frac{1}{Z} \text{tr} e^{-\beta H} AB. \quad (1.14)$$

where $Z = \text{tr} e^{-\beta H}$ is the partition sum. We choose the C_i such that they are orthogonal, $\langle C_i C_j \rangle = \delta_{ij} \langle C_i^2 \rangle$. Any conserved quantity A can now be expanded in the C_i ,

$$A = \sum_i \frac{\langle AC_i \rangle}{\langle C_i^2 \rangle} C_i. \quad (1.15)$$

Suzuki [17] shows that the difference $\chi^T - \chi^R(0)$ (which as we argue above is identical to the Drude weight, see Eq. (1.12)) can be expressed as a sum over *all* C_j :

$$D = \frac{\beta}{V} \sum_{j=0}^{\infty} \frac{\langle C_j J \rangle^2}{\langle C_j^2 \rangle} \geq \frac{\beta}{V} \sum_{j=0}^N \frac{\langle C_j J \rangle^2}{\langle C_j^2 \rangle}. \quad (1.16)$$

More useful than the equality in Eq. (1.16) is often the inequality [16] which is obtained when the sum is restricted to a finite subset of conservation laws. Such a finite sum over simple expectation values can often be calculated rather easily using either analytical or numerical methods. This allows to obtain lower bounds to the Drude weight with less effort. The Mazur inequality has recently been used heavily [2, 18, 19, 20, 21] to discuss the transport properties of one-dimensional systems. The goal of the next chapter is to obtain lower bounds to the dc conductivity in the case of small perturbations and finite dc conductivity, in the spirit of the Mazur inequality.

1.6 Splitting the Current

From equation (1.16) it is clear that *only* the conserved part of the current J contributes to the Drude weight. (This is what we expect, as the non-conserved part has to decay in a finite time.) To make this observation explicit, we split the current under consideration into a part parallel to the C_i and one that is orthogonal,

$$J = J_{\parallel} + J_{\perp},$$

⁵Basis means that the C_i span the space of conserved operators. Represented in an eigenbasis $\{|n\rangle\}$ of the Hamiltonian, the matrix elements $\langle n|C_i|m\rangle$ of C_i vanish when $E_n \neq E_m$, i.e. the C_i are block-diagonal in energy.

with

$$J_{\parallel} = \sum_i \frac{\langle C_i J \rangle}{\langle C_i^2 \rangle} C_i, \quad (1.17)$$

which results in a separation of the conductivity,

$$\sigma(z) = \sigma_{\parallel}(z) + \sigma_{\perp}(z). \quad (1.18)$$

Since the conductivity $\sigma(z)$ is given by a current-current correlation function and the current J_{\parallel} (J_{\perp}) is diagonal (off-diagonal) in energy, cross-correlation functions $\langle J_{\parallel}; J_{\perp} \rangle$ vanish in Eq. (1.18).

According to Eq. (1.16), the Drude peak of the unperturbed system, $g = 0$, arises solely from J_{\parallel} as can be checked by substitution of Eq. (1.17) in Eq. (1.16),

$$\text{Re } \sigma_{\parallel}(\omega) = \pi D \delta(\omega), \quad (1.19)$$

while $\sigma_{\perp}(z)$ appears in Eq. (1.3) as the regular part, $\text{Re } \sigma_{\perp}(\omega) = \sigma_{\text{reg}}(\omega)$.

In this work we focus on $\sigma_{\parallel}(\omega)$, since the small perturbation is not going to affect $\sigma_{\perp}(\omega)$ much, while $\sigma_{\parallel}(\omega = 0)$ diverges for $g \rightarrow 0$, see Fig. 1.1. As we are interested in the small g asymptotics only, we may neglect the contribution $\sigma_{\perp}(0)$ to the dc conductivity. The separation into parallel and perpendicular components of the current allow to rewrite Mazur's relation in a simple form:

$$D = \frac{\beta}{V} \langle J J_{\parallel} \rangle = \frac{\beta}{V} \langle J_{\parallel}^2 \rangle. \quad (1.20)$$

This relation is particularly useful when the current itself is conserved and $J_{\perp} = 0$. This is for example the case for the heat current J_Q in the XXZ Heisenberg spin chain which will be discussed below, see section 3.5.

1.7 Memory Matrix Formalism

The conserved currents of the unperturbed model H_0 are violated by the small perturbation gH_1 . However, if the perturbation is small, some of them will decay slowly, and typically those which decay with the slowest rate will contribute most to the conductivity. Thus, to study them, a hydrodynamic approach seems to be reasonable. The relation between hydrodynamic equations and correlation functions has been studied in Ref. [22]. To separate the dynamics of the slow modes from the rest, one can use projection operator techniques which project the dynamics onto the slow modes. In this section we will therefore review the so-called memory matrix formalism [23], introduced by Mori and Zwanzig [24, 25] for this purpose. In the next chapter we will show that this approach can be used to obtain a lower bound for the dc conductivity in terms of a perturbation theory for the small parameter g .

We start by defining a scalar product⁶ in the space of quantum mechanical operators,

$$(A|B) = \frac{1}{V} \int_0^\beta d\tau \langle A^\dagger(0)B(i\tau) \rangle - \beta \langle A^\dagger \rangle \langle B \rangle \quad (1.21)$$

Note that the second term can always be omitted by replacing A by $A - \langle A \rangle$. With this notation, the time evolution is given by the Liouville-(super)operator $L = [H, \cdot] = L_0 + gL_1$ with $(LA|B) = (A|LB) = (A|L|B)$, and the time evolution of an operator may be expressed as

$$|A(t)\rangle = |e^{iHt} A e^{-iHt}\rangle = e^{iLt}|A\rangle.$$

This more complicated (as compared to Eq. (1.14)) choice of a scalar product on the space of operators is necessary to account for the essentially dynamical situation. The Drude weight is a thermodynamic quantity (relation (1.11)) and thus can be calculated from static correlation functions (relation (1.20)). This is no longer true for the dc conductivity for finite g and equation (1.21) turns out to be the most convenient for our purpose. Note that in terms of this scalar product the Kubo formula (1.7) may be expressed as

$$\sigma(\omega) = \int_0^\infty dt e^{i\omega t} (J(t)|J). \quad (1.22)$$

Moreover, $(A|B)$ can be interpreted as a generalized thermodynamic susceptibility in analogy to Eqs. (1.10) and (1.11). In particular, $\chi^T = (J|J)$.

As the next step we choose a – for the moment – arbitrary set of operators $\{C_i\}$, which represent the chosen set of slow modes. As the only restriction we require that the current be included in the space spanned by the C_i .

$$|J\rangle = \sum_i \frac{(C_i|J)}{(C_i|C_i)} |C_i\rangle. \quad (1.23)$$

In most applications, the C_i include the relevant slow modes of the system. For notational convenience, we assume that the $\{C_i\}$ are orthogonal,

$$(C_i|C_j) = \delta_{ij} (C_i|C_i). \quad (1.24)$$

In terms of these we may define the projector P onto (and Q away from) the space spanned by these ‘slow’ modes

$$P = \sum_i |C_i\rangle (C_i|C_i)^{-1} \langle C_i| = 1 - Q. \quad (1.25)$$

⁶Note that usually [23] this scalar product is defined with an additional factor of β^{-1} , to make it dimensionless. We use a different convention because it is more convenient: One gets rid of factors of β one would otherwise have to include in all physical correlation functions, e.g. $\chi = (J|J)$ vs. $\chi = \beta(J|J)$.

Within this formalism, one obtains from Eq. (1.22) the following simple, yet formal expression for the conductivity:

$$\sigma(\omega) = \left(J \left| \frac{i}{\omega - L} \right| J \right). \quad (1.26)$$

Using a number of simple manipulations, one can show [23, 24, 25] that the conductivity can be expressed as a matrix product,

$$\sigma(\omega) = \sum_{ij} (J|C_i) (M(\omega) + iK - i\omega C)^{-1}_{ij} (C_j|J), \quad (1.27)$$

where

$$M_{ij}(\omega) = \left(\dot{C}_i \left| Q \frac{i}{\omega - LQ} \right| \dot{C}_j \right) \quad (1.28)$$

is the so-called *memory matrix*,

$$K_{ij} = \left(\dot{C}_i | C_j \right) \quad (1.29)$$

is a frequency independent matrix and

$$C = (C_i|C_j) = \delta_{ij}(C_i|C_i) \quad (1.30)$$

is the diagonal matrix of susceptibilities. The formal expression (1.27) for the conductivity is exact, and completely general, i.e. valid for an arbitrary choice of the modes C_i , provided only that the current can be written in terms of the slow modes, Eq.(1.23). The C_i do not even have to be ‘slow’.

Due to the projection operators Q , the memory matrix (1.28) is in general difficult to evaluate. To obtain correlation functions that can be evaluated easily one uses approximations to M , and it is in context with those approximations that the choice of the projectors (or equivalently the choice of slow modes $\{C_i\}$) becomes crucial. Different choices of slow modes can deliver qualitatively different approximations to the conductivity. This will be discussed in detail in the forthcoming chapter.

If we choose $J = C_1$, the dc conductivity is given by the (1, 1)-component of the matrix

$$(M(0) + K)^{-1}. \quad (1.31)$$

More generally, the (m, n) -component of Eq. (1.31) describes the response of the ‘current’ C_m to a homogeneous external field coupling solely to C_n . We note that, since a matrix of transport coefficients has to be positive (semi)definite, this also holds for the matrix $M(0) + K$.

To avoid technical complications associated with the presence of K , we restrict our analysis in the following to time reversal invariant systems and choose the C_i such that they have either signature +1 or -1 under time

reversal.⁷ In the dc limit, $\omega = 0$, components of Eq. (1.31) connecting modes of different signatures vanish. Thus, $M(0) + K$ is block-diagonal with respect to the time reversal signature, and consequently we can restrict our analysis to the subspace of slow modes with the same signature as the current J . However, if C_m and C_n have the same signature, then $(C_m | \dot{C}_n) = 0$, and thus K vanishes on this restricted space. The dc conductivity therefore takes the form

$$\sigma_{\text{dc}} = \sum_{ij} (J | C_i) (M(0)^{-1})_{ij} (C_j | J). \quad (1.32)$$

Making the above choice, $C_1 = J$, the expression is further simplified and one gets

$$\sigma_{\text{dc}} = (\chi^T)^2 (M(0)^{-1})_{11}. \quad (1.33)$$

Note again, that this is an exact expression when approximations to $M(\omega)$ have not been used yet. Furthermore, we have derived an expression for the memory matrix which is structurally similar to the expression (1.6). Thus we arrive at the conclusion that $M(0)/\chi^T$ plays the role of a scattering rate. This lays the foundations for a perturbative analysis aimed at in section 1.3 and carried out in the next chapter.

1.8 Conservation Laws and Slow Modes

To conclude this chapter, we make some general remarks on conservation laws, slow modes and integrable systems. As conserved quantities dictate the value of the Drude weight, it is worthwhile to halt for a moment's sake and to elaborate on the nature of conservation laws themselves.

We already have used the notion of the set of all conservation laws, $\{C_i\}$ in sections 1.5 and 1.6. As an example, the projector to some energy eigenstate $|n\rangle\langle n|$ would be a candidate for such a conservation law, and is trivially conserved. Such an operator, however, is typically a highly non-local object and an explicit knowledge of it is neither practically achievable nor is it desirable. To consider the abstract set $\{C_i\}$ was useful to learn about the nature of the Drude weight and also will be useful in the next section when we derive lower bounds to the conductivity, expressed through approximations to the memory matrix.

This set $\{C_i\}$ of trivially conserved quantities has to be contrasted with what one usually refers to as constants of the motion (or integrals of motion), which are conserved quantities Q_i associated with symmetries of the

⁷As $\Theta^2 = \pm 1$ for states with integer or half-integer spin, the combinations $A \pm \Theta A \Theta^{-1}$ have signatures ± 1 provided the operator A does not change the total spin by half an integer, which is the case for all operators with finite cross-correlation functions with the physical currents.

Hamiltonian and are the subject of Noether's theorem. The latter, non-trivial conservation laws are often explicitly known and are quite generally well defined local quantities for which a density and a current can be defined in the usual sense (see section 1.1). Thus, these are the quantities one commonly wants to work with.

In the context of hydrodynamics and transport, more often than not, these local conservation laws are those which protect the current from decaying. And even if they are not conserved (due to, say, impurities which break translational invariance), they typically are the slowest modes in the system and their decay rate determines the decay rate and dc conductivity of the current. For example, momentum conservation is responsible for the infinite electrical conductivity in a superconductor and the dissipation of momentum in a normal metal gives the electrical conductivity a finite value. However, there are exceptions to this rule. As we will see in chapter 3, the spin current in the XXZ Heisenberg spin chain is *not* protected by any of the known non-trivial local conservation laws, although there is an infinite number of them (see below). Nevertheless, the spin conductivity is characterized by a finite Drude weight, which means that actually it's *non-local* conservation laws that protect the *local* spin current.

Generally, whichever are the relevant slow modes, local or non-local conservation laws, constants of the motion or not, the philosophy of our treatment is always the same: The relevant modes of the perturbed model have to be among the set of exactly conserved quantities of the unperturbed model, and one chooses some of them as the slow modes in the definition of the memory matrix. Using approximations to the memory matrix delivers lower bounds to the asymptotic ($g \rightarrow 0$) value of the dc conductivity, and the result can systematically be improved by including more and more slow modes in the analysis.

The cautious reader may wonder why in the XXZ model there is an infinite number of constants of the motion. The reason is that this model is integrable, which takes us to the next topic of this section. While no fool-proof definition of integrability exists in mathematical terms, integrability is used to express that one can gain complete knowledge of the solution of the equation of motion, in terms of an explicit expression for the solution, which in principle can be evaluated. For *classical* systems with a *finite* number N of degrees of freedom, integrability is tantamount to the existence of exactly N constants of the motion Q_i which are in convolution, $\{Q_i, Q_j\} = 0$, and the dynamics of the system is uniquely determined by the values of the Q_i . The existence of the Q_i is related to the existence of invariant tori as described by the Hamilton-Jacobi formalism.

One can straightforwardly transfer this whole concept to *quantum* systems. The Q_i become conserved operators, $[H, Q_i] = 0$, and according to the correspondence principle the Poisson bracket is translated as a commu-

tator, $[Q_i, Q_j] = 0$. The requirement that the Q_i determine the dynamics, can be translated to the quantum situation as the requirement that the eigenstates of the Hamiltonian be completely characterized by eigenvalues of the Q_i . This implies that the Q_i constitute a set of good quantum numbers, i.e. that each eigenstate of the Hamiltonian can be uniquely labeled by eigenvalues of the Q_i . The concept just described is well known from quantum mechanics text books and is referred to by saying that the Q_i constitute a complete set of commuting operators (CSCO). What is usually *not* pointed out in these textbooks is the fact that the existence of a CSCO is rather the exception than the rule among physical models.

However, a problem with the quantum definition of integrability becomes apparent when it comes to the counting of degrees of freedom. One could argue, for instance, that a single quantum-mechanical particle in one dimension has an infinite number of degrees of freedom, as the value of the wave function can take infinitely many values at any of the infinitely many points in space. This point of view, however, is not very helpful, and it is customary to assign to the quantum system the same number of degrees of freedom as the corresponding classical problem. However, such a treatment brings with it additional subtleties. For example, it is not at all clear, whether the quantum counterpart of an integrable classical system is itself integrable, and even if it is, the constants of the motion of the quantum system are not necessarily straightforwardly obtained by a quantization of the constants of the motion of the classical system. As an other example, there are quantum systems which have no classical analogue at all, as for example the XXZ Heisenberg spin-1/2 chain. In this particular model, however, the determination of the number of degrees of freedom seems to be rather straightforward, and corresponds to the number of spins in the chain.

In going to an infinite number of degrees of freedom $N \rightarrow \infty$, one has to face the problem of an infinite number of constants of the motion. While in many cases there is no recipe to gain knowledge of all of the constants of the motion, in the case of the XXZ chain, integrability is guaranteed as the model is solvable by Bethe ansatz, which provides explicit expressions for all eigenstates of the Hamiltonian in terms of complicated (and often an infinite number of) integrals. Even more conveniently, a recipe to construct the hierarchy of the infinite number of constants of the motion, the existence of which is implied by integrability, is known, and therefore one can easily obtain explicit expressions for them.

While integrable systems, in general, are a seldom phenomenon, one dimensional systems are a special case. Here integrability appears to be rather common, which is often attributed to the reduced number of possibilities for the dynamics of the individual constituents. One example is the XXZ model, but more generally, the effective low energy theory of an arbitrary gapless spin chain (or any other massless 1D quantum model) is

given by the Luttinger liquid Hamiltonian, which is integrable. Real one dimensional quantum systems often can consequently be described as an integrable model plus some perturbation which at low temperatures can be considered to be small. Models like a one dimensional gas of bosons with point interaction (also referred to, for some reasons, as the nonlinear Schrödinger equation) or the aforementioned XXZ model, in contrast, are integrable *at any temperature*.

In this work, we are not so much interested in the well studied properties of the integrable systems themselves, but rather in the question of how are transport properties of integrable systems affected by small perturbations which destroy integrability. The whole chapter 3 is devoted to the study of this question.

Chapter 2

Lower Bounds for Conductivities of Correlated Quantum Systems

In this chapter we show how one can calculate lower bounds for conductivities of correlated quantum systems for the scenario described in the last chapter. As outlined above, the unperturbed model H_0 can also be an *interacting* Hamiltonian characterized by an infinite conductivity at finite temperatures. The small perturbation gH_1 renders the conductivity finite. We derive lower bounds for the relevant conductivities in the asymptotic limit $g \rightarrow 0$ and show how they can be improved systematically using the memory matrix formalism. We also investigate under what conditions our lower bound may become exact. The subsequent chapters contain numerous direct applications of the bounds derived here.

2.1 Motivation

Transport properties of complex materials are not only important for many applications but are also of fundamental interest as their study can give insight into the nature of the relevant quasi particles and their interactions.

Compared to thermodynamic quantities, the transport properties of interacting quantum systems are notoriously difficult to calculate even in situations where interactions are weak. The reason is that conductivities of non-interacting systems are usually infinite even at finite temperature, implying that even to lowest order in perturbation theory an infinite resummation of a perturbative series is mandatory. To lowest order this implies that one usually has to solve an integral equation, often written in terms of (quantum-) Boltzmann equations or – within the Kubo formalism – in terms of vertex equations. The situation becomes even more difficult if the interac-

tions are so strong that an expansion around a non-interacting system is not possible. Also numerically, the calculation of zero-frequency conductivities of strongly interacting clean systems is a serious challenge and even for one-dimensional systems reliable calculations are available for high temperatures only [1, 2, 3, 5, 26, 27].

Variational estimates, e.g. for the ground state energy, are powerful theoretical techniques to obtain rigorous bounds on physical quantities. They can be used to guide approximation schemes to obtain simple analytic estimates and are sometimes the basis of sophisticated numerical methods like the density matrix renormalization group [28].

Taking into account both the importance of transport quantities and the difficulties involved in their calculation it would be very useful to have general variational bounds for transport coefficients.

2.2 Boltzmann Equation and Variational Bounds

A well known example where a bound for transport quantities has been derived is the variational solution of the Boltzmann equation, discussed extensively by Ziman [29]. The linearized Boltzmann equation in the presence of a static electric field can be written in the form

$$e\mathbf{E}\mathbf{v}_{\mathbf{k}}\frac{df^0}{d\epsilon_{\mathbf{k}}} = \sum_{\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'}\Phi_{\mathbf{k}'} \quad (2.1)$$

where $W_{\mathbf{k},\mathbf{k}'}$ is the integral kernel describing the scattering of quasiparticles and we have linearized the Boltzmann equation around the Fermi (or Bose) distribution $f_{\mathbf{k}}^0 = f^0(\epsilon_{\mathbf{k}})$ using $f_{\mathbf{k}} = f_{\mathbf{k}}^0 - \frac{df^0}{d\epsilon_{\mathbf{k}}}\Phi_{\mathbf{k}}$. Therefore, the current is given by $\mathbf{I} = -e \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \frac{df^0}{d\epsilon_{\mathbf{k}}}\Phi_{\mathbf{k}}$ and the dc conductivity is determined from the inverse of the scattering matrix W using $\sigma = -e^2 \sum_{\mathbf{k}\mathbf{k}'} \frac{df^0}{d\epsilon_{\mathbf{k}}} v_{\mathbf{k}}^i W_{\mathbf{k},\mathbf{k}'}^{-1} v_{\mathbf{k}'}^i \frac{df^0}{d\epsilon_{\mathbf{k}'}}$. This result can be obtained by maximizing a functional $F[\Phi]$ (see [29, 30, 31, 32]) with

$$\begin{aligned} \sigma &= e^2 \max_{\Phi} F[\Phi] \geq e^2 \max_{a_i} F \left[\sum_i a_i \phi_i \right] \quad (2.2) \\ F[\Phi] &= \frac{2 \left(\sum_{\mathbf{k}} v_{\mathbf{k}}^i \Phi_{\mathbf{k}} \frac{df^0}{d\epsilon_{\mathbf{k}}} \right)^2}{\sum_{\mathbf{k},\mathbf{k}'} (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})^2 W_{\mathbf{k},\mathbf{k}'}} \end{aligned}$$

where on the rhs. of the first line one maximizes over the scalar prefactors of the trial functions ϕ_i . For the denominator in the second line we used that $\sum_{\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'} = 0$ reflecting the conservation of probability. The variational formula (2.2) is actually closely related [29] to the famous H-theorem of Boltzmann which states that entropy always increases upon scattering.

A lower bound for the conductivity can be obtained by varying Φ only in a subspace of all possible functions. This allows for example to obtain analytically good estimates for conductivities *without* inverting an infinite dimensional matrix or, equivalently, solving an integral equation, see Ziman's book for a large number of examples [29].

The applicability of Eq. (2.2) is restricted to situations where the Boltzmann equation is valid, i.e. in the presence of quasi particles. Bounds for the conductivity in more general setups are not known. As we have seen, for non-dissipative systems with infinite conductivity (described by a Hamiltonian H_0) it is possible to get a lower bound for the so-called Drude weight.

Our goal is to find a variational lower bound for conductivities in the spirit of Eq. (2.2) for this very general situation, without any requirement on the existence of quasi particles. For technical reasons (see below) we restrict our analysis to situations where H is time reversal invariant.

In the following, we use the memory matrix formalism to formulate an inequality for transport coefficients for weakly perturbed systems. We will argue that the inequality is valid under the conditions which we specify. Finally, we investigate under which conditions the lower bounds become exact and briefly discuss applications of our formula. But first we insert a short section in which we attempt a naive perturbative expansion of the conductivity which helps to identify issues that have to be resolved by a more thorough analysis.

2.3 Perturbation theory for $1/\sigma$

Let us give an example of a naive perturbative derivation (see also Ref. [3]) to gain some insight about what problems can turn up in a perturbative derivation as the one presented in this chapter. According to our assumptions, the conductivity is diverging for $g \rightarrow 0$ and therefore it is useful to consider the scattering rate $\Gamma(\omega)/\chi$ (with the current susceptibility χ of Eq. (1.10)) defined by

$$\sigma(\omega) = \frac{\chi}{\Gamma(\omega)/\chi - i\omega}. \quad (2.3)$$

If J is conserved for $g = 0$ (i.e. for $J = J_{\parallel}$, see above), the scattering rate vanishes, $\Gamma(\omega) \equiv 0$, for $g = 0$, which results in a finite Drude weight. A perturbation around this singular point results in a finite $\Gamma(\omega)$. In the limit $g \rightarrow 0$ we can expand (2.3) for any *finite* frequency ω in Γ to obtain

$$\omega^2 \text{Re } \sigma(\omega) = \text{Re } \Gamma(\omega) + \mathcal{O}(\Gamma^2/\omega). \quad (2.4)$$

We can read this as an equation for the leading order contribution to $\Gamma(\omega)$, which now is expressed through the Kubo formula for the conductivity. By

partially integrating twice in time we can write $\Gamma(\omega) = \tilde{\Gamma}(\omega) + \mathcal{O}(g^3)$ with

$$\text{Re } \tilde{\Gamma}(\omega) = \text{Re } \frac{1}{z} \frac{1}{V} \int_0^\infty dt e^{izt} \langle [J(t), J(0)] \rangle_0 \Big|_{z=\omega+i0}, \quad (2.5)$$

where $\dot{J} = i[H, J] = ig[H_1, J]$ is linear in g and therefore the expectation value $\langle \dots \rangle_0$ can be evaluated with respect to H_0 (which may describe an interacting system). Thus we have expressed the scattering rate via a simple correlation function of the time derivative of the current.

To determine the dc conductivity one is interested in the limit $\omega \rightarrow 0$ and it is tempting to set $\omega = 0$ in Eq. (2.5). We have, however, derived Eq. (2.5) in the limit $g \rightarrow 0$ at finite ω and *not* in the limit $\omega \rightarrow 0$ at finite g . The series Eq. (2.4) is well defined for finite $\omega \neq 0$ only and in the limit $\omega \rightarrow 0$ the series shows singularities to arbitrarily high orders in $1/\omega$.

At first sight this makes Eq. (2.5) useless for calculating the dc conductivity. One of the main results of this chapter is that, nevertheless, $\tilde{\Gamma}(\omega = 0)$ can be used to obtain a lower bound to the dc conductivity

$$\sigma(\omega = 0) \geq \frac{\chi^2}{\tilde{\Gamma}(0)} \quad \text{for } g \rightarrow 0. \quad (2.6)$$

2.4 Conjecture

To obtain a controlled approximation to the memory matrix in the limit of small g , it is important to identify the relevant slow modes of the system. For the C_i (appearing in 1.7) we choose quantities which are conserved by H_0 , $[H_0, C_i] = 0$, such that $\dot{C}_i = ig[H_1, C_i]$ is linear in the small coupling g . As argued above, we require that the singularities of correlation functions of the unperturbed system are exclusively due to exact conservation laws C_i , i.e. that the Drude peak appearing in Eq. (1.3) is the only singular contribution, see the end of section 1.4 and appendix A.3 for details. Furthermore, we choose $J = J_\parallel$, as discussed in section 1.6, and consider only C_i with the same time reversal signature as J (see the end of section 1.7). We also will make the following simplifications which still will keep all essential features of our proof. As can be seen from a comparison of Eqs. (1.32) and (1.33), one may further simplify the situation by the particular choice $C_1 = J_\parallel$. Finally, without loss of generality, we choose the C_i to be not only orthogonal but also normalized, $(C_i|C_j) = \delta_{ij}$.

To formulate our central conjecture we introduce the following notions. We define $M_n(\omega)$ as the (exact) $n \times n$ memory matrix obtained by setting up the memory matrix formalism for the first n slow modes $\{C_i, i = 1, \dots, n\}$. Note that the definitions of the relevant projectors P and Q also depend on this choice, and that for any choice of n one gets $\sigma = (M_n^{-1})_{11}$. We now introduce the approximate memory matrix \tilde{M}_n motivated by the following

arguments: \dot{C}_i is already *linear* in g and thus the leading contribution to $M(\omega)$ is of order g^2 . We want to keep the leading order contribution only and therefore in Eq. (1.28) we approximate L by L_0 and replace $(\cdot|\cdot)$ by $(\cdot|\cdot)_0$ as we evaluate the scalar product with H_0 instead of H for the thermal average as well as the time evolution appearing in Eq. (1.21). By definition, the C_i are conserved, implying $L_0|C_i) = 0$ and thus $L_0P = 0$ (see Eq. (1.25)) or equivalently $L_0Q = L_0$. Furthermore, as $(C_j|\dot{C}_i) = 0$ due to our choice that all of the C_i have the same time reversal symmetry, one has $Q|\dot{C}_i) = |\dot{C}_i)$. Therefore, the projector Q does not contribute within this approximation. We thus define the $n \times n$ matrix \tilde{M}_n by

$$\tilde{M}_{n,ij} = \lim_{\omega \rightarrow 0} \left(\dot{C}_i \left| \frac{i}{\omega - L_0} \right| \dot{C}_j \right)_0. \quad (2.7)$$

Note that \tilde{M}_n is a sub-matrix of \tilde{M}_m for $m > n$ and therefore the approximate expression for the conductivity $\sigma \approx (\tilde{M}_n^{-1})_{11}$ does depend on n while $(M_n^{-1})_{11}$ is independent of n .

Note that \tilde{M}_1 is identical to the naive perturbative for $\tilde{\Gamma}$ derived in the previous section 2.3, where the validity of this formula is also discussed.

The central conjecture of this chapter is, that for small g $(\tilde{M}_n^{-1})_{11}$ gives a lower bound to the dc conductivity for any n , or, more precisely,

$$\sigma|_{1/g^2} = (\tilde{M}_\infty^{-1})_{11} \geq \dots \geq (\tilde{M}_n^{-1})_{11} \geq \dots \geq \tilde{M}_1^{-1}. \quad (2.8)$$

Here $\sigma|_{1/g^2} = (1/g^2) \lim_{g \rightarrow 0} g^2 \sigma$ denotes the leading term $\propto 1/g^2$ in the small- g expansion of σ . Note that $\tilde{M}_n \propto g^2$ by construction. \tilde{M}_∞ is the approximate memory matrix where *all*¹ conservation laws have been included. In some special situations, discussed in Ref. [3], one has $\sigma \sim 1/g^4$ and therefore $\sigma|_{1/g^2} = \infty$.

Equation (2.6) in the previous section 2.3 is a special case of the inequality above, for the scattering rate $\tilde{\Gamma}/\chi$ may be expressed as $\tilde{\Gamma}/\chi^2 = \tilde{M}_1$.

Two steps are necessary to prove Eq. (2.8). The simple part is actually the inequalities in Eq. (2.8). They are a consequence of the fact that the matrices \tilde{M}_n are all positive definite and that \tilde{M}_n is a sub-matrix of \tilde{M}_m for $m \geq n$. More difficult to prove is that the first equality in (2.8) holds. To show this we will need an additional assumption, namely, that the *regular* part of all correlation functions (to be defined below) remains finite in the limit $g \rightarrow 0$, $\omega \rightarrow 0$. In this case, the perturbative expansion around \tilde{M}_∞ in powers of g is free of singularities at finite temperature (which is not the case for $\tilde{M}_{n < \infty}$). This in turn implies that $\lim_{g \rightarrow 0} M_\infty/g^2 = \tilde{M}_\infty/g^2$ and therefore $\sigma|_{1/g^2} = (\tilde{M}_\infty^{-1})_{11}$.

Next, we present the two parts of the proof.

¹The C_i span the space of *all* conservation laws, including those which do not commute with each other.

2.4.1 Inequalities

We start by investigating the (1,1)-component of the inverse of the positive definite symmetric matrix \tilde{M}_∞ . It is convenient to write the inverse as

$$(\tilde{M}_\infty^{-1})_{11} = \max_{\varphi} \frac{(\varphi^T \mathbf{e}_1)^2}{\varphi^T \tilde{M}_\infty \varphi} \quad (2.9)$$

where \mathbf{e}_1 is the first unit vector. The same method is used to derive Eq. (2.2) in the context of the Boltzmann equation. The maximum is obtained for $\varphi = \tilde{M}_\infty^{-1} \mathbf{e}_1$. By restricting the variational space in (2.9) to the first n components of φ we reproduce the sub-matrix \tilde{M}_n of \tilde{M}_∞ and obtain

$$\begin{aligned} (\tilde{M}_\infty^{-1})_{11} &\geq \max_{\varphi = \sum_1^m \varphi_i \mathbf{e}_i} \frac{(\varphi^T \mathbf{e}_1)^2}{\varphi^T \tilde{M}_\infty \varphi} = (\tilde{M}_m^{-1})_{11} \\ &\geq \max_{\varphi = \sum_1^{n < m} \varphi_i \mathbf{e}_i} \frac{(\varphi^T \mathbf{e}_1)^2}{\varphi^T \tilde{M}_\infty \varphi} = (\tilde{M}_{n < m}^{-1})_{11} \end{aligned}$$

By choosing different values for m and $n < m$, this proves all inequalities appearing in (2.8).

2.4.2 Expansion of the Memory Matrix

We proceed by expanding the exact memory matrix M_n , where $P_n = 1 - Q_n$ is a projector on the first n conservation laws, in powers of g . Using that $LQ_n = L_0 + gL_1Q_n$, we obtain the geometric series

$$M_{n,ij}(\omega) = \sum_{k=0}^{\infty} g^k \left(\dot{C}_i \left| Q_n \frac{i}{\omega - L_0} \left(L_1 Q_n \frac{1}{\omega - L_0} \right)^k \right| \dot{C}_j \right). \quad (2.10)$$

Note that this is not a full expansion in g , as the scalar product (1.21) is defined with respect to the full Hamiltonian $H = H_0 + gH_1$. We will turn to the discussion of the remaining g -dependence later.

In general, one can expand

$$L_1 = \sum_{m,n} \lambda_{mn} |A_m\rangle \langle A_n|$$

in terms of some basis A_m in the space of operators. Therefore Eq. (2.10) can be written as a sum over products of terms with the general structure

$$\left(A \left| Q_n \frac{1}{\omega - L_0} \right| B \right). \quad (2.11)$$

In the following we would like to argue that such an expansion is regular for $n = \infty$ if *all* conservation laws have been included in the definition of

Q . As argued in Appendix 2.3, we have to investigate whether the series coefficients in Eq. (2.10) diverge for $\omega \rightarrow 0$. The basis of our argument is the following: as Q_∞ projects the dynamics to the space perpendicular to all of the conservation laws, the associated singularities are absent in Eq. (2.11) and therefore the expansion of M_∞ is regular.

To show this more formally, we split up $B = B_\parallel + B_\perp$ in (2.11) into a component parallel and one perpendicular to the space of *all* conserved quantities, $|B_\parallel\rangle = P_\infty|B\rangle$. With this notation, the action of L_0 becomes more transparent:

$$\frac{1}{\omega - L_0}|B\rangle = \frac{1}{\omega}|B_\parallel\rangle + \frac{1}{\omega - L_0}|B_\perp\rangle. \quad (2.12)$$

As we assume that all divergences can be traced back to the conservation laws, we take the second term to be regular. It is only the first term which leads in Eq. (2.11) to a divergence for $\omega \rightarrow 0$, provided that $(A|Q_n|B_\parallel)$ is finite. If we consider the perturbative expansion of $M_{n<\infty}$, where $P_n = 1 - Q_n$ projects only to a subset of conserved quantities, then finite contributions of the form $(A|Q_n|B_\parallel)$ exist and the perturbative series in g will be singular (see also Appendix 2.3). Considering M_∞ , however, Q_∞ projects out *all* conservation laws and therefore by construction $Q_\infty|B_\parallel\rangle = Q_\infty P_\infty|B\rangle = 0$. Thus the first term in (2.12) does not contribute in (2.11) for $n = \infty$ and the expansion (2.10) of M_∞ is therefore regular.

The only remaining part of our argument is to show that in the limit $g \rightarrow 0$ one can safely replace $(\cdot|\cdot)$ by $(\cdot|\cdot)_0$. Here it is useful to realize that $(A|B)$ can be interpreted as a (generalized) static susceptibility. In the absence of a phase transition and at finite temperatures, susceptibilities are smooth, non-singular functions of the coupling constants and therefore we do not expect any further singularities from this step. If we define a phase transition by a singularity in some generalized susceptibility, then the statement that susceptibilities are regular in the absence of phase transitions even becomes a mere tautology.

Combining all arguments, the expansion (2.10) of $M_\infty(\omega \rightarrow 0)$ is regular, and using $(\dot{C}_i|Q_\infty = (\dot{C}_i|$ (see discussion before Eq. (2.7)) its leading term, $k = 0$ is given by \tilde{M}_∞ . We therefore have shown the missing first equality of our central conjecture (2.8).

2.5 Discussion

In this chapter we have established that in the limit of small perturbations, $H = H_0 + gH_1$, lower bounds to dc conductivities may be calculated for situations where the conductivity is infinite for $g = 0$. In the opposite case, when the conductivity is finite for $g = 0$, one can use naive perturbation theory to calculate small corrections to σ without further complications.

The relevant lower bounds are directly obtained from the memory matrix formalism. Typically[33, 34, 35] one has to evaluate a small number of correlation functions and to invert small matrices. The quality of the lower bounds depends decisively on whether one has been able to identify the ‘slowest’ relevant modes in the system.

There are many possible applications for the results presented in this chapter. The mostly considered situation is the case where H_0 describes a non-interacting system[33]. For situations where the Boltzmann equation can be applied, it has been pointed out a long time ago by Belitz [36] that there is a one-to-one relation of the memory matrix calculation to the variational Ansatz for the Boltzmann equation, see Eq. (2.2). In this chapter we were able to generalize this result to cases where a Boltzmann description is not possible. For example, if H_0 is the Hamiltonian of a Luttinger liquid, i.e. a non-interacting bosonic system, then typical perturbations are of the form $\cos \phi$ for which a simple transport theory in the spirit of a Boltzmann or vertex equation does not exist to our knowledge.

Another class of applications are systems where H_0 describes an *interacting* system, e.g. an integrable one-dimensional model[3] or some non-trivial quantum-field theory[37]. In these cases it can become difficult to calculate the memory matrix and one has to resort to use either numerical[3] or field-theoretical methods[37] to obtain the relevant correlation functions.

An important special case are situations where H_0 is characterized by a *single* conserved current with the proper symmetries, i.e. with overlap to the (heat-, spin- or charge-) current J . For example, in a non-trivial continuum field theory H_0 , interactions lead to the decay of all modes with exception of the momentum P . In this case the momentum relaxation and therefore the conductivity at finite T is determined by small perturbations gH_1 like disorder or Umklapp scattering which are present in almost any realistic system. As $\tilde{M}_\infty = \tilde{M}_1$ in this case, our results suggest that for small g the conductivity is *exactly* determined by the momentum relaxation rate $\tilde{M}_{PP} = \lim_{\omega \rightarrow 0} i(\dot{P} | (\omega - L_0)^{-1} | \dot{P})$,

$$\sigma = \frac{\chi_{PJ}^2}{\tilde{M}_{PP}} \quad \text{for } g \rightarrow 0. \quad (2.13)$$

Here we used that $J_{\parallel} = P(P|J)/(P|P)$ with $\chi_{PJ} = (P|J)$ and we have restored all factors which arise if the normalization condition (1.24) is not used. In the next section, 2.6, we check numerically that this statement is valid for a realistic example within the Boltzmann equation approach.

A number of assumptions entered our arguments. The strongest one is the restriction that all relevant singularities arise from exact conservation laws of H_0 . We assumed that the regular parts of correlation functions are finite for $\omega = 0$. There are two distinct scenarios in which this assumption does not hold. First, in the limit $T \rightarrow 0$, often scattering rates vanish

which can lead to divergences of the nominally regular parts of correlation functions. Furthermore, at $T = 0$ even infinitesimally small perturbations can induce phase transitions – again a situation where our arguments fail. Therefore our results are not applicable at $T = 0$. Second, finite temperature transport may be plagued by additional divergences for $\omega \rightarrow 0$ not captured by the Drude weight. In some special models, for instance, transport is singular even in the *absence* of exactly conserved quantities (e.g. non-interacting phonons in a disordered crystal[29]). In all cases known to us, these divergences can be traced back to the presence of some slow modes in the system (e.g. phonons with very low momentum). While we have not kept track of such divergences in our arguments, we nevertheless believe that they do *not* invalidate our main inequality (2.8) as further slow modes not captured by exact conservation laws will only increase the conductivity. It is, however, likely that the *equality* (2.13) is not valid for such situations. In section 2.6 we analyze in some detail within the Boltzmann equation formalism under which conditions (2.13) holds.

As an aside, we note that the singular heat transport of non-interacting disordered phonons, mentioned above, is well described within our formalism if we model the clean system by H_0 and the disorder by H_1 , see the extensive discussion by Ziman[29] within the variational approach which can be directly translated to the memory matrix language, see Ref. [36].

It would be interesting to generalize our results to cases where time reversal symmetry is broken, e.g. by an external magnetic field. As time reversal invariance entered non-trivially in our arguments, this seems not to be simple. We nevertheless do not see any physical reason why the inequality should not be valid in this case, too. One example where no problems arise are spin chains in a uniform magnetic field[38] where one can map the field to a chemical potential using a Jordan-Wigner transformation. Then one can directly apply our results to the time reversal invariant system of Jordan-Wigner fermions.

2.6 Single Slow Mode

In this section we check whether in the presence of a *single* conservation law with finite cross correlations with the current the inequality (2.8) can be replaced by the equality (2.13). This requires us to compare the true conductivity, which in general is hard to determine, to the result given by \tilde{M}_1 . Thus we restrict ourselves to the discussion of models for which a Boltzmann equation can be formulated and the expression for the conductivity can be calculated at least numerically. In the following we first show numerically that the equality (2.13) holds for a realistic model. In a second step we discuss the precise regularity requirement of the scattering matrix such that

Eq. (2.13) holds.

To simplify numerics, we consider a simple one-dimensional Boltzmann equation of interacting and weakly disordered Fermions. Clearly, the Boltzmann approach breaks down close to the Fermi surface due to singularities associated with the formation of a Luttinger liquid, but in the present context we are not interested in this physics as we only want to investigate properties of the Boltzmann equation. To avoid the restrictions associated with momentum and energy conservation in one dimension we consider a dispersion with two minima and four Fermi points,

$$\epsilon_k = -\frac{k^2}{2} + \frac{k^4}{4} + \frac{1}{10}. \quad (2.14)$$

The Boltzmann equation reads

$$\begin{aligned} v_k \frac{df_k^0}{d\epsilon_k} E &= \sum_{k'qq'} S_{kk'}^{qq'} [f_k f_{k'} (1-f_q)(1-f_{q'}) \\ &\quad - f_q f_{q'} (1-f_k)(1-f_{k'})] \\ &\quad + g^2 \sum_{k'} \delta(\epsilon_k - \epsilon_{k'}) [f_k (1-f_{k'}) - f_{k'} (1-f_k)] \\ &= \sum_{k'} W_{kk'} \Phi_{k'} \end{aligned} \quad (2.15)$$

where the inelastic scattering term $S_{kk'}^{qq'} = \delta(\epsilon_k + \epsilon_{k'} - \epsilon_q - \epsilon_{q'}) \delta(k + k' - q - q')$ conserves both energy and momentum. In the last line we have linearized the right hand side using the definitions of the introductory chapter. The velocity v_k is given by $v_k = \frac{d}{dk} \epsilon_k$. The scattering matrix splits up into an *interaction* component and a *disorder* component, $W_{kk'} = W_{kk'}^0 + g^2 W_{kk'}^1$. As we do not consider Umklapp scattering, $W_{kk'}^0$ conserves momentum, $\sum_{k'} W_{kk'}^0 k' = 0$, and one expects that momentum relaxation will determine the conductivity for small g .

For the numerical calculation we discretize momentum in the interval $[-\pi/2, \pi/2]$, $k_n = n\delta k = n\pi/N$ with integer n . (At the boundaries the energy is already too high to play any role in transport.) The delta function arising from energy conservation is replaced by a Gaussian of width δ . The proper thermodynamic limit can for example be obtained by choosing $\delta = 0.3/\sqrt{N}$. The numerics shows small finite size effects.

In Fig. 2.1 we compare the numerical solution of the Boltzmann equation to the single mode memory matrix calculation or, equivalently[36], to the variational bound obtained by setting $\Phi_k = k$ in Eq. (2.2)

$$\tilde{\sigma} = \frac{\left(\sum_k v_k^i k \frac{df_k^0}{d\epsilon_k} \right)^2}{\sum_{k,k'} k W_{kk'} k'} = \frac{\left(\sum_k v_k^i k \frac{df_k^0}{d\epsilon_k} \right)^2}{g^2 \sum_{k,k'} k W_{kk'}^1 k'}. \quad (2.16)$$

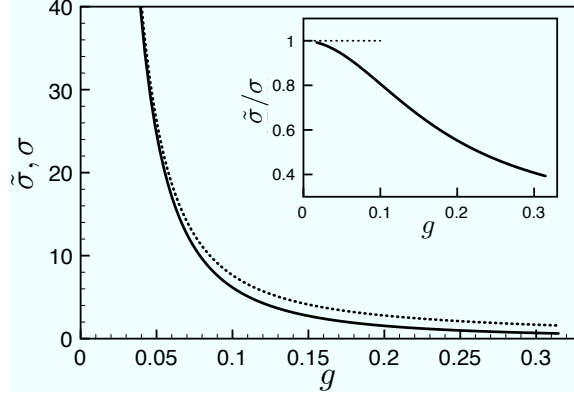


Figure 2.1: Comparison of the result of a single mode memory matrix calculation (solid line), Eq. (2.16), to the full numerical solution of the Boltzmann equation (dotted line) for $T = 0.05$ and $N = 500$. The memory matrix is always a lower bound to the Boltzmann result and converges towards it as the disorder strength g is reduced, as shown in the inset (ratio of the single mode approximation to the Boltzmann result).

As can be seen from the inset, in the limit of small g one obtains the exact value for the conductivity, which is what we intended to demonstrate.

Next we turn to an analysis of regularity conditions which have to be met in general by the scattering matrix $W_{kk'}$ such that convergence is guaranteed in the limit $g \rightarrow 0$. According to the assumptions of this section, for $g = 0$ the variational form of the Boltzmann equation (2.2) has a unique solution $\bar{\Phi}_k$ (up to a multiplicative constant), with $F(\bar{\Phi}_k) = \infty$, $\sum_{k'} W_{kk'}^0 \bar{\Phi}_{k'} = 0$ and $\sum_k v_k \bar{\Phi}_k df^0/d\epsilon_k > 0$.

In the presence of a finite, but small g we write the solution of the Boltzmann equation as $\Phi = \bar{\Phi} + \Phi^\perp$, where Φ^\perp has no component parallel to $\bar{\Phi}$ (i.e. $\sum_k \bar{\Phi}_k \Phi_k^\perp df^0/d\epsilon_k = 0$). By combining the two inequalities

$$F[\bar{\Phi}] \leq F[\Phi] \quad (2.17)$$

$$\Phi W \Phi = \bar{\Phi} g^2 W^1 \bar{\Phi} + \Phi_\perp W \Phi_\perp \geq \bar{\Phi} g^2 W^1 \bar{\Phi} \quad (2.18)$$

one concludes that Eq. (2.13) is valid, i.e. that

$$\lim_{g \rightarrow 0} \frac{F[\bar{\Phi}]}{F[\Phi]} = 1$$

under the condition that

$$\lim_{g \rightarrow 0} \sum_k v_k \bar{\Phi}_k \frac{df^0}{d\epsilon_k} = \sum_k v_k \bar{\Phi}_k \frac{df^0}{d\epsilon_k}$$

or, equivalently,

$$\lim_{g \rightarrow 0} \sum_k v_k \Phi_{\perp, k} \frac{df^0}{d\epsilon_k} = 0. \quad (2.19)$$

We therefore have to check whether Φ_{\perp} becomes small in the limit of small g .

Expanding the saddle-point equation for (2.2) we obtain

$$\begin{aligned} \sum_{k'} W_{kk'}^0 \Phi_{k'}^{\perp} &= v_k \frac{df^0}{d\epsilon_k} \frac{\sum_{k', k''} \bar{\Phi}_{k'} g^2 W_{k' k''}^1 \bar{\Phi}_{k''}}{\sum_{k'} v_{k'} \frac{df^0}{d\epsilon_{k'}} \bar{\Phi}_{k'}} \\ &\quad - \sum_{k'} g^2 W_{kk'}^1 \bar{\Phi}_{k'} + \mathcal{O}(g^2 W_1 \Phi_{\perp}, \Phi_{\perp} W_0 \Phi_{\perp}) \end{aligned}$$

As by definition Φ^{\perp} has no component parallel to $\bar{\Phi}$, we can insert the projector Q which projects out the conservation law in front of Φ_k^{\perp} on the left hand side. We therefore conclude that *if* the inverse of $W^0 Q$ exists, then Φ_{\perp} is of order g^2 , Eq. (2.19) is valid and therefore also Eq. (2.13). In our numerical examples these conditions are all met.

Under what conditions can one expect that Eq. (2.19) is not valid? Within the assumptions of this section we have excluded the presence of other zero modes of W^0 (i.e. conservation laws) with finite overlap with the current. But it may happen that W^0 has many eigenvalues which are arbitrarily small such that the sum in Eq. (2.19) diverges. In such a situation the presence of slow modes which cannot be identified with conservation laws of the unperturbed system invalidates Eq. (2.13).

Chapter 3

Transport in Almost Integrable Spin Chains

The heat conductivity $\kappa(T)$ of the integrable one-dimensional spin-1/2 nearest-neighbor Heisenberg model, is infinite even at finite temperatures as a consequence of the conservation laws associated with integrability. Small perturbations lead to finite but large transport coefficients which we calculate perturbatively using exact diagonalization and moment expansions. We show that there are two different classes of perturbations. While an inter-chain coupling of strength J_{\perp} leads to $\kappa(T) \propto 1/J_{\perp}^2$ as expected from simple golden-rule arguments, we obtain a much larger $\kappa(T) \propto 1/J'^4$ for a weak next-nearest-neighbor interaction J' . This can be explained by a new approximate conservation law of the J - J' Heisenberg chain.

Similarly, the spin conductivity $\sigma_s(T)$ in the gap-less regime (i.e. for anisotropies $-1 < \Delta < 1$) of the XXZ model, too, is infinite at finite temperatures T . Nevertheless there is a fundamental difference between the two cases. While the heat current is one of the integrals of motion of the XXZ model, the spin current can easily be shown to have no overlap with any of the infinitely many integrals of motion, implying that the conserved currents protecting the spin current have to be of non-local nature¹. We construct numerically a non-local conserved operator J_{\parallel} which is responsible for the finite spin Drude weight of the integrable model and calculate its decay rate for small J' . This allows us to obtain a lower bound for the spin conductivity $\sigma_s \geq c(T)/J'^2$, where, despite the conceptual difference of the spin current as opposed to the heat current, $c(T)$ is also finite for $J' \rightarrow 0$. We discuss the implication of our result for the general question how non-local conservation laws affect transport properties.

The outline of the chapter is as follows. First we will give a motivation for our analysis. Then several technical sections follow in which we develop

¹For examples of non-local operators, see the section about the spin current, 3.6.

the model and comment on the numerical methods we use. These sections cope with material common to both pieces of work. The final two sections in this chapter are devoted to a presentation of the results for the heat and the spin conductivity, respectively. Both pieces of analysis use the result from the last chapter and therefore they are devoted to the calculation of the ‘scattering rate’ $\tilde{\Gamma}(\omega)$ for different situations. The results are discussed at the end of each of these sections.

3.1 Motivation

The thermodynamic properties of many experimental systems (like, e.g., KCuF_3 , CuGeO_3 , $\text{MEM}[\text{TCNQ}]_2$, SrCuO_2 or Sr_2CuO_3) are well described by a one-dimensional (1D) nearest-neighbor spin-1/2 Heisenberg model [39]. In such systems, measurements of specific heat or susceptibilities are in quantitative agreement with exact results derived from the Bethe ansatz.

The situation is different when transport is considered. The transport properties of the XXZ Heisenberg chains, which is equivalent to a model of spinless Fermions with nearest neighbor interactions, has been studied extensively both theoretically [40, 41, 26, 42, 43, 44, 6, 19, 5, 3] and experimentally [45, 46, 47, 38, 9]. In theory, both the heat conductivity κ and the spin conductivity σ_s (or, equivalently, the electric conductivity in the Fermionic language) are infinite and have a finite Drude weight at any temperature [44].

In real materials the unavoidable presence of (small) perturbations like longer range spin-spin interactions, inter-chain couplings, disorder or spin-phonon interactions, breaks the integrability and renders the conductivities finite. This has to be contrasted with the behavior of thermodynamic quantities and most other correlation functions which—at least for finite temperatures—vary smoothly as a function of small perturbations (assuming that no phase transitions are induced). Obviously the general question arises of how transport can be calculated in “almost integrable models”, i.e., how strongly is the transport affected by small couplings which break the integrability.

When the perturbations are small, the heat conductivity is known to remain very large [18, 35, 48, 4]. This is reflected in experiments which show a huge contribution to the heat conductivity from the spin chain component of the system. In contrast, no experimental data is available for the spin conductivity and there are good reasons to expect that the situation might be quite different in this case, see the section about non-local conservation laws below.

The question, how transport is affected by small integrability breaking perturbations, is not only important for systems well described by integrable

Heisenberg or Hubbard models but is also of relevance for a much broader class of quasi-1D materials. The reason is that effective low-energy theories in 1D are notoriously integrable. For example, an arbitrarily complicated two-leg spin-ladder is, at low energies, well described by an integrable Sine-Gordon model as long as the energy gap Δ_E is much smaller than microscopic energy scales like J . The term “well-described” implies again that the integrable model can be used for an accurate description of thermodynamics. To understand transport, however, one has to study again the effects of *small* perturbation (suppressed by powers of Δ_E/J) on transport.

A further reason for our investigations is the general theoretical question of how singular are integrable models and how are they affected by perturbations. The analog question is well studied in classical systems with small numbers of degrees of freedom, c.f. the famous Kol'mogorov-Arnol'd-Moser theorem [49]. But already infinitesimal perturbations of classical systems with an *infinite* number of degrees of freedom may drive the system into chaotic behavior, and not much is known about many-particle quantum systems.

3.2 The XXZ Model and its Currents

Here we will introduce the Hamiltonian that will be worked with in this section. The unperturbed model H_0 is the XXZ Heisenberg spin chain with nearest-neighbor coupling only.

$$H_0 = \sum_i h_i, \quad (3.1)$$

$$h_i = J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) \quad (3.2)$$

Perturbations will include the next-nearest neighbor coupling

$$H_1 = \sum_i h'_i, \quad (3.3)$$

$$h'_i = J'(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta' S_i^z S_{i+2}^z) \quad (3.4)$$

and the (isotropic) coupling between chains,

$$\tilde{H}_1 = \sum_i h_i^\perp, \quad (3.5)$$

$$h_i^\perp = J_\perp \sum_{\langle \alpha\beta \rangle} \mathbf{S}_i^\alpha \cdot \mathbf{S}_i^\beta \quad (3.6)$$

where $\mathbf{S} = (S^x, S^y, S^z)^T$. To maintain consistency with our earlier notation we will sometimes use a slightly different normalization for the perturbation: Defining the coupling parameter $g = J'/J \ll 1$ or $g = J_\perp/J \ll 1$ we then

maintain the form $H = H_0 + gH_1$ and then it is understood that in Eqs. (3.3) and (3.5) the coupling constants should be replaced by J . This should be sufficient for confusion.

The reader not familiar with the used symbols may consult the pedagogical appendix on spin operators B.1 at this point.

Next, let us elaborate on relevant properties of the XXZ chain. The XXZ Heisenberg chain is integrable as it is solvable by the Bethe Ansatz method [50]. This means that analytic expressions for the wave functions of the XXZ model are known in terms of integro-differential equations. A consequence of integrability is the existence of an infinite set of integrals of the motion, which have been given in explicit form by Grabowski and Mathieu [40, 51]. These constants of the motion constitute a complete set of commuting operators, Q_n with $[Q_n, Q_m] = 0$ for all n, m . In principle, their eigenvalues can be used to label all eigenstates of the system. Let us consider the Q_n more closely. The first of these conserved quantities is also the simplest one, namely the z-component of the total spin, $Q_1 = \sum_i S_i^z$. All other Q_n can be constructed by a simple recursive formula [40], $Q_{n+1} = [B, Q_n]$ with the so-called boost operator $B = 1/(2i) \sum_j j h_j$. For example, a single application of the boost operator on Q_0 yields the Hamiltonian itself,

$$H_0 = Q_2 = \sum_i h_i, \quad (3.7)$$

$$h_i = J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \quad (3.8)$$

and the next step in the hierarchy yields the energy current operator, which for the isotropic case $\Delta = 1$ may simply be written as a triple product:

$$J_Q = Q_3 = J^2 \sum_i \mathbf{S}_i \cdot (\mathbf{S}_{i+1} \times \mathbf{S}_{i+2}). \quad (3.9)$$

All these conservation laws have a property which will become important for the discussion about non-local operators: the Q_n are *local* operators in the sense that each Q_n can be written in terms of a local ‘‘density’’ $q_{n,i}$ at site i ,

$$Q_n = \sum_i q_{n,i}, \quad (3.10)$$

where $q_{n,i}$ is local as it contains only spin operators S_j^α on maximally n adjacent sites, $i \leq j < i+n$. The current associated with a locally conserved density (c.f. any of the Q_n) can be obtained from the continuity equation $\partial_t \rho(x) + \nabla j(x) = 0$, which in its discrete form (setting the lattice spacing to unity, $a = 1$) reads

$$i[H_0, q_{n,i}] = j_{n,i} - j_{n,i+1}. \quad (3.11)$$

This equation can readily be solved for $j_{n,i}$ and yields for the spin current

$$J_s = \frac{i}{2} \sum_i j_{2,i} = \sum_i (S_i^- S_{i+1}^+ - S_i^+ S_{i+1}^-) \quad (3.12)$$

and for the heat (or energy) current $J_Q = Q_3$, i.e. Eq. (3.9), respectively. (As there is no convective flow in the spin chain, heat and energy current are the same.)

3.3 Exact Diagonalization

A common method to evaluate correlation functions numerically is referred to as ‘exact diagonalization’ and will be described in the following. The method uses the matrix elements of the appearing operators in an eigenbasis of the Hamiltonian. Therefore one diagonalizes the Hamiltonian numerically and transforms the operators to the eigenbasis. If the matrix elements are known, one can use the spectral (or Lehmann) representation, in terms of which correlation functions are given by a sum over the matrix elements. E.g. for $\beta\omega \ll 1$ (i.e. in the high temperature or the low frequency limit) the conductivity may be written as follows:

$$\text{Re } \sigma(\omega) = \frac{\pi\beta}{V\mathcal{Z}} \sum_{mn} e^{-\beta E_m} |\langle m|J|n\rangle|^2 \delta(\omega - (E_n - E_m)), \quad (3.13)$$

where $\mathcal{Z} = \sum_m e^{-\beta E_m}$ is the partition sum. Of course, an exact diagonalization of the Hamiltonian can be achieved for finite system sizes only. Therefore the correlation function is given as a set of delta functions of frequency scattered over the real axis, each coming with a weight determined by the matrix elements of J . It is only in the limit of infinite system size (the thermodynamic limit) that the correlation function becomes a smooth function of frequency. Under the assumption that the thermodynamic limit is approached continuously as one increases system size, one can attempt to draw a histogram for the finite size correlation function which shall be an approximation to the real correlation function in the thermodynamic limit. This can be achieved by means of a technique referred to as ‘binning’. It consists of a subdivision of the real axis into a number of equal intervals and summing the weights of the delta peaks lying within each interval. The resulting histogram is the approximation to the real correlation function. The intervals (or bins) should be large enough to contain a number of delta peaks which can be considered as macroscopic, but should be small enough to obtain a histogram which on a scale dictated by the coupling constants can be considered as continuous. These two criteria² are competing and can

²Here we have formulated the criteria in a rather qualitative fashion. Although possible in several ways, a quantification of the methods is not necessary in the cases discussed

be met to a higher degree when one increases the system size. Thus it is desirable to calculate the correlation functions for large systems. However, the calculational effort of the diagonalization grows exponentially with system size as the number of states in a chain of length N is given by 2^N . In our case, this limits the number of spins in the chain that are amenable to exact diagonalization to $N = 20$.

To make statements about the thermodynamic limit, it is necessary to assure oneself of the fact that finite size effects are small and can be neglected. Thus it is necessary to compare curves obtained for different system sizes. If the difference between the histograms for systems of size N with adjacent N decreases sufficiently to make possible an extrapolation to $N = \infty$, then one usually concludes that finite size effects are negligible.

The last consideration also affects our argument about the numerical cost. While the effort grows exponentially with system size, the information gain by increasing the system size by one or two often decreases quickly. In fact, often systems with $N = 16$ already reproduce most features of the correlation function quite reliably. A further increase of the parameter N then often happens out of sportsmanship. There are, however, situations where genuinely new information can be gained from considering, say, $N = 18$, because it clearly shows distinct features the identification of which is not possible for $N = 16$ due to poor statistics.

As the exact diagonalization technique is quite common, we do not discuss it beyond the qualitative description above, and restrict ourselves to briefly discuss implementation details which are specific to our situation of the XXZ Heisenberg model, instead.

To avoid open boundaries we choose periodic boundary conditions. The thermodynamic limit would be the same with both approaches, but periodic boundary conditions have the additional advantage of higher symmetry, which allows to reduce the dimension of the matrices which have to be diagonalized. The drawback of periodic boundary conditions is that not all temperature regimes are accessible. For $T \ll J$ correlations decay algebraically with distance only [52] and thus large finite size effects can be expected for this regime. One is thus restricted to the high temperature regime $T \gtrsim J$, where correlation functions decay exponentially. All our calculations are performed in the high temperature limit, $T \rightarrow \infty$, where the correlation length vanishes. The results presented here are, however, qualitatively the same for finite $T \gtrsim J$. The advantage of the limit $T \rightarrow \infty$ is that the statistics provided by the calculated correlation functions is best: All delta peaks are equally weighted.

The numerically most expensive step is actually the diagonalization of

here. In our simple implementation we keep the number of bins constant (equal to 1023) across different system sizes, which proves to be sufficient for our purpose.

huge matrices. What is achievable on modern computers available to us (both from memory and time standpoint) are matrices up to a size of $10\,000 \times 10\,000$. If we would attempt to diagonalize the full Hamiltonian directly, this would limit the accessible system size to $N = 13$, as the size of the Hamiltonian matrix is given by the number of states in the system, $2^{13} = 8\,192 \lesssim 10\,000$. However, the Hamiltonian preserves the z-component of the total spin, $S^z = \sum_i S_i^z$, and thus the Hamiltonian is block-diagonal with respect to S^z . One thus can diagonalize in subspaces of the Hilbert space with given spin- S^z eigenvalue. This already would allow us to diagonalize system sizes up to $N = 15$ or $N = 16$, as the dimension of the largest subspace (i.e. the one with the smallest $|S^z|$) is given by $\binom{N}{\lfloor N/2 \rfloor}$ and we have $\binom{15}{7} = 6\,435$ and $\binom{16}{8} = 12\,870$. However, it is possible to reduce the dimension of the matrices necessary to diagonalize further by taking into account one more ‘good’ quantum number, and the most straightforward one is provided by the translation operator T . The translation operator ‘rotates’ a state by one site to the right,

$$T|\uparrow\uparrow\uparrow\downarrow\downarrow\rangle = |\downarrow\uparrow\uparrow\downarrow\downarrow\rangle. \quad (3.14)$$

For a system with N sites one has the identity $T^N = 1$. Furthermore, $T^{-1}T = 1$ and considering the action of T^{-1} to the left it is clear that T is unitary, $T^{-1} = T^\dagger$. Given an arbitrary state $|\psi\rangle$, we can construct eigenstates of the translation operator

$$|\psi\rangle \rightarrow |k\rangle_\psi = \sum_{n=1}^N e^{-2\pi i \frac{k}{N} n} T^n |\psi\rangle \quad (3.15)$$

with

$$T|k\rangle_\psi = e^{2\pi i \frac{k}{N}} |k\rangle_\psi. \quad (3.16)$$

Thus k is the (lattice) momentum of state $|k\rangle_\psi$ (as momentum generates translations) and it can take N distinct values. If we go to a common eigenbasis of S^z and T , the dimension of the largest matrix to be diagonalized for given N is roughly³ equal to $\frac{1}{N} \binom{N}{\lfloor N/2 \rfloor}$ which allows us to go to system sizes up to $N = 20$, as $\frac{1}{20} \binom{20}{10} \lesssim 10\,000$. System sizes above $N = 16$ show already a respectable statistics and comparison with systems up to size $N = 20$ can give an accurate estimate of the appearing finite size effects.

The recipe for obtaining the desired correlation functions is then as follows. First, determine the Hamiltonian, and all terms appearing in the correlation function, in a subspace of the Hilbert space with given S^z and T

³Not from every state can one construct eigenstates of T with given momentum k : For example take the state $|\psi\rangle = |\uparrow\downarrow\uparrow\downarrow\rangle$ for $N = 4$, for which no states with $k = 1$ and $k = 3$ exist.

eigenvalues. Each of the subspaces can be treated separately. This includes calculation of each matrix element. To produce the numerical data presented below, this step has been implemented in the programming language “c”. As a next step we have to diagonalize the Hamiltonian matrix. This can be achieved most efficiently with existing diagonalization routines. We have used the so-called LAPACK library. Diagonalization provides us with the eigenvalues and the eigenvectors of the Hamiltonian. In the third step, one transforms the other operators into the just obtained eigenbasis of the Hamiltonian. The transformation matrix is given by the eigenvectors. The correlation function now can be calculated from its spectral representation. In this final step the binning is applied which was described above.

3.4 Frequency Moments Reconstruction

The reconstruction of a frequency dependent correlation function from its moments is an alternative to exact diagonalization. It provides us with an independent method for the approximate determination of a correlation function, which allows to cross-check the results. We have used this method solely in the context of heat conductivity in the isotropic Heisenberg spin chain with next nearest neighbor perturbation, see section 3.5. In fact, we have utilized this method prior to using the exact diagonalization technique because we expected large finite size effects from exact diagonalization, based on exact diagonalization studies [53] for the heat conductivity itself, which close to the integrable point showed considerable finite size effects. However, those effects are connected to the singular properties of the conductivity and it turns out that these finite size effects are absent for the type of correlation functions we are interested in, namely approximations to the memory matrix. In the following we will describe the method of frequency moments.

The basis of the method is the observation that the frequency moments appear as coefficients in a high frequency expansion of the correlation function:

$$\chi^R(z) = \mathcal{P} \int \frac{d\omega}{\pi} \frac{\chi^C(\omega)}{\omega - z} \quad (3.17)$$

$$= - \sum_{p=1}^{\infty} \frac{1}{z^p} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^p \frac{\chi^C(\omega)}{\omega} \quad (3.18)$$

$$\equiv - \sum_{p=1}^{\infty} \frac{1}{z^p} \mu_p \quad (3.19)$$

where we introduced the p th frequency moment of the correlation function

$\chi(\omega)$ (defined as in appendix A.2) which reads

$$\mu_p \equiv \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^p \frac{\chi^C(\omega)}{\omega}. \quad (3.20)$$

By partial integration one directly obtains that

$$\mu_p = \langle [(id/dt)^p J(t), J(0)] \rangle|_{t=0} \quad (3.21)$$

$$= \langle [\dots \underbrace{[[J, H], H] \dots}_{p \times}, J] \rangle. \quad (3.22)$$

Thus the frequency moments can be obtained from equal-time commutators. Therefore, the moments are often easier to calculate than the correlation function itself. While we have determined the moments of $\chi^R(\omega)$, we are rather interested in the moments of the scattering rate $\tilde{\Gamma}(\omega)$. Fortunately, it turns out that both quantities have the same moments to leading order in g . This can be seen as follows. In the expression for the regular part of the conductivity (1.13), the imaginary part of $\chi^R(0)$ vanishes and therefore all (but the first, which would include the Drude weight) moments of the real part of the conductivity are given by the imaginary part of moments of $\chi^R(\omega)$. Furthermore, in leading order in g we have equation (2.4), which tells us that moments of the conductivity are also moments of the memory matrix. We can write

$$\int \frac{d\omega}{\pi} \omega^p \text{Re } \tilde{\Gamma}(\omega) = \text{Im } \mu_{p+1}. \quad (3.23)$$

The moments can be calculated rather straightforwardly in the high temperature limit $T \rightarrow \infty$. In appendix B.3 we give implementation details on the calculation of the moments. We have succeeded to calculate the first 14 non-vanishing moments for $\tilde{\Gamma}(\omega)$. Choosing periodic boundary conditions, one would need a system of at least 30 sites to reproduce these moments from exact diagonalization.

As soon as the moments are known, one can attempt to reconstruct the scattering rate using different methods. This part of the task is less straightforward and may involve different subtleties, depending on the method used. Since we are interested in the low frequency limit, it is useless to insert the moments into the expansion (3.19) and one has to resort to methods which attempt to reconstruct the behavior in the vicinity of $\omega = 0$. We have tried three different methods, namely a continued fraction expansion, the Nickel method [54, 55], and the maximum entropy method [56]. Each of these algorithms has its own advantages and disadvantages and each of them delivers different reconstructions of $\tilde{\Gamma}(\omega)$. We have found the maximum entropy to be the most useful in our case (see Fig. 3.5). This method finds the most probable of all curves which have the given moments, assuming that nothing

else is known about the curve. This is achieved by maximizing the entropy functional $-\int f(\omega) \ln f(\omega) d\omega$ among the set of all curves with the given moments. By using curves reconstructed from different numbers of moments, one can then extrapolate the number of moments to infinity. Doing so for the point $\tilde{\Gamma}(\omega = 0)$ one obtains an estimate for the lower bound to the conductivity.

We have used the frequency moments reconstruction method only in the case of the heat conductivity in the isotropic Heisenberg chain with weak next nearest neighbor coupling. As outlined below, we find that exact diagonalization gives more reliable results and less finite size effects using a more straightforward method. Thus for all other calculations only exact diagonalization is used.

3.5 Heat Conductivity

In this section we present numerical results for the leading order contribution to the scattering rate of heat current

$$g^2\Gamma_2(\omega) = \tilde{\Gamma}(\omega) = \frac{\beta}{V} \frac{1}{\omega} \int_0^\infty dt e^{i\omega t} \langle [J_Q(t), J_Q(0)] \rangle_0 \quad (3.24)$$

(compare Eqs. (2.5,2.6) and the discussion at the end of 2.4) in the XXZ model with next-nearest neighbor and inter-chain coupling (see section 3.2) obtained via exact diagonalization and frequency moments reconstruction. According to the last chapter this provides a rigorous lower bound to the heat conductivity $\kappa(\omega = 0)$, see Eq. (2.8). In the case of the isotropic spin chain and next nearest neighbor (nnn) perturbation we also evaluate higher order contributions $g^3\Gamma_3(\omega)$ and $g^4\Gamma_4(\omega)$ to the scattering rate. Expressions for the higher order contributions are derived in appendix B.4.

The real heat current in the perturbed system has a contribution $\propto J'$, (i.e. $J_Q = J_0 + gJ_1$) as the continuity equation has to be solved with the new energy density, also containing a term $\propto J'$. Therefore, the operator \dot{J}_Q appearing in equation (3.24) contains two contributions which are linear in J' , $\dot{J}_Q = ig[H_0, J_1] + ig[H_1, J_0]$. However, the last chapter suggests to use only the exact conservation laws of the unperturbed Hamiltonian as slow modes in the memory matrix. In fact, it is easy to see that terms that are coming with a commutator with the unperturbed Hamiltonian (here $ig[H_0, J_1]$) do not contribute to the scattering rate at $\omega = 0$: As the correlation function is evaluated with respect to H_0 , any such term can be integrated by parts and makes a contribution proportional to ω . The calculations presented in this chapter, nevertheless, include that irrelevant additional term which alters the results at $\omega \neq 0$ only. The reason for this is the lack of awareness about

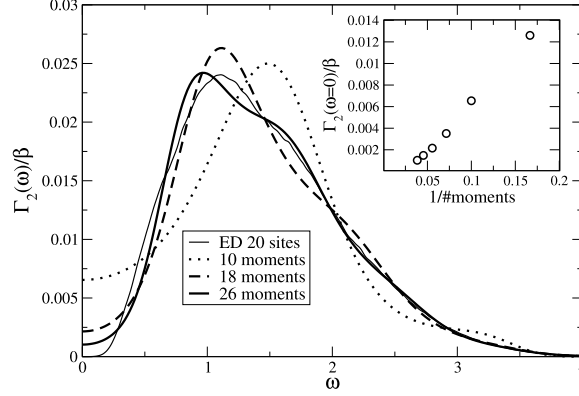


Figure 3.1: Leading order contribution to the scattering rate $\Gamma(\omega)$ from exact diagonalization of a 20-site Heisenberg chain (thin solid line) with weak nnn coupling J' (at $T = \infty$). To this order the scattering rate vanishes at $\omega = 0$, implying anomalous transport. The same result is obtained if $\Gamma_2(\omega)$ is reconstructed from N moments ($N = 10\dots 26$) using the maximum entropy method. The inset shows that $\Gamma_2(\omega = 0) \rightarrow 0$ for $N \rightarrow \infty$.

the irrelevance of these contributions at the date of accomplishment⁴. For completeness we give the form of the heat current we use in our calculations. In the continuity equation we use a symmetrized version of the h_i ,

$$h_i = \frac{J}{2} \sum_{\alpha} (\mathbf{S}_{i-1}^{\alpha} \cdot \mathbf{S}_i^{\alpha} + \mathbf{S}_i^{\alpha} \cdot \mathbf{S}_{i+1}^{\alpha}) + 2g' \mathbf{S}_{i-1}^{\alpha} \cdot \mathbf{S}_{i+1}^{\alpha} + 2g_{\perp} \sum_{\langle \alpha \beta \rangle} \mathbf{S}_i^{\alpha} \cdot \mathbf{S}_i^{\beta}$$

which, for the isotropic case $\Delta = \Delta' = 1$ leads to the following expression for the heat current $J_Q = \sum_i j_i$:

$$j_i = \frac{J^2}{2} \sum_{\alpha} \left[2\mathbf{S}_{i-1}^{\alpha} \cdot (\mathbf{S}_i^{\alpha} \times \mathbf{S}_{i+1}^{\alpha}) + g'(3\mathbf{S}_{i-2}^{\alpha} - 4\mathbf{S}_i^{\alpha} + 3\mathbf{S}_{i+2}^{\alpha}) \cdot (\mathbf{S}_{i-1}^{\alpha} \times \mathbf{S}_{i+1}^{\alpha}) + g_{\perp} \sum_{\langle \alpha \beta \rangle} (\mathbf{S}_{i-1}^{\alpha} - \mathbf{S}_{i+1}^{\alpha}) \cdot (\mathbf{S}_i^{\alpha} \times \mathbf{S}_i^{\beta}) \right] + \mathcal{O}(g'^2).$$

Next we present the results.

⁴As an aside we note that J_1 is not even uniquely defined and the results for $\tilde{\Gamma}(\omega)$ for $\omega \neq 0$ also depend on the choice of J_1 . The reason is that the definition of the Hamiltonian density is not unique, $H = \sum_i h_i = \sum_i \tilde{h}_i$, and different choices of h_i lead to different results for J_1 . While dynamic correlation functions depend on this gauge freedom, static susceptibilities at $\omega = 0$ are independent.

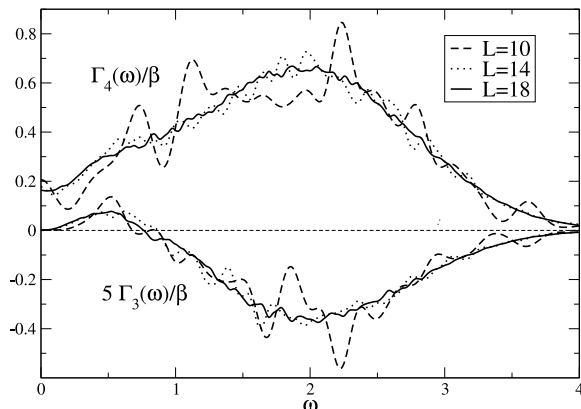


Figure 3.2: Third and fourth order contributions to the scattering rate for various system sizes (see Fig. 3.1), the first non-vanishing contribution being of order g^4 . Note that finite-size effects are small.

First, we consider the isotropic ($\Delta = 1$) Heisenberg spin chain with a weak and isotropic ($\Delta' = 1$) nnn coupling. Figure 3.1 shows the leading order contribution $\Gamma_2(\omega)$ to the scattering rate determined from an evaluation of Eq. (3.24) for large T using exact diagonalization. As similar physical quantities (at large T) have been reported [53] to show surprisingly large finite size effects (not observed in our case) we have also reconstructed Γ_2 from an analytic calculation of its first 26 moments, $\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \Gamma_2(\omega) = \langle [\partial_t^{n-1} J_Q, J_Q] \rangle$, using a high-temperature expansion for an infinite system. We have used various methods to obtain $\Gamma_2(\omega = 0)$ from these moments, as described in section 3.4. Although the curves of the reconstructed $\tilde{\Gamma}(0)$ over the number of moments $1/N$ differ depending on which method is used for reconstruction, all methods consistently show that $\Gamma_2(\omega \rightarrow 0)$ vanishes. (For results from maximum entropy reconstruction, see the inset in Fig. 3.1.) Our exact diagonalization results also show that this is not an artifact of the $T \rightarrow \infty$ limit as the limit is, contrary to our expectations, smooth (see, e.g., Fig. 3.2).

We would like to emphasize that the vanishing of the scattering rate $\Gamma(0)$ to lowest order is very surprising both formally and physically. Formally, one would expect that any “generic” correlation function of type (3.24) has a finite $\omega = 0$ limit at any finite temperature. Physically, golden-rule arguments suggest that the breaking of integrability leads to a decay rate of the heat current of order J^2 . In the following, we will first investigate the role of higher order corrections and then the influence of other terms which break integrability.

Corrections to Γ up to order J^4 are derived starting from Eq. (2.4), where our lowest order result, Γ_2 , is used to determine the term of order Γ^2 . The $\partial_t J_Q - \partial_t J_Q$ correlation function is then evaluated to order J^3 and J^4

using the wave functions and energies obtained from the exact diagonalization of H_0 . The contributions to orders J^3 and J^4 are given in Appendix B.4 and the results are shown in Fig. 3.2. Since $\text{Re } \Gamma(\omega)$ has to be positive and $\Gamma_2(0) = 0$, it is not surprising that $\Gamma_3(0)$ also vanishes. $\Gamma_4(0)$, however, is clearly finite. We therefore conclude that the heat conductivity in the limit $J' \rightarrow 0$, $\Delta = \Delta' = 1$, has the form

$$\kappa \approx \frac{J^7}{T^2 J^4 f(T/J)} \approx \frac{0.054(1) J^7}{T^2 J^4} \quad \text{for } T \rightarrow \infty, \quad (3.25)$$

where f is an (unknown) function of T/J only, with $f(x \rightarrow \infty) \approx 18.5$ estimated from our exact diagonalization results shown in Fig. 3.2. Together with the analytical explanation given below this is the main result of this section.

3.5.1 Readjusted Conservation Law

We start with the observation that the time derivative of the heat current is linear in g as $[H_0 + gH_1, J_Q] = \mathcal{O}(g)$. How can the naive golden-rule argument which suggests a decay rate proportional to g^2 fail? This can happen if the presence of slow modes modifies the long-time behavior of the $\partial_t J_Q$ correlation function as discussed, e.g. in [35, 4, 57]. We therefore try to construct a new slow mode of the perturbed system $H_0 + gH_1$ starting from the conserved heat current J_0 of the integrable model H_0 . Hence, we seek a solution \tilde{J}_1 to the equation

$$[H_0 + gH_1, J_0 + g\tilde{J}_1] = \mathcal{O}(g^2). \quad (3.26)$$

As $[H_0, J_0] = 0$, we have to construct a \tilde{J}_1 with

$$[H_0, \tilde{J}_1] = -[H_1, J_0]. \quad (3.27)$$

While we will use this equation for the following analysis, it is desirable to obtain a better understanding of what it actually tells us. We choose a common eigenbasis of H_0 and J_0 for the Hilbert space, i.e. a basis in which $H_0 = \sum_n E_n |n\rangle\langle n|$ and $J_0 = \sum_n J_n |n\rangle\langle n|$. In this basis, Eq. (3.27) reads

$$(E_n - E_m) \langle n | \tilde{J}_1 | m \rangle = (J_m - J_n) \langle n | H_1 | m \rangle. \quad (3.28)$$

This equation is trivial to solve for $\langle n | \tilde{J}_1 | m \rangle$ if $E_n \neq E_m$. However, considering an energy-diagonal block, $E_n = E_m$, a solution to $\langle n | \tilde{J}_1 | m \rangle$ can only exist provided that either $J_n = J_m$ or $\langle n | H_1 | m \rangle = 0$. Therefore, the existence of a solution to Eq. (3.27) can exist iff the perturbation H_1 does *not* have matrix elements connecting states $|n\rangle$ and $|m\rangle$ of the same energy and of different values of the current J_0 . In fact, the dc-conductivity, as

the $\omega \rightarrow 0$ limit of a current-current correlation function, only involves the energy-diagonal blocks of the current operators, and, in leading order in g , only the energy-diagonal blocks of the perturbation H_1 can contribute to the scattering rate at $\omega = 0$. Only those matrix elements of H_1 can lead to a degradation of the current which connect states with different values of the current, $J_n \neq J_m$, and other matrix elements contribute only to higher order in g . The existence of \tilde{J}_1 therefore implies a vanishing of the approximate memory matrix, Eq. (3.24), at $\omega = 0$. This also can be seen more formally: With $J_Q = J_0 + gJ_1$ we find

$$-i\dot{J}_Q = [gH_1, J_0] + [H_0, gJ_1] + \mathcal{O}(g^2), \quad (3.29)$$

$$= g[H_0, J_1 - \tilde{J}_1] + \mathcal{O}(g^2). \quad (3.30)$$

As a consequence, the leading order contribution $\Gamma_2(\omega)$ to the scattering rate—by partial integration—may be written as $\Gamma_2(\omega) = \omega^2 A(\omega)$, where $A(\omega)$ is the $(J_1 - \tilde{J}_1)$ self correlator in the unperturbed system. We therefore conclude that $\kappa(\omega = 0)$ diverges at least as $1/g^4$ if \tilde{J}_1 exists. This trick of studying “readjusted” approximate conservation laws may well be useful for many other systems with slow modes.

We turn our attention to relation (3.27). To find a solution \tilde{J}_1 we make the most general ansatz for it. \tilde{J}_1 is a translationally invariant operator of finite range consisting of a linear combination of products of spin operators. By inserting the ansatz into Eq. (3.27) we obtain a system of linear equations for the unknown coefficients. This overdetermined system of equations turns out to have a solution in the case of an isotropic ($\Delta' = 1$) nnn perturbation of the Heisenberg model with

$$\tilde{J}_1 = -g'J^2 \sum_i (\mathbf{S}_{i+1} + \mathbf{S}_{i+2}) \cdot (\mathbf{S}_i \times \mathbf{S}_{i+3}). \quad (3.31)$$

The explicit construction of \tilde{J}_1 proves the absence of a J'^2 contribution to the scattering rate as discussed above. Note that it is not possible to construct a \tilde{J}_1 such that the commutator in Eq. (3.26) is of order g^3 rather than g^2 . Therefore the presented readjustment procedure cannot be generalized to higher orders.

While (3.31) can easily be generalized to the case of an anisotropic XXZ chain with $\Delta \neq 1$, no solution for \tilde{J}_1 exists in the case of an anisotropic nnn perturbation with $\Delta' \neq 1$. We therefore expect (and confirm numerically) that in the limit of small J' and small but finite $(\Delta' - 1)$

$$\kappa \approx \frac{J^5/T^2}{J'^2(1 - \Delta')^2 h(T/J)} \approx \frac{0.21(2) J^5/T^2}{J'^2(1 - \Delta')^2} \text{ for } T \rightarrow \infty, \quad (3.32)$$

where h is an (unknown) function of T/J only, the value of which we can determine from the results shown in Fig. 3.3 in the limit $T \rightarrow \infty$. This

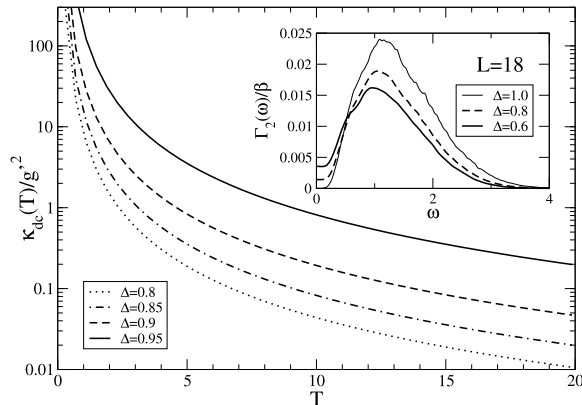


Figure 3.3: Calculated heat conductivity of the anisotropic frustrated chain as a function of temperature for various anisotropies $\Delta = \Delta'$. Inset: leading order contribution to the scattering rate for the isotropic case (thin solid line) as well as with weak anisotropies for $T \rightarrow \infty$.

figure also shows the T dependence of κ for $T \gtrsim J$ where we use Eq. (2.6) and χ is calculated to order g^0 using exact diagonalization. Large finite size corrections prohibit calculations for $T \ll J$ within exact diagonalization.

In many experimental systems we expect that the leading term which breaks integrability arises from a weak coupling J_{\perp} between chains (or spin-phonon interactions [4] or impurities) but not from nnn-coupling. For this perturbation, Eq. (3.31) has no solution, and $\kappa \sim 1/J_{\perp}^2$ can be evaluated at high temperatures from Eq. (3.24) using exact diagonalization, see Fig. 3.4. Our value for the ladder in the limit $J_{\perp} \rightarrow 0$, $\kappa \approx 0.18J^5/(J_{\perp}^2T^2)$, seems to be consistent with results of Zotos [58] obtained for finite J_{\perp} using Lanczos diagonalization.⁵

3.5.2 Conclusion

To summarize, we have analyzed the heat transport in spin chains near the integrable point. In the presence of a small next-nearest neighbor coupling J' , which breaks integrability, one can construct a new approximate conservation law. As a result, the heat conductivity remains extremely high, $\kappa \sim 1/J'^4$. For other perturbations like a weak inter-chain coupling J_{\perp} this construction is not possible and $\kappa \sim 1/J_{\perp}^2$. Thereby we have shown that

⁵There is a systematic deviation between our result and Zotos' result of a few percent. This can be traced back to the fact that Zotos uses the $S^z = 0$ block of the Hamiltonian only while we calculate the grand canonical ensemble and sum over all values of S^z . As the two ensembles are equivalent when $N \rightarrow \infty$, we identify the deviation as a finite size effect.

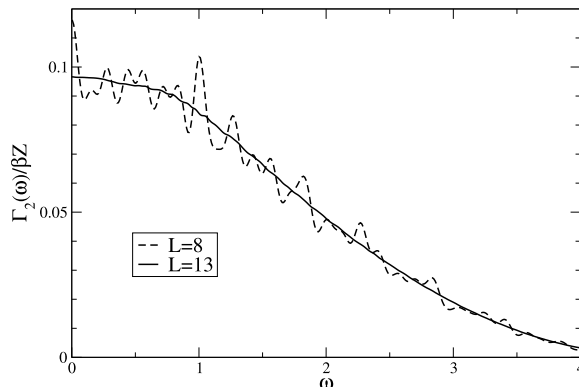


Figure 3.4: Leading order (in J_{\perp}/J) contribution to the scattering rate of weakly coupled spin chains for $T \rightarrow \infty$. The finite value at $\omega = 0$ leads to a conductivity $\kappa \approx 0.091(3)J^5/(ZJ_{\perp}^2T^2)$ per chain where Z is the number of nearest-neighbor chains.

transport in “almost integrable models” depends not only quantitatively, but also qualitatively on the precise way how integrability is destroyed. It would be interesting to study experimentally systems in which the strength of J' and J_{\perp} can be varied systematically, e.g., by chemical substitutions or by pressure.

3.6 Non-Local Conservation Laws and Spin Conductivity

This section is devoted to the study of the spin conductivity in the perturbed XXZ Heisenberg model. As anticipated in the introduction to this chapter, the situation is conceptually different from the heat conductivity. The spin conductivity is infinite in the gap-less regime $-1 < \Delta < 1$ and is characterized by a finite Drude weight $D(T) > 0$ as is observed both numerically (by exact diagonalization) and analytically (via Bethe Ansatz) [42, 43, 59]. However, the spin current has no overlap with any of the constants of the motion which are present due to integrability, $\langle J_s Q_n \rangle = 0$, as can be shown by simple symmetry arguments⁶ (also see [43]) and therefore do not contribute to the Drude weight. As outlined above, these constants of the motion are local quantities (see the discussion at the end of section 3.2), and in fact they are the *only* known operators that are both conserved *and* local (in the sense defined above). Thus, the current must be protected

⁶ J_s changes sign under spin reversal ($S^z \rightarrow -S^z, S^+ \rightarrow S^-$ and $S^- \rightarrow S^+$) while all the Q_n are invariant under this transformation.

by conserved quantities which are *not* local, as only conserved quantities contribute to the Mazur-Suzuki sum (1.16).

This is an important statement for the following reason. Only local ‘charges’ q_k are associated with a continuity equation $\partial_t q_k + j_{k+1} - j_k = 0$, where j_k is the corresponding current density. As a theoretical commonplace, therefore only for local slow modes a hydrodynamic description can be formulated. (Note that while our formalism of the last chapter started from a hydrodynamic approach, it does not rely on the continuity equation. Therefore it can be used to study non-local modes as well.) A main motivation to study the spin current in the XXZ model is the question, to what extent non-local conservation laws are relevant in the sense that they lead to experimentally observable consequences in real materials.

An example which shows that perturbation theory for local and non-local quantities can be drastically different has been discussed in Ref. [60]. There, it has been shown that an arbitrarily small inter-chain coupling can destroy a non-local order parameter (e.g. the string order of a spin-1 Haldane chain) in a gapped system. Formally, the perturbations turn out to be proportional to the length of the system. In contrast, local order parameters are always robust against small perturbations for all gapped systems.

In principle one can try to investigate the transport properties for small J' directly by calculating the spin-conductivity from an exact diagonalization of the XXZ chain in the presence of finite J' . In such a calculation Heidrich-Meisner *et al.* [48] were able to show that the spin Drude weight vanishes in the thermodynamic limit, but a reliable determination of the resulting finite spin-conductivity is rather difficult even for large J' . Furthermore, finite size effects grow rapidly [48] for small J' .

In the following, we will use a different approach based on a perturbation theory in J' . We construct numerically a non-local operator J_{\parallel} which is conserved for $J' = 0$ and responsible for the finite Drude weight of the unperturbed XXZ Heisenberg chain. In a second step we derive a lower bound for the spin conductivity of the perturbed system using the results of the last chapter 2 and show that the spin conductivity is proportional to $1/J'^2$. Finally, we analyze to what extent J_{\parallel} is a non-local operator and discuss how the result can be interpreted. Section 3.7 investigates the role of special values of the anisotropies where the Heisenberg model possesses extra symmetries.

3.6.1 Setup

As stated above, Eq. (1.16) implies that the finite Drude weight is associated to constants of motion C_i of H_0 with $\langle C_i J_s \rangle \neq 0$ which we need to identify for our further analysis. More precisely, we split the current operator into

two pieces,

$$J_s = J_{\parallel} + J_{\perp}, \quad (3.33)$$

as described in section 1.6. One has

$$J_{\parallel} = \sum_i \frac{\langle J_s C_i \rangle}{\langle C_i^2 \rangle} C_i. \quad (3.34)$$

J_{\parallel} can be interpreted as the projection of the the spin current to the space of conserved quantities, i.e. the conserved part of J_s and, indeed, one obtains directly from Eq. (1.16):

$$D_s = \frac{\beta}{N} \langle J_{\parallel}^2 \rangle. \quad (3.35)$$

As described above, the known local conservation laws Q_n do not contribute to J_s , i.e. $\langle J_{\parallel} Q_n \rangle = 0$. J_{\parallel} is a very complex non-local operator which is difficult to construct and handle analytically. For finite size systems with up to 20 sites, however, one can construct J_{\parallel} numerically using the exact eigenstates of H_0 . As the C_i span the space of energy diagonal operators, we just keep the energy diagonal part of J_s , i.e.

$$\langle n | J_{\parallel} | m \rangle = \delta_{E_m E_n} \langle n | J_s | m \rangle. \quad (3.36)$$

For a finite value of the perturbation J' the Drude weight (3.35) is absent, as is known from numerical studies [53, 48] which were, however, not able to investigate the regime of small J' due to large finite size effects in this limit.

In the last chapter we have shown that a lower bound for the leading order contribution to the conductivity σ_s can be obtained in the limit of small J' by evaluating the correlation function $\tilde{\Gamma}$ with respect to H_0 :

$$\text{Re } \tilde{\Gamma}(\omega) = \frac{1}{N} \int_0^{\infty} dt e^{i\omega t} \langle [\dot{J}_{\parallel}(t), \dot{J}_{\parallel}(0)] \rangle_0. \quad (3.37)$$

As $[J_{\parallel}, H_0] = 0$, $\tilde{\Gamma}(\omega)$ is proportional to J'^2 . The inequality for the spin conductivity reads

$$\sigma_s \geq \frac{\chi^2}{\tilde{\Gamma}(0)} \quad (3.38)$$

where $\chi = \beta \langle J_{\parallel} J_s \rangle / N = D_s$ is the generalized (spin current) susceptibility and $\tilde{\Gamma}(\omega) / \chi$ can be interpreted as a scattering rate of J_{\parallel} , see Ref. [61] for details. Next we will present our analysis of the correlation function Eq. (3.37).

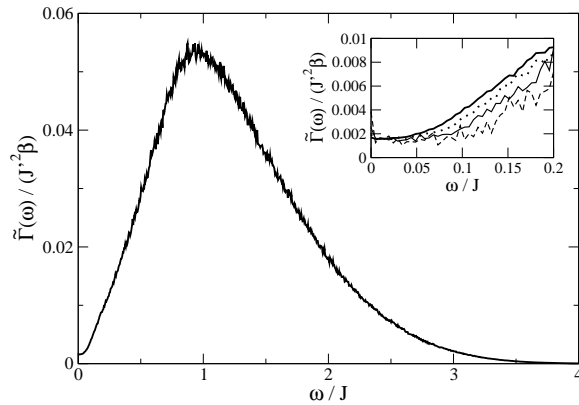


Figure 3.5: Leading order contribution to the spin current relaxation rate for $\Delta = 0.75$ and system size $L = 20$ for $T \rightarrow \infty$. Finite size effects are small and $\tilde{\Gamma}(\omega)$ is finite at $\omega = 0$ as can be seen in more detail in the inset (thick line $L = 20$, dotted line $L = 18$, thin line $L = 16$, dashed line $L = 14$).

3.6.2 Numerical results

We investigate $\tilde{\Gamma}(\omega)$ and the generalized susceptibility χ numerically in the $T \rightarrow \infty$ limit via exact diagonalization for system sizes up to $L = 20$ and for various anisotropies Δ using periodic boundary conditions. In this high temperature limit, the spin-spin correlation length vanishes and therefore finite size effects are smallest. Results for finite $T \gg J$ (not shown) are essentially identical.

The results for an intermediate $\Delta = 0.75$ are shown in Fig. 3.5. $\tilde{\Gamma}(\omega)$ drops rapidly for small frequencies but saturates at a finite value. This saturation value $\lim_{\omega \rightarrow 0} \tilde{\Gamma}(\omega)$ is almost independent of system size (see inset). This indicates that finite size effects are small despite the fact that J_{\parallel} is expected to be a non-local operator. We therefore conclude that for small J'

$$\sigma_s \geq \frac{c(T)}{T J'^2}. \quad (3.39)$$

in the thermodynamic limit. This is the main result of this section: the spin-conductivity of a slightly perturbed XXZ Heisenberg chain is very large, despite the fact, that the spin current is not protected by any local conservation law. For $\Delta = 0.75$ we obtain for example $c(T \rightarrow \infty) = 0.92 J^3$. For any finite temperature we expect that the same result holds: in the limit of small J' the spin conductivity is proportional to $1/J'^2$.

In Fig. 3.6 the behavior of the scattering rate $\tilde{\Gamma}/\chi$ as a function of Δ is shown. Interestingly, the scattering rate seems to vanish in the isotropic limit $\Delta \rightarrow 1$, $\tilde{\Gamma} \propto J'^2(1-\Delta)^2$. We have previously [3] observed the same effect for the scattering rate of the heat current, which turns out to be proportional

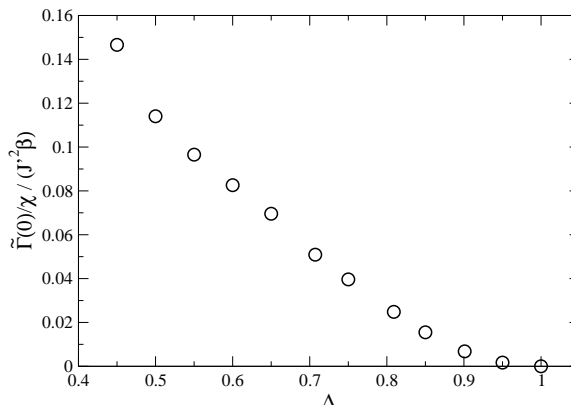


Figure 3.6: Scattering rate $\tilde{\Gamma}(0)/\chi$ as a function of the anisotropy parameter Δ for $L = 18$, $T = \infty$. For the isotropic system, $\Delta = 1$, $\tilde{\Gamma}(0)$ is zero, see text. The errors are comparable to the size of the symbols and are discussed in more detail in section 3.7.

to $1/J^4$ at the isotropic point. The reason for this unexpected result is that for the isotropic case one can construct an operator $Q'_3 = Q_3 + J'\Delta Q_3$ such that the commutator $[Q'_3, H_0 + H_1]$ is of order J^2 rather than linear in J' . As a consequence, the decay rate of the heat current at the isotropic point is proportional to J'^4 . Very likely, the same mechanism applies to J_{\parallel} , too. A subtle and controversial issue [43, 48, 59] is the value of the Drude weight, $D_s = \chi$, for $\Delta = 1$. Both from numerics and from Bethe ansatz, there is evidence pointing either to a finite [48, 59] or vanishing [43, 59] Drude weight in the thermodynamic limit. If the Drude weight vanishes for $\Delta = 1$, our results are only of relevance for $\Delta < 1^7$.

In section 3.7 we discuss a further effect: the Drude weight D_s appears to be a discontinuous function of Δ as for special values of the anisotropies $\Delta = \cos(\pi/n)$, $n = 3, 4, 5, \dots$, one obtains different values for D_s compared to anisotropies slightly away from these points. For the scattering rate $\tilde{\Gamma}/\chi$ these effects are much smaller and possibly absent in the thermodynamic limit.

3.6.3 Non-Locality of J_{\parallel}

As stressed in the introduction, the spin current J_s is orthogonal to all known local conservation laws Q_n of the XXZ Heisenberg chain. This suggests that J_{\parallel} , the conserved part of J_s , is a non-local operator which cannot be written in the form of Eq. (3.10). To quantify this statement, we expand the

⁷If $D(T) = 0$, then the conductivity is finite anyway and there is no point in using the memory matrix formalism.

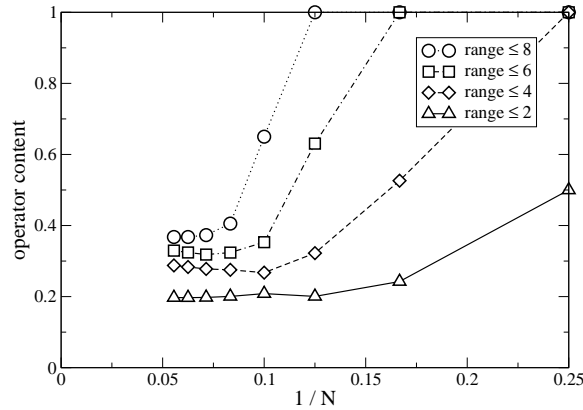


Figure 3.7: Relative weight $\sum_{m=1}^n c_m$, see Eq. (3.41), of local operators with range up to n ($n = 2, 4, 6, 8$) contributing to J_{\parallel} as a function of inverse system size from $N = 4$ to $N = 18$.

numerically constructed J_{\parallel} in local operators A_{ni} which contain products of spin-operators on n adjacent sites,

$$J_{\parallel} = \sum_{ni} a_{ni} \frac{A_{ni}}{\langle A_{ni}^2 \rangle^{1/2}}, \quad (3.40)$$

where the A_{ni} define a complete orthogonal basis in the space of operators, $\langle A_{ni} A_{mj} \rangle = 0$ for $n \neq m$ or $i \neq j$. The A_{ni} are written as sums of products of spin-operators, where each product contains spins on n adjacent sites. Here we use – as above – the ($T = \infty$) expectation value as the scalar product in the space of operators. In Eq. (3.40) obviously only translationally invariant hermitian operators contribute which also conserve S_z . For $n = 1$ there is just one such operator, $A_{11} = \sum_i S_i^z$, for $n = 2$ one finds 3 such terms $A_{21} = \sum_i S_i^z S_{i+1}^z$, $A_{22} = \sum_i S_i^+ S_{i+1}^- + h.c.$, $A_{23} = i \sum_i (S_i^+ S_{i+1}^- - h.c.)$. The 10 operators of range 3, A_{3i} , contain both products of two spin operators, e.g. $\sum_i S_i^z S_{i+2}^z$ and products of three spin-operators, e.g. $\sum_i S_i^z S_{i+1}^z S_{i+2}^z$.

The ratio

$$c_n = \frac{\sum_i |a_{ni}|^2}{\sum_{i,m} |a_{mi}|^2} \quad (3.41)$$

shown in Figs. 3.7 and 3.8 describes which fraction of the operator J_{\parallel} can be expressed in terms of operators of range n . For example, if one determines the c_n for H one obtains $c_2 = J^2 / (J^2 + J'^2)$ and $c_3 = J'^2 / (J^2 + J'^2)$. By construction one gets $\sum_{n=0}^N c_n = 1$ for a system with N sites.

What types of behavior can be expected for c_n ? First, one has to investigate whether c_n is finite or zero in the thermodynamic limit $N \rightarrow \infty$. For example, for the square of a translationally invariant local operator (e.g. H_0^2),

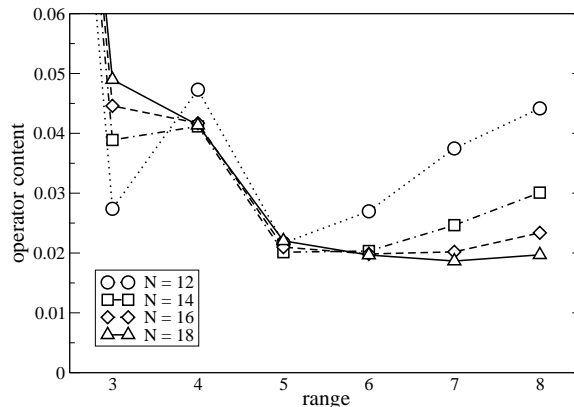


Figure 3.8: Relative weight c_n of local operators of range n ($n = 3, \dots, 8$) contributing to J_{\parallel} for different system sizes. Note that in the thermodynamic limit most of the weight is carried by operators involving more than 8 consecutive sites (see Fig. 3.7).

one finds that c_n drops proportionally to $1/N$, such that $\lim_{N \rightarrow \infty} c_n = 0$ for all $n > 0$. Even if $\lim_{N \rightarrow \infty} c_n$ is finite for each n , one can ask how rapidly $\lim_{N \rightarrow \infty} c_n$ drops for $n \rightarrow \infty$ and whether $\sum_{n=0}^{\infty} \lim_{N \rightarrow \infty} c_n$ equals 1 or is smaller.

As shown in Fig. 3.7, the c_n converge to finite values for $N \rightarrow \infty$. For $n = 2$, this is a necessary consequence of the fact that the spin current is a range 2 operator and that the Drude weight of the spin current is finite. As the latter is proportional to $\langle J_s J_{\parallel} \rangle^2$ this implies that J_{\parallel} has a finite overlap with a range 2 operator in the thermodynamic limit.

A qualitative result of Fig. 3.7 is, however, that even operators up to range 8 have less than 40% of the total weight of J_{\parallel} (but $c_8 \approx 0.02$ is already very small). As $\sum_{n=1}^{\infty} c_n = 1$, the c_n have to drop faster than $1/n$ for large n in the thermodynamic limit. Fig. 3.8 shows that the c_n decay extremely slowly with n . In this sense J_{\parallel} appears to be a rather nonlocal operator but we cannot decide from our numerics whether $\sum_{n=0}^{\infty} \lim_{N \rightarrow \infty} c_n = 1$ or smaller.

3.7 Spin Conductivity close to and at $\Delta = \cos \pi/n$

Next we discuss the behavior of the spin conductivity for anisotropies $\Delta = \cos(\pi/\nu)$. At these special points it is known that there are further symmetries which, for example, simplify the Bethe ansatz equations considerably [62, 63]. Interestingly, at these special points thermodynamic quantities show unexpected logarithmic corrections [63].

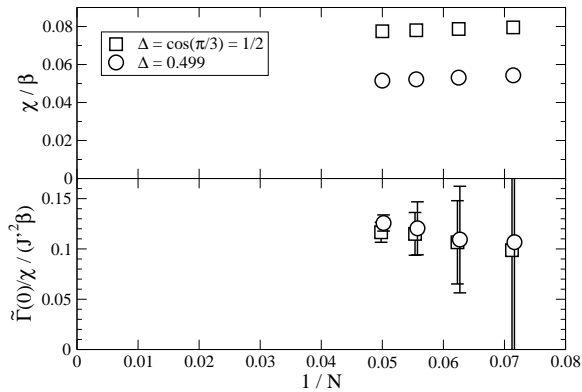


Figure 3.9: Drude weight $D = \chi$ (upper panel) and scattering rate $\tilde{\Gamma}(0)/\chi$ (lower panel) for the anisotropy $\Delta = \cos(\pi/3) = 1/2$ and a nearby value $\Delta = 0.499$ as a function of inverse system size $1/N$. The error bars represent the uncertainty inherent in the fitting procedure.

In Ref. [41], Naef and Zotos found numerically that the Drude weight at these special points differs for finite systems significantly from the values obtained for slightly different anisotropies. They concluded, however, that these differences vanish in the thermodynamic limit. This effect has also been observed by Heidrich-Meisner et al. in Ref. [48], where it was noted that the effect is absent in systems with odd number of sites N , in which case $\chi(\Delta)$ is smooth and reproduces the values at $\Delta = \cos(\pi/\nu)$ for even N . In that work the phenomenon is attributed to finite size effects, too. While we have reproduced the numerical results of Naef and Zotos, we can not find any signatures of a convergence. One would expect, that with increasing system size either the Drude weight D_s converges, or that some weight of the conductivity is shifted from around $\omega = 0$ towards this point. From the analysis in Ref. [41] one sees no indication of the latter. Concerning the first possibility, in Fig. 3.9 we show the Drude weight of the integrable model, $D_s = \chi$, and the scattering rate, $\tilde{\Gamma}(0)/\chi$, as a function of $1/N$ both for $\Delta = \cos \pi/3 = 1/2$ and $\Delta = 0.499$. Apparently, different values are obtained for $N \rightarrow \infty$ for χ while the effect for the scattering rate $\tilde{\Gamma}(0)/\chi$ is much smaller (and possibly absent). We note, that subtle logarithmic finite size effects can possibly invalidate this analysis. In other studies (see c.f. [64]) it has been shown that similar logarithmic corrections may become visible at extremely large $N \approx 1000$ systems only.

3.7.1 Conclusion

In this section we have shown that the spin-conductivity of a one-dimensional anisotropic spin-chain is strongly enhanced close to the integrable point. It

diverges (at least) as $1/J'^2$ for $J' \rightarrow 0$. This is the expected behavior for a situation where a local conservation law prohibits the decay of the current at the integrable point. However, as emphasized by Zotos, Naef and Prelovsek [18], the spin-current is orthogonal to all known local conservation laws of the XXZ chain.

There are two possible interpretations of this result. First, the conserved part J_{\parallel} of the spin current could nevertheless be ‘sufficiently’ local to define a slow hydrodynamic mode. Second, the theoretical prejudice, that only local conservation laws (i.e. those associated with a continuity equation) lead to slow modes, may be wrong. In this respect, the results of section 3.6.3, where this question is investigated, are ambiguous. On the one hand, we could prove that J_{\parallel} is a highly non-local operator involving products of operators acting on widely separated sites. On the other hand, the relative weight of range- n operators, c_n , is finite in the thermodynamic limit.

In this section we have shown that the transport properties of simple one-dimensional problems depend quantitatively and qualitatively on ‘exotic’ and rather complex conserved quantities. For the future, it would be interesting to gain a more analytic understanding of these conservation laws.

Chapter 4

Disorder Effects on the Spin Chain

This chapter is devoted to the study of the heat conductivity in real spin chain materials. The subject is motivated by several experiments of the last decade which measured values of the heat conductivity [45, 46] which were so high that they were, in the first place, quite unexpected. In fact, these experiments were the main motivation for a range of theoretical work on transport in one dimensional spin chains. It was suspected early on that the integrability of the Heisenberg model might be responsible for the high contribution to the heat conductivity. Therefore, the problem is to explain the mechanisms which lead to a finite, but large value. Of particular interest is the behavior of the heat conductivity as a function of temperature. The experiments show a broad peak of the (spin chain component of the) heat conductivity around room temperature and a characteristic decay for both lower and higher temperatures. This suggests, that different mechanisms are responsible for the decay at higher and at lower temperatures. Indeed, towards higher temperatures the heat conductivity is known to be suppressed by the coupling of the spin chain to lattice vibrations, which introduces a source of scattering for the heat current. Towards lower temperatures, disorder is known to become relevant which, again, is a source of scattering. While most of the theoretical work that has been kicked off by these experiments concentrates on analytic properties of the integrable Heisenberg chain approached via Bethe ansatz and numerical studies of small perturbations ‘inside’ the chain (e.g. next nearest neighbor, inter-chain couplings, magnetic field) via exact diagonalization techniques, studies that try to fit the experimental data are low in number. The most well-known of them is the paper by Chernyshev and Rozhkov [65] in which they use semi-phenomenological methods to reproduce the experimental data. While the fit to experiments is reasonably good, they neglect the scattering between spinons which may

lead to wrong results in certain regimes [66]. Here we attempt a more microscopic calculation of the heat conductivity. On the high temperature side (the region above the maximum) such a microscopic calculation has been carried out a few years ago by Shimshoni, Andrei and Rosch [4], where the effect of the coupling of clean spin chains to the three dimensional phonon bath has been elucidated by calculating the same correlation functions as in the last chapter for a different model.

This chapter comprises three major parts. In the first, introductory section we present the Luttinger liquid formulation of spin chains. The second section is devoted to the study of the effect of weak disorder in the spin chain, and a discussion whether this can reproduce experimental data below the conductivity maximum. In the final section we will try to actually fit the experimental data using results from Ref. [4] (decay by coupling to phonons) and the second section (decay by coupling to disorder). For this, we will put all contributions into one memory matrix. In the end, we will find that the fitting is not completely successful. While the basic feature – the characteristic maximum of the spin chain contribution to the heat conductivity – is retained, the qualitative features on both sides of the maximum fail to reproduce the measurements. On the disorder side (lower temperatures), we find that weak disorder is not sufficient to explain some of the experiments. For these one would need to take into account strong disorder, which cannot be treated as easily in our model setting. On the phonon side, we find that, strictly, the results of Ref. [4] do not apply in the temperature regime relevant for the experiment. The mismatch on each side is discussed in detail.

We note, that as is always the case with the memory matrix formalism, there is no guarantee that one has not accidentally omitted the most relevant slow modes. In the present situation, yet another ambiguity complicates matters: A given perturbation may lead to several mechanisms for the decay of the current, corresponding to a number of contributions to the Hamiltonian. Of these contributions, the most effective scattering terms have to be identified. As the coupling constants of the various terms are often not known, the only information one can access is the temperature dependence of the various contributions, and one has to determine the effectiveness of a contribution solely by means of this temperature dependence. Strictly, such selection is possible in some asymptotics of the temperature only. In our case, we will keep – from an infinite set of possible terms – the contributions that would be most dominant in a certain limit which does not completely overlap with the relevant experimental regime. The optimistic theoretician's hope is that the result from this limit will sustain at the relevant temperatures. In this sense, the expectation, that in the end one will be able to fit the results to the experiments, should be taken with a grain of salt, anyway.

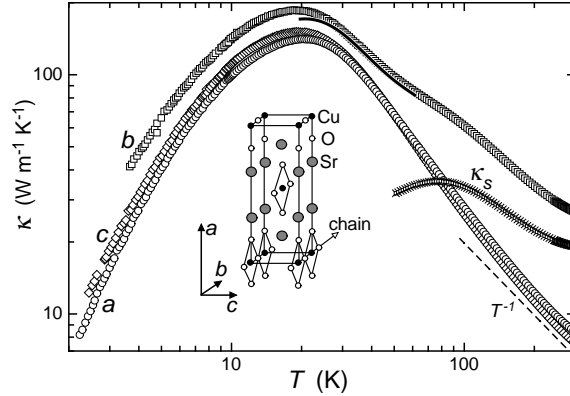


Figure 4.1: Heat conductivity in the spin chain compound Sr_2CuO_3 measured parallel and perpendicular to the direction of the chains. The difference of parallel and perpendicular contributions is also plotted. Source: [8].

4.1 Setup

In this section we review the relevant experimental situation and introduce and motivate the theoretical framework that we use for its description. The framework will be applied in the following sections.

4.1.1 Experiments

In [8] and [45] Sologubenko first reported his finding of an anomalous contribution to the heat conductivity $\kappa_s = \kappa - \kappa_p$ associated with the presence of spin chains in certain spin chain compounds. The experimental data for the compound Sr_2CuO_3 is shown in Fig. 4.1. The heat conductivity is measured perpendicular and parallel to the spin chain direction. One observes the typical *phonon peak* at around $T \sim 10\text{K}$ in all directions, whereas an excess contribution is observed along the spin chain direction. From the experimental analysis it is clear that the additional peak must be attributed to heat transport in the spin chain, and therefore we refer to this structure as the *spinon peak*, which has its maximum around $T \sim 70\text{K}$.

The special feature of the studied spin chain compound Sr_2CuO_3 is the extremely high value of the exchange coupling in the spin chain, $J \gg \Theta$, where Θ is the Debye temperature. In that system, $\Theta \approx 430\text{K}$ and $J \approx 2600\text{K}$. This separation of energy scales is also responsible for the fact that the spinon peak occurs at temperatures well above the phonon peak. Also, the spinon velocity, which is proportional to the exchange coupling, ($v = \pi/2Ja$ in the isotropic Heisenberg chain, see [67]) is much larger than

the phonon velocity, which may be determined¹ from the Debye temperature, ($v_p \approx 0.5\Theta_D a$), and the ratio is given by $v_p/v \sim 1/20$.

The excess contribution to the heat conductivity measured in the direction of the spin chains amounts to about double the expected phonon contribution at $T = 200K$ ($\kappa_s(T) \gtrsim \kappa_p(T)$). It was noted very early [8] that this huge contribution might be linked to the integrability of the spin-1/2 Heisenberg chain. Here we note that meanwhile other materials have been found in which the excess contribution from the spin chain is much more pronounced, c.f. [9].

The phonon heat conductivity smoothly changes from $\kappa_p \sim T^{-\alpha}$ with $\alpha \approx 1.3$ above the low temperature maximum to $\alpha \approx 1$ at room temperature. The amount of disorder in the system seems to legitimize the assumption that above the phononic low temperature maximum at $T_{\max} \sim 20K$ the heat conductivity is determined by the effect of disorder in the spin chain. The spin chains are almost isotropic, i.e. it is well described by the XXZ-model with $\Delta = 1$, which is the spin-1/2 Heisenberg chain.

4.1.2 Low energy dynamics

As in the whole range of the experiment we are in a regime where $T \ll J$, it is advisable to consider an effective low energy theory for the spin chain. The low energy dynamics of the spin chain is described by the Luttinger liquid Hamiltonian. One can map the spin chain onto this model in two steps. First, by performing a Jordan-Wigner transformation of the XXZ spin chain one obtains as an intermediate stage a one dimensional gas of spinless electrons. An effective low energy theory of the electron gas can be obtained by linearizing the spectrum around the Fermi point. This allows to apply the bosonization technique and the Luttinger liquid Hamiltonian is obtained. While the XXZ model maps onto the Luttinger liquid which, as it should, is characterized by a finite drude weight for the heat conductivity, perturbations to the spin chain (e.g. next-nearest neighbor coupling, coupling to the phonons, disorder, etc.) will introduce scattering terms, additionally to the Luttinger liquid Hamiltonian, which are responsible for the decay of the current. In the low energy limit $T \rightarrow 0$ these additional terms are *irrelevant* and therefore can be treated perturbatively for $T \ll J$ (see Fig. 4.2). We can therefore express the conductivity by accounting for the

¹In reality, the phonon velocity depends both on the energy, the direction of the phonons, and can be multiple-valued due to the presence of multiple bands, and the Debye temperature is a well defined quantity only in the framework of the Debye approximation. By assuming that the Debye approximation (linear, isotropic spectrum, only one band) well describes the physics of the phonons, the two quantities can be related. The assumption of an isotropic phonon velocity would lead to $v_p = 0.3\Theta_D a$, but the phonon velocity is enhanced in the direction of the chains, which we account for by correcting the prefactor to 0.5 [68].

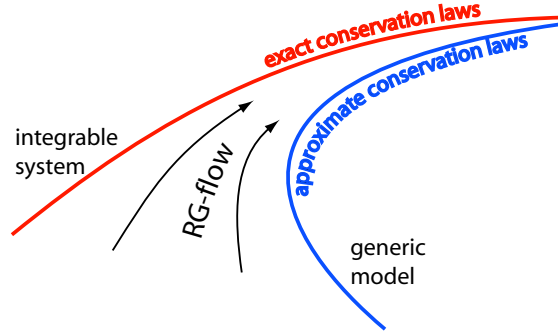


Figure 4.2: Schematic depiction of the RG-flow as temperature is decreased. A generic system with perturbations has a $T = 0$ fixed point which is integrable. At finite but low enough temperatures the perturbations are small and therefore can be treated perturbatively.

irrelevant terms in terms of a memory matrix formalism.

The mapping of the XXZ chain to the Luttinger liquid is standard and can be found in textbooks (see c.f. [52]). Here we restrict ourselves to give the effective Hamiltonian and the associated irrelevant terms and to define the fields. We shall adopt the conventions in Giamarchi's book [52].

4.1.3 Luttinger liquid Hamiltonian

The low energy fixed point of many gapless one dimensional systems is given by the Luttinger liquid Hamiltonian,

$$H_{\text{LL}} = v \int \frac{dx}{2\pi} \left(K(\pi\Pi(x))^2 + \frac{1}{K}(\partial_x\phi(x))^2 \right) \quad (4.1)$$

with the bosonic conjugate fields $\phi(x)$ and $\Pi(x)$ satisfying

$$[\phi(x), \Pi(x')] = i\delta(x - x'). \quad (4.2)$$

The Hamiltonian (4.1) is obtained by bosonization of a fermionic model. The fermionic fields are expressed in terms of the bosonic fields:

$$\psi_{R/L} = \frac{1}{\sqrt{2\pi a}} e^{i(\pm\phi - \theta)} \quad (4.3)$$

where θ is defined by $\partial_x\theta(x) = \pi\Pi(x)$. The right and left moving fields $\psi_R(x)$ and $\psi_L(x)$ describe the low energy excitations of the fermions, i.e. they originate from a linearization of the spectrum around the Fermi points $\pm k_F$

with $k_F = \frac{\pi}{2a}$,

$$\psi(x) = e^{ik_F x} \psi_R(x) + e^{-ik_F x} \psi_L(x). \quad (4.4)$$

The fermionic field $\psi(x)$ is connected to the spin operators of the spin chain in terms of the Jordan-Wigner transformation:

$$S_i^z = c_i^\dagger c_i - \frac{1}{2} \quad (4.5)$$

$$S_i^+ = c_i^\dagger e^{i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j} \quad (4.6)$$

$$S_i^- = e^{-i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j} c_i \quad (4.7)$$

where the creation and annihilation operators at site i are connected to the corresponding continuous field via $c_i^{(\dagger)} = \sqrt{a} \psi^{(\dagger)}(r_i)$ where a is the lattice spacing. Talking about the spin chain in terms of the Jordan-Wigner fermions, one refers to the effective low energy excitation – described by the fields ψ_L and ψ_R – as *spinons*.

The coupling constants v and K which completely determine the low energy fixed point (4.1) are in general hard to determine. In the case of the XXZ model they can be calculated from Bethe ansatz [67] yielding

$$K = \frac{1}{1 - \frac{1}{\pi} \cos^{-1}(\frac{J_z}{J})}. \quad (4.8)$$

In describing the experimental situation sketched above we may set $J_z = J$ which gives $K = 1/2$ for the isotropic Heisenberg model. The *speed of light*, or spinon velocity v takes the value $v = \pi/2Ja$ for $\Delta = 1$.

In the following section(s) the Luttinger liquid plays the role of the unperturbed Hamiltonian. Elements of the memory matrix are – calculated in leading order in the perturbation – given by correlation functions evaluated with respect to the unperturbed model. For the Luttinger liquid, the correlation functions are known. Using the definitions

$$\langle \phi(x, t) \phi(0, 0) \rangle_{LL} \equiv G_\phi(x, t) = KG(x, t) \quad (4.9)$$

$$\langle \theta(x, t) \theta(0, 0) \rangle_{LL} \equiv G_\theta(x, t) = \frac{1}{K} G(x, t) \quad (4.10)$$

$$\langle \phi(x, t) \theta(0, 0) \rangle_{LL} \equiv \tilde{G}(x, t) \quad (4.11)$$

the basic propagators are given by

$$G(x, t) = -\frac{1}{4} \ln \frac{\sinh(\tau(x - vt + ia)) \sinh(\tau(x + vt - ia))}{(\tau a)^2} \quad (4.12)$$

$$\tilde{G}(x, t) = -\frac{i}{2} \text{Arg} [u \cosh(\tau x) + iw \sinh(\tau x)] \quad (4.13)$$

²An additional magnetic field would shift the Fermi level by an amount proportional to the magnetization. Here we restrict ourselves to time reversal invariant situations and assume that no external magnetic field is applied

where we have defined the *reduced temperature*

$$\tau = \frac{\pi T}{v} \quad (4.14)$$

which for the isotropic case takes the value $\tau = \frac{2}{a}(T/J)$. Correlators of arbitrary functions of the fields $\phi(x)$ and $\theta(x)$ can be evaluated by using Wick's theorem³. However, one is interested in correlation functions of operators given in terms of the spin-operators of the original spin chain model. The recipe to calculate such correlation functions is therefore as follows. First one expresses the spin operators through the bosonic fields ϕ and θ . Then one performs the necessary Wick contractions. This step leaves us with integrals over functions of $G(x, t)$ and $\tilde{G}(x, t)$ and their derivatives. These integrals in turn can either be evaluated numerically or – by using further approximations – be treated analytically.

4.1.4 Memory Matrix

While the low energy fixed point of our model is described by the Luttinger liquid which obeys an infinite number of conserved charges assuring its integrability, at finite temperatures $T > 0$ additional terms (as those arising from perturbations) break integrability and thus determine the decay of currents and hence the transport properties. To determine the transport properties, we calculate matrix elements of the memory matrix, which are given by correlation functions of time derivatives of the slow modes (which are chosen as conserved currents C of the Luttinger liquid), $\partial_t C = i[H, C]$. Among the terms which arise from different perturbations there also will be those which commute with the currents. For the full Hamiltonian we write

$$H = H_0 + gH_1 + H_{\text{irr}} \quad (4.15)$$

where H_0 is the unperturbed model (in our case it is the Luttinger liquid Hamiltonian, or, when phonons are also taken into account, the Hamiltonian of the pure phonon bath) and H_{irr} arises from corrections which also commute with the slow modes (see below), $[H_0 + H_{\text{irr}}, C] = 0$. We therefore need to select the contributions to gH_1 arising from perturbations that are relevant for the decay of the currents, $\partial_t C = ig[H_1, C]$.

In the memory matrix formalism, one choses a set of slow modes, denoted by C_i , which are not specified yet. The leading order contribution to the heat conductivity is given by

$$\kappa \geq \frac{1}{T} \chi^T \tilde{M} \chi \quad (4.16)$$

³Wick's theorem is applicable as the Luttinger liquid theory is Gaussian.

where χ is a vector of generalized susceptibilities

$$\chi_i = (J_Q | C_i) \quad (4.17)$$

and \tilde{M} is the leading contribution to the memory matrix,

$$\tilde{M}_{i,j} = \lim_{\omega \rightarrow 0} \left(F_i \left| \frac{i}{\omega - L_0} \right| F_j \right), \quad (4.18)$$

where we have introduced the generalized *forces* $F_i = -\partial_t C_i = i[C_i, gH_1]$. The memory matrix can be evaluated in terms of the retarded response function calculated with respect to the unperturbed model (compare with Eq. (1.9)),

$$\langle A; B \rangle_\omega^0 = \frac{i}{V} \int_0^\infty dt e^{i\omega t} \langle [A(t), B(0)] \rangle_0, \quad (4.19)$$

in terms of which we find

$$\tilde{M}_{i,j} = \lim_{\omega \rightarrow 0} \frac{\langle F_i; F_j \rangle_\omega^0 - \langle F_i; F_j \rangle_{\omega=0}^0}{i\omega}, \quad (4.20)$$

compare with Eq. (1.8). In the limit $\omega \rightarrow 0$ we can interpret this as a derivative with respect to ω :

$$\tilde{M}_{i,j} = -i \frac{\partial}{\partial \omega} \langle F_i; F_j \rangle_\omega^0 \Big|_{\omega=0} \quad (4.21)$$

which, using Eq. (4.19), can be written as

$$\tilde{M}_{i,j} = \frac{i}{V} \int_0^\infty dt t \langle [F_i(t), F_j(0)] \rangle_0. \quad (4.22)$$

Using the fact that $\langle A(t)B(0) \rangle^* = \langle A(-t)B(0) \rangle$, we arrive at our final working expression

$$\tilde{M}_{i,j} = \frac{i}{V} \int_{-\infty}^\infty dt t \langle F_i(t) F_j(0) \rangle_0. \quad (4.23)$$

This expression is useful in our context because in terms of the effective low energy theory it is the time correlation functions that are known and are most comfortable to work with.

After we have determined gH_1 , the task is thus to calculate the generalized forces, the calculation of the correlation functions $\langle F_i(t) F_j \rangle_0$ and the time integral. Let us assume that we have determined all relevant scattering contributions to the Hamiltonian. We write

$$gH_1 = \sum_n H_n^S. \quad (4.24)$$

Then we can write the generalized forces as

$$F_i = i \sum_n [C_i, H_n^S] \equiv \sum_n F_{in} \quad (4.25)$$

leading to a large number of contributions to each matrix element of the memory matrix. Of all these contributions we need to select the most relevant ones. Next we will identify a class of irrelevant (in the RG sense) perturbations that is always present in the system. Although these will turn out not to be responsible for the decay of the current, it is instructive to consider them, as the relevant contributions arising from disorder and from the coupling to phonons (to be discussed in the following sections) are related to this class of perturbations.

4.1.5 Intrinsic Perturbations

In this subsection we discuss the various ways in which such terms do arise. Let us look at a generic, anti-ferromagnetic, translationally invariant spin-1/2 chain with finite range interactions,

$$H = \frac{1}{2} \sum_{ij} J_{ij} (S_i^+ S_j^- + S_i^- S_j^+) + \sum_{ij} J_{ij}^z S_i^z S_j^z \quad (4.26)$$

where $J_{ij} = J_{i-j} > 0$ and $J_{i-j} = 0$ for $|i-j| > n$ with some finite n . The motivation for such a choice is evident: While an XXZ model may be a good approximation to the spin chains in the CuO_2 compounds, small values of additional couplings inside the real chain will be present, such as a coupling of next nearest neighbors. Although small in magnitude, these couplings break the integrability of the XXZ chain and it is crucial to take into account their effect on transport properties. An exact derivation of the effective low energy theory would involve repeated RG transformations, leading to the luttinger liquid plus (provided the chain is gap-less) irrelevant terms. However, since the microscopic values of the couplings are not known, anyway, one can instead write up all terms that are allowed by symmetry and assume generic values for their couplings. This task has been performed by Shimshoni et al. in [4] and in the following we present their results. The symmetries of the spin chain are the spin rotation invariance around the z -axis, discrete translation by a lattice spacing, inversion and time reversal. It is convenient to think about the spin chain in terms of the Jordan-Wigner fermions and thus to know how these symmetries translate to the fermionic language. The spin rotation invariance leads to charge conservation and translation invariance leads to momentum conservation up to multiples of the reciprocal lattice vector, $G = 2\pi/a$. The right and left moving fields transform according to

$$\psi_L \rightarrow \psi_R, \quad \psi_R \rightarrow \psi_L \quad (4.27)$$

under parity and

$$\psi_L \rightarrow \psi_R^\dagger, \quad \psi_R \rightarrow \psi_L^\dagger, \quad i \rightarrow -i \quad (4.28)$$

under time reversal. Of all terms preserved under these symmetry transformations, we keep only those which have the ability to degrade currents. Terms conserving the number of spinons around each Fermi point, i.e. commuting with the operator

$$J_0 = N_R - N_L, \quad (4.29)$$

the number of right movers minus the number of left movers, do not affect the conductivity directly. Also, any translationally invariant term (including terms arising from band curvature or normal scattering) conserve momentum and therefore are invariant under *continuous* translations of the fermions. Therefore, these terms commute with the generator of continuous translations,

$$P_T = -i \int dx (\psi_R^\dagger \partial_x \psi_R + \psi_L^\dagger \partial_x \psi_L). \quad (4.30)$$

According to the philosophy of chapter 2, to calculate the leading order contribution to the heat conductivity, it is sufficient to consider the heat current operator of the *fixed point*. Now, as can be shown [4], the heat current in the Luttinger liquid is proportional to the translation operator (4.30), implying that the leading order contribution to the memory matrix does not depend on contributions to the Hamiltonian which are translationally invariant. Therefore, these terms are irrelevant to our analysis and we have to take into account terms which relax momentum. Typically, such terms involve the annihilation of a left mover and the creation of a right mover. Additionally, lattice momentum can be transferred to the lattice in multiples of the reciprocal lattice vector. This class of operators we shall refer to as Umklapp processes⁴. The leading Umklapp terms compatible with the above symmetries are different for even and odd number of processes n which scatter from one Fermi point to the other, due to time reversal symmetry. With the momentum transfer

$$\Delta k_{nm} = n2k_F - mG \quad (4.31)$$

the Umklapp terms are given by

$$H_{nm}^U = g_{nm}^U \int dx \prod_{j=0}^{n-1} (\psi_R^\dagger(x+ja)\psi_L(x+ja) + h.c.) \quad (4.32)$$

for even n and by

$$H_{nm}^U = g_{nm}^U \int dx (\psi_R^\dagger(x)\psi_R(x) + \psi_L^\dagger(x)\psi_L(x)) \prod_{j=1}^n (\psi_R^\dagger(x+ja)\psi_L(x+ja) + h.c.) \quad (4.33)$$

⁴Strictly speaking, only processes which transfer momentum to the lattice should be termed ‘Umklapp’. Here we adopt the conventions in Ref. [4]

for odd n . It is these processes that dominate the decay of the heat current in the generic spin chain. The most relevant slow modes of the full Hamiltonian are the operators P_T and J_0 of Eqs. (4.30) and (4.29)⁵.

For later reference, we also note that the translation operator (4.30) commutes with all translationally invariant terms ($\Delta k_{nm} = 0$) and therefore with all possible low energy processes. On the other hand, processes *with* momentum transfer $\Delta k \neq 0$ are exponentially suppressed by a factor $\exp(-v|\Delta k|/T)$ [4]. Therefore, intrinsic perturbations can not relax the heat current sufficiently for $T \ll J$. One needs to take into account impurities and/or phonons to relax the current. Also, the Umklapp terms identified above are relevant in connection to the discussion that follows.

4.2 Impurity Scattering

This section discusses the role of disorder in the material on the heat conductivity. The goal is a description of the experimental results of Refs. [8, 45] (see Fig. 4.1) in the temperature regime below the spinon peak, i.e. below $T \approx 100K$.

4.2.1 Relevant Operators

Disorder in the system can have various sources, including point defects and different sorts of dislocations, which are spatially extended misalignments of the lattice. Here we focus on the effect of point defects. The different kinds of point defects can roughly be classified into vacancies, extra impurities, impurity substitution and isotope substitution. A vacancy is a single missing atom and an extra impurity is an extra atom, not fitting into the crystal structure. Such defects introduce considerable mechanical strain into the lattice and therefore cost a big amount of energy. It is less costly not to disrupt the geometric structure of the lattice, and therefore impurities, i.e. foreign types of atoms, will try to take positions otherwise occupied by native atoms. Nevertheless, impurity atoms typically will have a different radius and valence structure, and therefore, too, lead to a less severe local distortion of the crystal. The least severe effect is caused by isotopes of the native atoms, which are always present, even if the crystal would be perfect (i.e. no dislocations or vacancies) and no foreign atoms would be present. The main effect of isotopes is a mass difference of single atoms, affecting the lattice vibrations of the crystal. However, isotopes have identical valence structure and magnetic properties as the host, and therefore do not affect the spin chain, only the phonons are affected. As we are interested in the

⁵In fact, in Ref. [4] it is shown that not only do both P_T and J_0 commute with H_0 and all other irrelevant terms, but that also for any particular combination $H_0 + H_{nm}^U$ there exists a linear combination of P_T and J_0 which is conserved.

effect of disorder on the spin chains, we do not consider isotope scattering. Furthermore, we want to apply our well developed perturbative techniques and require the perturbations not to be too severe.

We therefore consider impurities and defects which have one of two effects. First, those which introduce mechanical strain into the lattice and locally distort the crystal. These distortions lead among other things to a local displacement in the position and shape of the orbitals carrying the spins. As the exchange coupling between spins sensitively depends on the overlap between orbitals, impurities and off-chain defects thus introduce local perturbations in the exchange coupling constants. Second, impurities may have a different electronic structure, carrying a number of electrons differing from the atoms they substitute, therefore showing different magnetic properties as the spin of the atom may be changed. Again, if such impurities are located in the spin chain, substituting one of the spins, they effectively may cut the chain. If the magnetic impurity is located outside of the chain, the interaction with the chain may be weak enough to describe the effect through a random magnetic field mediated by the impurity atoms which the spin chain is exposed to.

It is known, that in 1D systems, even the ‘weak’ impurities discussed above have a dramatic effect on the low energy excitations. The impurity Hamiltonian is a relevant perturbation in the RG sense, and this is true whether one considers single impurities in a 1D electron gas [69] or in a spin chain [70], or quenched (dilute) disorder in one of these cases [71, 72]. Therefore, in the limit $T \rightarrow 0$, one can not treat the disorder perturbatively. One can see that perturbation theory has to break down by attempting a perturbative expansion at finite temperatures. The leading order contribution from a perturbation (say, to the free energy) then has the form [52]

$$F = F_0 \left[1 + \left(\frac{T}{\epsilon_F} \right)^{-\alpha} + \mathcal{O}(\delta J^2) \right] \quad (4.34)$$

where α is the scaling dimension of the impurity Hamiltonian H_{imp} . Relevant perturbations are characterized by a positive scaling dimension, implying that the perturbation diverges as $T \rightarrow 0$. However, what is also seen from this relation is that relevant terms, too, can be treated perturbatively above a certain temperature. Namely, if

$$T \gg T_c \equiv \left(\frac{\delta J_{\text{imp}}}{J} \right)^{1/\alpha} \epsilon_F \quad (4.35)$$

then the leading order contribution from perturbation theory is much smaller than the unperturbed contribution, which is the criterion for the validity of the expansion. Therefore, we can treat disorder perturbatively for weak enough disorder and not too low temperatures, $T \gg T_c$. We note that in our case the Fermi energy is given by the exchange coupling, $\epsilon_F = J$.

Clearly, if there is a defect directly in the chain, say, one takes out a spin, then this can be considered to be a rather severe perturbation, and δJ_{imp} would be comparable to J . On the other hand, if an impurity is located several atomic distances apart from the chain, then the effect on the chain may be considered to be small and we can go for a perturbative treatment. Little is known about the position of the impurities in the real materials we are considering, whether they interrupt the chain or whether they are apart from it [68]. Since non-perturbative calculations are more difficult, if possible at all, therefore we restrict ourselves to situations where a perturbative treatment is amenable and will apply our memory matrix machinery to them⁶.

Next, take a closer look at the possible kinds of disorder we are able to treat. There are two kinds of impurities we wish to discuss. First, we assume non-magnetic impurities that apply local mechanical stress to the lattice. This kind of impurities introduce a spatial dependence in the exchange coupling J , assuming that the variation is small. To account for this kind of impurities we make the replacement

$$J \rightarrow J + \delta J(x), \quad \overline{\delta J(x)} = 0, \quad \overline{\delta J(x)\delta J(x')} = D_J \delta(x - x').$$

Such a variation in the coupling constants will in general lead to a variation in all coupling constants of the generic spin chain, in the spinon velocity v , the interaction parameter K and all coupling constants g_{nm}^U associated with the processes we previously termed Umklapp processes. We will present a detailed calculation of the contribution of these terms to the memory matrix below.

In addition to these terms, disorder breaks parity and therefore disorder couples to backscattering terms which break parity and therefore were omitted in the list of Umklapp operators in the clean situation above. The leading contribution has already been determined elsewhere[72]. It reads in terms of the fermionic and the bosonic fields respectively

$$\begin{aligned} H_{\text{imp}} &= i \int dx \delta J(x) (\psi_L^\dagger(x) \psi_R(x) - \psi_R^\dagger(x) \psi_L(x)) \\ &= \int dx \delta J(x) \sin(2\phi(x)). \end{aligned} \tag{4.36}$$

This contribution is the simplest one that involves scattering between left and right movers and changes sign under parity.

The second kind of impurity we are able to treat are magnetic impurities which are far enough from the chain, such that their effect can be considered to be that of an effective weak random magnetic field which the chain is

⁶If you've lost your keys at night, the first place you'll search for them is under the street-lamp. (L. D. Landau)

exposed to. Such a contribution breaks time reversal and effectively leads to a random magnetic field. For simplicity we assume that the coupling is only along the z-axis⁷. Thus we introduce a weak random magnetic field⁸ along the z-direction, $\delta h(x)$, with

$$\overline{\delta h(x)} = 0, \quad \overline{\delta h(x)\delta h(x')} = D_h \delta(x - x'). \quad (4.37)$$

The contribution to the Hamiltonian, likewise, has been determined in [72] and reads

$$\begin{aligned} H_{\text{imp}} &= \int dx \delta h(x) (\psi_L^\dagger(x) \psi_R(x) + \psi_R^\dagger(x) \psi_L(x)) \\ &= \int dx \delta h(x) \cos(2\phi(x)). \end{aligned} \quad (4.38)$$

Note that this backscattering term corresponds to the leading contribution for odd n ($n = 1$) from the ‘Umklapp’ terms Eq. (4.33) but with the additional density term $\partial_x \phi$ removed. The additional $\partial_x \phi$ was necessary to preserve time reversal, which here is explicitly broken.

Both contributions, magnetic and non-magnetic dilute disorder, are known to have scaling dimension $\alpha = 2 - 2K$. In the isotropic case, $K = 1/2$, this implies for the temperature the requirement $T \gg \sqrt{D_J}$ and $T \gg \sqrt{D_h}$ respectively, the perturbative treatment to be allowed. These terms will turn out to give the dominant contributions to the memory matrix and a detailed calculation is given further below. We note that these two terms lead to the same temperature dependence for the memory matrix, therefore we will consider only one of them.

4.2.2 Choice of Slow Modes

So far we have identified the potentially relevant contributions to the Hamiltonian, which are responsible for the decay of the currents, but we have not specified yet which slow modes C_i we chose. There are two obvious conservation laws of the Luttinger liquid (and also of the terms irrelevant for relaxation, H_{irr}). Namely, the translation operator of Eq. (4.30) and the particle current,

$$J_0 = N_R - N_L \quad (4.39)$$

which is simply the difference of right movers and left movers. It turns out that both of these operators have a physical significance in the spin chain, too. The translation operator is proportional to the heat current,

⁷The leading order contribution involves only contributions that arise from the same component of the magnetic field due to $\langle S^\alpha S^\beta \rangle \propto \delta_{\alpha\beta}$ with $\alpha, \beta = x, y, z$.

⁸In fact, the source of the random magnetic field is not relevant: An additional term $\sum_i \delta h_i S_i^z$ in the Hamiltonian would lead to the same δh expression in terms of Jordan-Wigner fermions or Luttinger bosons.

$J_Q = -v^2 P_T$ and the particle current can be interpreted as the spin current operator, $J_s = vKJ_0$, see Ref. [4]. In terms of the bosonic fields, these operators take the form

$$J_Q = -v^2 \int dx \Pi(x) \partial_x \phi(x), \quad (4.40)$$

$$J_s = vK \int dx \Pi(x), \quad (4.41)$$

and we shall choose these two operators as the slow modes. While clearly we could have chosen additional slow modes as well (there is an infinite number of conserved charges in the Luttinger liquid) these two slow modes will give us a rigorous lower bound to the heat conductivity, and chances are, that we will obtain a good approximation to the true conductivity.

4.2.3 Preparations for the Calculation

Now we have developed all pieces that are necessary to carry out the calculation of the memory matrix. We have expressed a lower bound to the heat conductivity in terms of the approximate memory matrix, Eq. (4.16), and have worked out a simple expression for the memory matrix (4.23) which we will be able to calculate straightforwardly. Furthermore, we have chosen the slow modes and also have collected the relevant scattering terms. We are therefore in the position to determine the generalized forces. Then we can express the correlation function $\langle F_i(t) F_j \rangle_0$ in terms of boson propagators Eqs. (4.12) and (4.13) by using Wick contractions. Technical details on how the contractions are carried out are given in appendix C.2. This step will leave us with functions of the boson propagators and derivatives thereof. Simple derivation of the correlation functions (defined in Eqs. (4.12) and (4.13)) gives

$$G^{(2)}(0, t) = \frac{\tau^2}{2 \sinh^2(\tau(vt - ia))} \quad (4.42)$$

$$G^{(4)}(0, t) = \frac{\tau^4 (3 + 2 \sinh^2(\tau(vt - ia)))}{\sinh^4(\tau(vt - ia))} \quad (4.43)$$

$$\tilde{G}^{(3)}(0, t) = \tau^3 (\coth(\tau(vt - ia)) - \coth^3(\tau(vt - ia))) \quad (4.44)$$

only these derivatives will appear. The single time integral that will be left in all cases of perturbations can be reduced to one single integral relation,

$$\int_{-\infty}^{\infty} d\xi \xi (i \sinh(\xi - i\alpha))^{-\gamma} = -i \cos\left(\frac{\pi\gamma}{2}\right) B\left(\frac{\gamma}{2}, \frac{1}{2} - \frac{\gamma}{2}\right) (\pi/2 - \alpha), \quad (4.45)$$

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the so-called beta function. We will encounter this integral repeatedly, therefore it is advisable to define the

shorthand

$$I(\gamma) = \cos\left(\frac{\pi\gamma}{2}\right) B\left(\frac{\gamma}{2}, \frac{1}{2} - \frac{\gamma}{2}\right). \quad (4.46)$$

$I(\gamma)$ is a smooth and positive function of γ . Particular values that will be encountered are $I(\gamma = 1) = \pi$ and $I(\gamma = 3) = \pi/2$. Finally we turn our attention to the calculations.

4.2.4 Calculation of the Subleading Contributions

Next we will calculate the contributions to the memory matrix which will turn out to be subleading in retrospect. The leading contributions are treated subsequently.

Effect of disorder

As outlined above, to leading order in the perturbation, the disorder contributes through the additional contribution H^{dis} to the Hamiltonian only, which in turn determines the ‘generalized forces’ $F_p^{\text{dis}} = i[H^{\text{dis}}, J_p]$ through which the memory matrix is defined. The density $h^{\text{dis}}(x)$ of this contribution to the Hamiltonian reads

$$\begin{aligned} h^{\text{dis}}(x) &= \frac{1}{2\pi} \left[vK \left(\frac{\delta v(x)}{v} + \frac{\delta K(x)}{K} \right) (\pi\Pi(x))^2 + \right. \\ &+ \left. \frac{v}{K} \left(\frac{\delta v(x)}{v} - \frac{\delta K(x)}{K} \right) (\partial_x \phi(x))^2 \right] \\ &+ \sum_{nm} \frac{\delta g_{nm}^U(x)}{(2\pi a)^n} \left(e^{i\Delta k_{nm}x} e^{i2n\phi} (\partial_x \phi)^{\delta_{n \text{ odd}}} + h.c. \right). \end{aligned}$$

The generalized forces F_q are evaluated as follows:

$$\begin{aligned} F_Q^{\text{dis}} &= i[J_Q, H] \\ &= F_Q + i \int dx' [J_Q, h^{\text{dis}}(x')] \\ &= F_Q + \int dx \delta J(x) f_Q^{\text{dis}}(x) \end{aligned}$$

Here $F_Q = i[J_Q, H - H^{\text{dis}}]$ denotes the contribution not associated with disorder, and captures the effect of the spinon-‘Umklapp’ terms to the Hamiltonian. These contributions and the associated contributions to the memory matrix have already been evaluated in [4]. In the last line we have introduced the reduced density f_Q^{dis} , i.e. the density of F_Q^{dis} with the fluctuations in the exchange coupling $\delta J(x)$ extracted, as we assume the fluctuations in the coupling parameters v , K and g_{nm} all to be induced by these fluctuations.

For convenience, we introduce constants relating the fluctuations:

$$\begin{aligned}\delta v(x) &= A_v \delta J(x) \\ \delta K(x) &= A_K \delta J(x) \\ \delta g_{nm}(x) &= A_{nm} \delta J(x)\end{aligned}$$

With these definitions, the reduced density becomes

$$\begin{aligned}f_Q^{\text{dis}}(x) &= -iv^2 \int dx' [\Pi(x) \partial_x \phi(x), h^{\text{dis}}(x')] \\ &= -iv^3 K (A_v + A_K) \int dx' [\Pi(x) \partial_x \phi(x), (\pi \Pi(x'))^2] \\ &\quad -iv^3 / K (A_v - A_K) \int dx' [\Pi(x) \partial_x \phi(x), (\partial_x \phi(x'))^2] \\ &\quad -iv^2 \sum_{mn} \frac{A_{nm}}{(2\pi a)^n} \int dx' \\ &\quad \left[\Pi(x) \partial_x \phi(x), \left(e^{i\Delta k x'} e^{i2n\phi} (\partial_x \phi)^{\delta_{n \text{ odd}}} + h.c. \right) \right] \\ &= v^3 K (A_v + A_K) \partial_x (\pi \Pi(x))^2 + v^3 / K (A_v - A_K) \partial_x (\partial_x \phi(x))^2 \\ &\quad -v^2 \sum_{mn} \frac{A_{nm}}{(2\pi a)^n} \left[e^{i\Delta k x} \partial_x \left(e^{i2n\phi(x)} (\partial_x \phi(x))^{\delta_{n \text{ odd}}} \right) + h.c. \right]\end{aligned}$$

The commutators have been evaluated following the rules given in appendix C.1. Similarly, the force associated with the spin current becomes

$$\begin{aligned}F_s^{\text{dis}} &= i[J_s, H] = i[J_s, H^U] + i[J_s, H^{\text{dis}}] \\ &= F_s + ivK \int dx dx' \delta R(x') [\Pi(x), h^{\text{dis}}(x')] \\ &= F_s + \int dx \delta R(x) f_s^{\text{dis}}(x) \\ f_s^{\text{dis}}(x) &= i(A_v - A_K) v^2 \int dx' [\Pi(x), (\partial_{x'} \phi(x'))^2] \\ &\quad + ivK \sum_{nm} A_{nm} \frac{g_{nm}^U}{(2\pi a)^n} \left[\Pi(x), \left(e^{i\Delta k x'} e^{i2n\phi(x')} (\partial_{x'} \phi(x'))^{\delta_{n \text{ odd}}} + h.c. \right) \right] \\ &= -2(A_v - A_K) v^2 \partial_x^2 \phi(x) \\ &\quad + vK \sum_{nm} \frac{i2n A_{nm}}{(2\pi a)^n} \left(e^{i\Delta k x} e^{i2n\phi(x)} (\partial_x \phi(x))^{\delta_{n \text{ odd}}} - h.c. \right)\end{aligned}$$

Disorder averaging

It is the right moment to take a look at disorder averaging. The disorder average over the correlation function that appears in the definition of the

memory matrix Eq. (4.23) can be evaluated as follows:

$$\begin{aligned}
\overline{\langle F_p^{\text{dis}}(t) F_q^{\text{dis}} \rangle}^0 &= \langle F_p(t) F_q \rangle_0 + \int dx dx' \overline{\delta R(x) \delta R(x')} \langle f_p^{\text{dis}}(x, t) f_q^{\text{dis}}(x', 0) \rangle_0 \\
&= \langle F_p(t) F_q \rangle_0 + D \int dx dx' \delta(x - x') \langle f_p^{\text{dis}}(x, t) f_q^{\text{dis}}(x', 0) \rangle_0 \\
&= \langle F_p(t) F_q \rangle_0 + D \int dx \langle f_p^{\text{dis}}(x, t) f_q^{\text{dis}}(x, 0) \rangle_0 \\
&= \langle F_p(t) F_q \rangle_0 + DV \langle f_p^{\text{dis}}(0, t) f_q^{\text{dis}}(0, 0) \rangle_0.
\end{aligned}$$

The mixed terms do not contribute due to $\overline{\delta J(x)} = 0$. In the last step we have used the translational invariance of the correlation function. Therefore we see that no integration in space is necessary and we are left with only the time integral appearing in Eq. (4.23). The first (unperturbed) contribution has been calculated by Shimshoni *et al.* [4] and is exponentially suppressed in the limit $T \ll J$. Inserting the second contribution into Eq. (4.23), the volume factor V cancels. Also, the memory matrix is proportional to the disorder strength D . We now are ready to carry out the contractions.

Identification of the correlators

We have to evaluate the following correlators for $\langle f_Q; f_Q \rangle_0$:

$$\begin{aligned}
&\langle \partial_x (\pi \Pi(0, t))^2 \partial_x (\pi \Pi(0, 0))^2 \rangle_0 \\
&2 \langle \partial_x (\pi \Pi(0, t))^2 \partial_x (\partial_x \phi(0, 0))^2 \rangle_0 \\
&\langle \partial_x (\partial_x \phi(0, t))^2 \partial_x (\partial_x \phi(0, 0))^2 \rangle_0 \\
&2 \langle \partial_x (e^{i2n\phi(0, t)} (\partial_x \phi(0, t))^{\delta_{n \text{ odd}}}) \partial_x (e^{-i2n\phi(0, 0)} (\partial_x \phi(0, 0))^{\delta_{n \text{ odd}}}) \rangle_0
\end{aligned}$$

for $\langle f_Q; f_s \rangle$:

$$\begin{aligned}
&\langle \partial_x (\pi \Pi(0, t))^2 \partial_x^2 \phi(0, 0) \rangle_0 \\
&\langle \partial_x (\partial_x \phi(0, t))^2 \partial_x^2 \phi(0, 0) \rangle_0 \\
&\langle \partial_x (e^{i2n\phi(0, t)} (\partial_x \phi(0, t))^{\delta_{n \text{ odd}}}) e^{-i2n\phi(0, 0)} \rangle_0
\end{aligned}$$

and for $\langle f_s; f_s \rangle$:

$$\begin{aligned}
&\langle \partial_x^2 \phi(0, t) \partial_x^2 \phi(0, 0) \rangle_0 \\
&\langle e^{-i2n\phi(0, t)} e^{-i2n\phi(0, 0)} \rangle_0
\end{aligned}$$

The mixed contributions (Umklapp- f with non-Umklapp- f) vanish because the sum of the prefactors does not add to zero (see c.f. [52]). We treat the terms with and without exponentials separately.

Terms without exponentials

Using appendix C.2, we obtain the following expressions for the terms without exponentials: for $\langle f_Q; f_Q \rangle_0$:

$$\begin{aligned}\langle \partial_x(\pi\Pi(0,t))^2 \partial_x(\pi\Pi(0,0))^2 \rangle_0 &= -4K^{-2}G^{(4)}(0,t)G^{(2)}(0,t) \\ 2\langle \partial_x(\pi\Pi(0,t))^2 \partial_x(\partial_x\phi(0,0))^2 \rangle_0 &= 2\left(-4\tilde{G}^{(3)}(0,t)^2\right) \\ \langle \partial_x(\partial_x\phi(0,t))^2 \partial_x(\partial_x\phi(0,0))^2 \rangle_0 &= -4K^2G^{(4)}(0,t)G^{(2)}(0,t)\end{aligned}$$

for $\langle f_Q; f_s \rangle$:

$$\begin{aligned}\langle \partial_x(\pi\Pi(0,t))^2 \partial_x^2\phi(0,0) \rangle_0 &= 0 \\ \langle \partial_x(\partial_x\phi(0,t))^2 \partial_x^2\phi(0,0) \rangle_0 &= 0\end{aligned}$$

and for $\langle f_s; f_s \rangle$:

$$\langle \partial_x^2\phi(0,t) \partial_x^2\phi(0,0) \rangle_0 = KG^{(4)}(0,t).$$

Where the number in parentheses (superscripts to the propagators) denote derivation with respect to the spatial variable. The cross terms appearing in $\langle f_Q; f_s \rangle$ vanish since they include an odd number of operators. Inserting the expressions of Eqs. (4.44) (and using elementary algebra) we can readily reduce the integrals to the form of Eq. (4.45) with $\gamma = 2, 4, 6$. As a reminder, the occurring constants are defined as $\tau = \pi T/v$ and $v = \pi/2Ja$ at the isotopic point.

Collecting prefactors, we obtain the following contributions from the terms induced by the variation of the couplings $\delta K(x)$ and $\delta v(x)$ to the memory matrix:

$$M_{QQ}[\partial_x\Pi^2\partial_x\Pi^2] = \frac{8\pi^5}{15}D(A_v + A_K)^2\left(1 - \frac{T}{J}\right)T^4 \quad (4.47)$$

$$M_{QQ}[\partial_x\Pi^2\partial_x(\partial_x\phi)^2] = -\frac{16\pi^5}{15}D(A_v^2 - A_K^2)\left(1 - \frac{T}{J}\right)T^4 \quad (4.48)$$

$$M_{QQ}[\partial_x(\partial_x\phi)^2\partial_x(\partial_x\phi)^2] = \frac{8\pi^5}{15}D(A_v - A_K)^2\left(1 - \frac{T}{J}\right)T^4 \quad (4.49)$$

$$M_{ss}[\partial_x^2\phi\partial_x^2\phi] = 0. \quad (4.50)$$

The last contribution vanishes because the integral $\int dt tG^{(4)}$ vanishes. Using the limit $T \ll J$ we finally arrive at

$$M_{QQ}[\delta v, \delta K] = \frac{2\pi^5 v^4 D A_K^2}{15a^4} \left(\frac{T}{J}\right)^4$$

for the terms without g_{nm} -contributions together. As one could have expected, the result does not depend on A_v : This term is induced by a variation of the spinon velocity v which is a global prefactor for the kinetic

term. One could get rid of this variation by a redefinition of the length scale, $dx \rightarrow dx (1 + \delta v(x)/v)$.

The result carries a power of T/J which we will use as the only measure by which we judge which contributions to the memory matrix dominate and which are subleading, as we have no information about the strength of the disorder. As $T \ll J$, higher powers of T/J are suppressed as compared to lower powers. It will turn out that the other scattering terms (associated with the g_{nm} come with lower powers of temperature and therefore they dominate the relaxation of heat current in the spin chain.

Terms with exponentials

We next turn to the correlators including exponentials of the fields. As these contributions involve the scattering of left movers to right movers induced by disorder, we refer to them as backscattering terms. To start with, we note that the periodic fluctuation $e^{i\Delta kx}$ appearing in those terms does not contribute if the disorder acts locally, as we have assumed. In appendix C.4 we consider the effect of a finite range disorder potential and show that its effect consists of an additional multiplicative factor $\exp(-|\Delta k|^2 \chi^2/2)$, where χ is the width of the disorder potential, which exponentially suppresses contributions from terms with $\Delta k \neq 0$. For n even, the contribution with exponentials to the s, s component can be found in the literature (c.f. [52]) and delivers

$$\left\langle e^{i2n\phi(x)} e^{-i2n\phi(x')} \right\rangle_0 = e^{4n^2 G_\phi(x-x')}.$$

For the Q, Q component, the appearing derivatives can be pulled outside of the correlator. We thus have for even n

$$\begin{aligned} \left\langle \partial_x e^{i2n\phi(0,t)} \partial_x e^{-i2n\phi(0,0)} \right\rangle_0 &= -\partial_x^2 \left\langle e^{i2n\phi(0,t)} e^{-i2n\phi(0,0)} \right\rangle_0 \\ &= -\partial_x^2 e^{4n^2 G_\phi(0,t)} \\ &= -\left(16n^4 G_\phi'(0,t)^2 + 4n^2 G_\phi^{(2)}(0,t)\right) e^{4n^2 G_\phi(0,t)} \end{aligned}$$

and since $G'(0,t) = 0$, we are left with

$$\left\langle \partial_x e^{i2n\phi(0,t)} \partial_x e^{-i2n\phi(0,0)} \right\rangle_0 = -4n^2 G_\phi^{(2)}(0,t) e^{4n^2 G_\phi(0,t)}$$

The exponential reads

$$e^{4n^2 G_\phi(0,t)} = (\tau a)^{2Kn^2} (i \sinh(\tau(vt - ia)))^{-2Kn^2}$$

and therefore we can use the same integrals of Eq. (4.45) as before, but with a modified, non-integer $\gamma = 2 + 2Kn^2$. After collecting prefactors ($\alpha = ka$

and $k = \pi T/v$ and $v = 2Ja$ as in the foregoing integration) obtains

$$M_{QQ}^{n\text{even}}[\delta g_{nm}] = 2\pi DK \frac{n^2 v^2 A_n^2}{(2\pi a)^{2n}} 2^{2Kn^2} I(2 + 2Kn^2) \left(\frac{T}{J}\right)^{2Kn^2}, \quad (4.51)$$

$$M_{ss}^{n\text{even}}[\delta g_{nm}] = 2DK \frac{(2n)^2 A_n^2}{a^2 (2\pi a)^{2n}} 2^{2Kn^2-2} I(2Kn^2) \left(\frac{T}{J}\right)^{2Kn^2-2} \quad (4.52)$$

where we have defined $A_n = \sum_m A_{nm}$. We note that due to the symmetry properties of the propagator, the $\langle f_Q f_s \rangle$ -term vanishes for even n .

Clearly, smaller values of n (the number of spinons scattered in-elastically) are more relevant, as they lead to a contribution to the memory matrix which come with a lower power of the small parameter T/J . Inserting the value that is closest to experiment, $K = 1/2$ (corresponding to an isotropic chain), and choosing the smallest even $n = 2$, we obtain the result that the discussed two-spinon processes are – with a contribution $\sim (T/J)^4$ – as relevant for the decay of the heat current as are the contributions discussed in the previous section, while, with a power $(T/J)^2$ the contribution to M_{ss} is the only one so far to the decay of spin current.

For odd n one has additional derivatives. One can evaluate them by writing the product of exponential and $\partial_x \phi$ terms as a derivative of the exponential, which brings us back to the above situation, but with more derivatives. We obtain

$$\begin{aligned} & \left\langle \partial_x \left(e^{i2n\phi(x,t)} \partial_x \phi(x,t) \right) \partial_x \left(e^{-i2n\phi(0,0)} \partial_x \phi(0,0) \right) \right\rangle_0 \\ &= -\partial_x^2 \left\langle e^{i2n\phi(x,t)} \partial_x \phi(x,t) e^{-i2n\phi(0,0)} \partial_x \phi(0,0) \right\rangle_0 \\ &= -\partial_x^2 \left[- \left(G_\phi''(x,t) + 4n^2 G_\phi'(x,t)^2 \right) e^{4n^2 G_\phi(x,t)} \right] \end{aligned}$$

and at $x = 0$ one gets

$$\left[12n^2 G_\phi^{(2)}(0,t)^2 + G_\phi^{(4)}(0,t) \right] e^{4n^2 G_\phi(0,t)}$$

The calculation proceeds in full analogy to the above one (but slightly more complicated) and one obtains and collecting all the factors we get as a final result

$$M_{QQ}^{n\text{odd}}[\delta g] = R_Q \left(\frac{T}{J}\right)^{2Kn^2+2} \quad (4.53)$$

$$M_{ss}^{n\text{odd}}[\delta g] = R_s \left(\frac{T}{J}\right)^{2Kn^2} \quad (4.54)$$

with

$$R_Q = D \frac{\pi^3 v^2}{4a^2} K \frac{Kn^2(4 + 3Kn^2)}{Kn^2 + 3/2} 2^{2Kn^2} I(2Kn^2)$$

and a similar expression for R_s , which we omit. Again, as with even n , the cross terms $\langle f_s f_Q \rangle_0$ vanish.

Therefore, the most dominant contribution identified so far are the one spinon processes $n = 1$ which lead in the isotropic chain $K = 1/2$ to a power $\sim (T/J)^3$ to M_{QQ} and $\sim T/J$ to M_{ss} . However, as we show below, there are still more relevant contributions.

4.2.5 The Leading Contribution

From the above calculations, a certain scheme in the occurrence of the power is apparent. One can trace back the origin of each contribution to the exponent to the presence of a corresponding term in the operator in f_q . Each spatial derivative acting on some function of ϕ contributes another factor of (T/J) , and if exponentials are present, this contributes a factor according to the prefactor in the exponential, here $2Kn^2$. Furthermore, the time integration $\int dt t$ removes two powers of (T/J) . In this way, it is easy to find the expected exponent.

We make then the following observation. The formula for the contribution for odd and even n differ by a factor of $(T/J)^2$, which stems from the additional factors of $(\partial_x \phi)$ for odd n which had to be included in the Umklapp terms to preserve parity and time reversal. Then it is clear, that the presence of impurities which break these symmetries, lead to odd n contributions lacking the additional factor $\partial_x \phi$ and therefore lead to a corresponding contribution to the memory matrix which comes with a reduced exponent, leading to the same formula in powers of (T/J) as for even n . Note that the resulting terms are for $n = 1$ precisely those given in Eqs. (4.36) and (4.38). Therefore, the leading contributions from impurity scattering to the memory matrix elements comprise

$$M_{QQ}[\delta h] = R_Q \left(\frac{T}{J} \right)^{2Kn^2} \quad (4.55)$$

$$M_{ss}[\delta h] = R_s \left(\frac{T}{J} \right)^{2Kn^2-2}. \quad (4.56)$$

For the prefactors we obtain the expressions

$$R_Q = \frac{\pi}{2} v^2 2^{2Kn^2} \frac{(2nB)^2}{(2\pi a)^{2n}} I(Kn^2) D, \quad (4.57)$$

$$R_s = \frac{K^2}{\pi} v^2 2^{2Kn^2} \frac{B^2}{(2\pi a)^{2n}} \cos(\pi Kn^2) B \left(Kn^2, \frac{1}{2} - Kn^2 \right) D, \quad (4.58)$$

where either $B = 1$ in the case of terms arising from parity breaking, or $B = \sqrt{D_h/D}$ in the case of the term arising from time reversal breaking, associated with a random magnetic field with disorder strength D_h . We

emphasize once more, that this result holds for both cases, operators which break time reversal, $\psi_L^\dagger \psi_R + h.c.$ and those which break parity, $i(\psi_L^\dagger \psi_R - h.c.)$, Eqs. (4.36) and (4.38), respectively. The calculation leading to the above results is performed along the same lines as in the previous section and is omitted here for brevity.

The dominant contribution comes from $n = 1$ and we note for later reference that in the isotropic case $K = 1/2$ the relevant contribution to the heat current component of the memory matrix becomes

$$M_{QQ} = R_Q T = 2\pi^2 \frac{\overline{\delta h^2}}{(2\pi a)^{2n}} \frac{v^2}{J} \cdot T. \quad (4.59)$$

4.2.6 Memory Matrix Off-Diagonals

So far, we did not consider cross-terms M_{Q_s} . Such contributions could be shown to vanish identically in the case of the less relevant contributions. However, in the case of the new terms odd under either time-reversal or parity, non-vanishing contributions to the off diagonals of the memory matrix appear, as some contributions now have matching numbers of derivatives. (In the case of the time-reversal breaking terms these components are only present, if the fluctuations in the lattice spacing and those in the induced magnetic field are correlated.) The two possible contributions to M_{Q_s} stem from

$$\left\langle \partial_x e^{i2\phi(0,t)} e^{-i2\phi(0,0)} \partial_x \phi(0,0) \right\rangle_0 = -2i G_\phi^{(2)}(0,t) e^{4G_\phi(0,t)} \quad (4.60)$$

$$\left\langle \partial_x \left(e^{i2\phi(0,t)} \partial_x \phi(0,t) \right) e^{-i2\phi(0,0)} \right\rangle_0 = -2i G_\phi^{(2)}(0,t) e^{4G_\phi(0,t)} \quad (4.61)$$

thus there is only one integration we have to consider, which has been carried out already, namely

$$i \int_{-\infty}^{\infty} dt t G_\phi^{(2)}(0,t) e^{4G_\phi(0,t)} = \frac{\pi (\tau a)^{2Kn^2}}{4 v^2} I(Kn^2)$$

As the only occurrence of temperature is through the reduced temperature $\tau = \pi T/v$, this component of the memory matrix behaves as

$$M_{Q_s} \sim \left(\frac{T}{J} \right)^{2Kn^2}, \quad (4.62)$$

i.e. M_{Q_s} carries the same power of temperature as M_{QQ} . The heat conductivity is given by the QQ component of the inverse of the memory matrix. It has the structure

$$\left(\begin{pmatrix} T^{2K} & T^{2K} \\ T^{2K} & T^{2K-2} \end{pmatrix}^{-1} \right)_{QQ} \sim \frac{T^{2K-2}}{T^{4K} + T^{4K-2}} \quad (4.63)$$

and the T^{4K} contribution from the off-diagonals in the denominator is sub-leading. Therefore, the dominant contribution to the heat conductivity comes from the M_{QQ} term, $(M^{-1})_{QQ} \approx M_{QQ}^{-1}$. As a consequence, the contribution of the spin current is irrelevant in the sense that we would have obtained the same result for the heat conductivity if we would have omitted it as a slow mode in the first place. The physical reason behind this is that the spin current has a much higher decay rate than the heat current (indicated by the appearance of a lower power in T/J) and therefore can be neglected as a slow mode. The spin current is not a mode sufficiently slow to protect the decay of the heat current.

4.2.7 Discussion

To summarize, we have calculated various contributions to the memory matrix arising from dilute disorder in the system. The most relevant contributions stem from the absence of parity or time reversal symmetry, broken by the presence of the impurities. The associated contributions to the Hamiltonian are relevant in the RG sense, but can be treated perturbatively for weak perturbations and not too low temperatures.

We have found that non-vanishing contributions to the off-diagonals of the memory matrix exist, but these contributions do not affect the conductivity. In fact, one could have omitted the choice of the spin current as a slow mode in the first place, which would lead to exactly the same $T \ll J$ result.

Using the main result of this section, Eq. (4.55), we get for the heat current ($\kappa \leq 1/T\chi^2/M_{QQ}$ with $\chi \sim T^2$) in the isotropic case $K = 1/2$ the prediction

$$\kappa \sim T^2 \tag{4.64}$$

in our approximation. Therefore, we expect a quadratic increase in temperature for the spin chain contribution to heat conductivity at not too low temperatures. Towards even lower temperatures, the effect of the relevant perturbations on the low energy degrees are so strongly affected by the disorder, that the Luttinger liquid picture will not be adequate any more. Also at low temperatures, localization effects will set in that will lead to an exponential suppression of the conductivity. At $T = 0$ and $K < 1$, the tiniest amount of disorder is sufficient to localize the Jordan-Wigner fermions completely, leading to a vanishing conductivity $\kappa = 0$ in this case.

While we have discussed the effect of weak impurities, one can not exclude that there are strong impurities present in the real system, having a more drastic effect on transport properties. For example, one could imagine foreign atoms with a different spin or vacancies, substituting spins across the chains randomly. Such perturbations could lead to a much stronger effect, as they effectively cut the chains. Our perturbative treatment is not capable

of accounting for this kind of impurities, and different methods should be applied to describe that situation.

4.3 Full Memory Matrix: Coupling to Phonons

In this section we set up a complete microscopic description of the spinon contribution to the heat conductivity in spin chain compounds similar to SrCuO_2 and Sr_2CuO_3 described in Refs. [8, 45]. As above, we restrict ourselves to situations in which a perturbative treatment in terms of the memory matrix formalism is possible. While the contribution from impurity scattering of spinons – which describes the behavior of the heat conductivity below $T \approx 60\text{K}$ – has been discussed in the last chapter, in this chapter we will enlarge our theory by taking into account the coupling of the phonons to the spinons, which determine the decay of the spinon heat conductivity above $T \approx 100\text{K}$. Besides the scattering of the spinons by phonons we take care of a modeling of the phonon contribution to the heat conductivity. In particular, we discuss under what circumstances a simple separation of the observed heat conductivity into a phononic and a spinonic contribution $\kappa = \kappa_p + \kappa_s$ can be assumed and whether such a separation is appropriate for the experimental situation under consideration. We also perform an analysis of the occurring limits and will find that many features of the experimental system are reproduced correctly, while some are decisively not. We will discuss how the result can be improved.

The outline of the section is as follows. First, we will describe the phononic component of the heat conductivity. Then we will shortly review a work by Shimshoni *et al.* [4] where the heat conductivity in a clean spin chain coupled to phonons has been analyzed in detail. As the methods utilized there are the same memory matrix techniques used here, we can straightforwardly incorporate their results in a memory matrix formalism which takes into account both phonons and spinons and their mutual interaction. After formulating the full memory matrix, we will identify all contributions. A discussion of different regimes follows. In the end we will give a summary and outlook with suggestions for future work.

4.3.1 Contributions to the Memory Matrix

We recall that a lower bound to the heat conductivity can be obtained by calculating the approximate memory matrix, \tilde{M} , in terms of which

$$\kappa \geq \frac{1}{T} \chi^T \tilde{M}^{-1} \chi. \quad (4.65)$$

Next we chose an appropriate set of slow modes, consisting of the normalized translation operators $J_s = -v^2 P_s$ for the spin chain and $J_p = -v^2 P_p$ for the

phonon bath. Note that the normalization of the phonon translator is chosen with respect to the *spinon* velocity, for convenience. In terms of these slow modes, the vector of susceptibilities χ is given by

$$\chi = \begin{pmatrix} (J_Q|J_s) \\ (J_Q|J_p) \end{pmatrix}. \quad (4.66)$$

The heat current is given by $J_Q = -v^2 P_s - v_p^2 P_p$. As we evaluate the susceptibilities with respect to the unperturbed system (where the coupling between the spin chain and the phonon bath is considered as a small perturbation), the susceptibility vector reduces to

$$\chi = \begin{pmatrix} (J_s|J_s) \\ \gamma(J_p|J_p) \end{pmatrix}, \quad (4.67)$$

where we have introduced the small parameter $\gamma = (v_p/v)^2$.

The memory matrix \tilde{M} has various contributions. Assuming that the coupling between spinons and phonons vanishes, the memory matrix (in the basis $\{J_s, J_p\}$) is diagonal,

$$\tilde{M} = \begin{pmatrix} M_s & 0 \\ 0 & M_p \end{pmatrix} \quad (4.68)$$

and in this case the heat conductivity reduces to the sum of the contributions from the spin chain and phonons, respectively:

$$\kappa = \frac{1}{T} \chi_s^2 / M_s + \frac{1}{T} \chi_p^2 / M_p. \quad (4.69)$$

Here M_s includes the contributions from weak impurities, discussed in the last chapter, as well as intrinsic Umklapp scattering terms⁹ discussed in 4.1.5. The phonon memory matrix M_p is not known a priori. Since the phonon heat conductivity is dictated by various phenomena (to be discussed below) and a complete modeling of the phonon bath is both complicated and beyond our scope¹⁰, we will, concerning the pure phonon contribution to the memory matrix, take a phenomenological point of view, and chose it just in the right fashion to match the experimental results perpendicular to the chain direction (i.e. the pure phonon part).

The coupling to phonons generates an additional contribution to the memory matrix which has non-vanishing off-diagonal contributions in the above discussed basis. In particular, the coupling to phonons will invalidate the simple splitting of the total heat current into the respective contributions from the two subsystems, Eq. (4.69). In the following, we will identify each contribution in turn, to finally put all pieces together.

⁹While impurity scattering dominates the decay at low temperatures, $T \ll J$, towards intermediate temperatures $T \lesssim J$ intrinsic scattering limits the value of the conductivity.

¹⁰The phonon heat conductivity is not the subject of this thesis.

4.3.2 The Susceptibilities

According to Equation (4.67) we have to calculate the generalized susceptibilities given by the correlation function $(J_s|J_s)$, which is a property of the spin chain alone and the correlation function $(J_p|J_p)$, which is a property of the phonon bath alone, respectively. As all perturbations are considered to be weak enough to consider them perturbatively, their contribution to the conductivity is through the memory matrix, whereas perturbative corrections to the susceptibilities are subleading. The susceptibility of the spin-translation operator P_s has been calculated in [4] and is given by

$$\chi_s = (J_Q|J_s) = \frac{\pi}{3} vT^2.$$

The calculation of this expression assumes the low energy limit $T \ll J$ and can therefore be assumed to be valid in the whole experimental range.

The susceptibility χ_p of the phonon translation operator P_p is calculated in appendix C.3. While we give the result for two limiting cases, $T \ll \Theta_D$ and $T \gg \Theta_D$, no analytic expression exists for the general result. In the appendix we argue that the $T \ll \Theta_D$ result is a good approximation for T below about $0.15\Theta_D$, while the $T \gg \Theta_D$ result gives a reasonable approximation at around Θ_D , too. The part of the experimental curve which is of interest to us is $60K < T < 300K$ (and $\Theta_D \approx 430K$), which at first sight would suggest the low temperature result. However, the deviations from the real curve for χ_p in this regime are much smaller using the high-temperature approximation¹¹, in relative terms, than using the low temperature result. Therefore, to reproduce the experimental results, we chose the high energy limit, given by

$$(J_Q|J_p) = v_p^2 v^2 (P_p|P_p) = \frac{\Theta_D^3 v^2}{6\pi^2 v_p^3} T. \quad (4.70)$$

We note that the expressions for the susceptibilities for spinons and phonons carry different dimensionality, as the spin chain susceptibility is measured in units of length, whereas the phonon susceptibility is in units of volume. One has two possibilities to deal with this mismatch. Either one includes a summation over the whole (two dimensional) array of spin chains, or one determines the per spin chain contribution of the phononic susceptibility. Here we chose the latter route. The area of the cross section associated with one wire is about $\sim 3a^2$ in the compounds SrCuO_2 and Sr_2CuO_3 of interest to us [68]. Therefore we use, instead of Eq. (4.70), the phonon susceptibility ‘per spin chain’, $\chi_p = 3a^2 (J_Q|J_p)$. This is quietly assumed in all what follows.

¹¹What concerns the phonon susceptibility, its exact dependence on temperature is not crucial. For our purposes it is sufficient to work with the correct order of magnitude, as will become clear later.

4.3.3 Phonon Heat Conductivity

We recall the structure of the lattice heat conductivity κ_p measured perpendicular to the chain direction in the spin chain compounds. The temperature dependence is typical of an insulating crystal whose heat conduction is dominated by phonons and lacking phase transitions in the whole range of temperature.

The high temperature asymptotic behavior of the phononic heat transport is characterized by a decay of the heat conductivity $\kappa_p \sim T^{-\alpha}$ with a power of α typically varying between 1 and 2. The precise theory of the power law is complicated and has to do with the competition of cubic and quartic terms. The reason for the decay is the following. In this high temperature regime $T > \Theta$, the number of phonons in the system becomes $\propto T$ and it becomes more likely for a phonon to get scattered by other phonons.

As temperature is decreased below the debye temperature Θ_D , the probability of Umklapp scattering events becomes exponentially suppressed as the Umklapp processes freeze out. The heat conductivity rises accordingly.

However, the heat conductivity can not increase indefinitely. Any real physical system has finite dimensions and the phonons will scatter off the boundaries of the sample. This effect starts to dominate where the mean free path of the phonons is of the order of the system size, in our case at about $T = 6K$. This leads to the characteristic low temperature behavior $\kappa_p \sim T^3$ at the lowest temperatures.

The combination of these effects leads to the characteristic low temperature maximum of the phononic heat conductivity around $T \approx 10K$. However, there is an additional mechanism of scattering for phonons, namely scattering off impurities. This mechanism mainly dominates around the low temperature maximum of the phononic heat conductivity and leads to a lowering of the maximal value. If there are many impurities, the suppression can be strong enough to be relevant up to around the Debye temperature, in which case the effect of exponential suppression of U processes can be completely be shaded by disorder effects. This is the case for example in the copper-oxide compounds considered here, as the exponential behavior of the heat conductivity for $20K \lesssim T \lesssim \Theta_D = 400K$ can hardly be observed. The heat conductivity in this case can be fitted to $\kappa_p \sim T^{-\alpha}$ with an exponent varying between 1 and 1.3 right down to the boundary scattering region. In fact, isotope scattering is of comparable magnitude to Umklapp scattering in many substances, even at room temperature.

For our purpose, the precise source of phonon scattering is irrelevant, as we are interested in the excess spinon contribution. What may happen to be important is the power law dictating the scattering rate and therefore the conductivity. As throughout the relevant temperature range (where the excess spinon contribution is significant) the experimental observation is

consistent with a power law like behavior with an exponent close to 1, we therefore make the assumption that in the relevant temperature range the phonon heat conductivity behaves as $\kappa_p \sim 1/T$.

In modeling the phonons, we will do without the behavior of the conductivity at and below the phonon peak, and we use the high temperature expression for the susceptibility, as discussed above. We adjust the powers in temperature for the memory matrix by requiring the resulting conductivity to behave as $\kappa_p = \chi_p^2/(TM_p) \sim 1/T$. With the susceptibility given by $\chi_p = \gamma(J_p|J_p) \sim T$, we obtain

$$M_p = m_p T^2, \quad (4.71)$$

where the constant m_p is chosen to best fit the experimental result for the phononic heat conductivity.

4.3.4 Spinon Heat Conductivity

The main result of the last section was that the disorder induced memory matrix has the leading order contribution $M_s \sim T$, leading to the low temperature behavior $\kappa \sim T^2$ for the heat conductivity. Going towards higher temperatures, however, Umklapp scattering of spinons becomes relevant, in the same fashion as for the phonons. But in this case, the temperature scale at which Umklapp events start to dominate, is $T \sim J$. Therefore such a term will lead to a cutoff in the spinon contribution to heat conductivity (predicted by only impurities as $\kappa \sim T^2$) at temperatures close to $T \lesssim J$. We will see, that coupling to phonons provides a much more efficient source of scattering at a temperature regime well below J . Therefore, in this approximation we neglect contributions from intrinsic Umklapp scattering, and set

$$M_s = m_s \frac{T}{J} \quad (4.72)$$

where the constant m_s is proportional to the disorder strength D .

4.3.5 Coupling between Spinons and Phonons

The coupling of the phonons to a clean spin chain and its effect on the heat conductivity has been discussed in detail by Shimshoni *et al.* in Ref. [4], where the same methods used here found application. We shortly describe the setup and main results that concern us.

We write the joint Hamiltonian of the spin chain and the phonons as

$$H = H_s + H_p^{3D} + H_{sp} \quad (4.73)$$

where H_s describes the spin array (a simple sum over Hamiltonians of the form Eq. (4.15)), H_p^{3D} is the phonon Hamiltonian, and H_{sp} the interaction

between spins and phonons. One can model the 3D phonon bath (optical phonons are omitted) by a harmonic Hamiltonian similar to the Luttinger liquid,

$$H_p^{3D} = \int \frac{d^3x}{2\pi} \left[(\pi P)^2 + \sum_{\mu} v_{\mu}^2 (\partial_{\mu} q)^2 \right] \quad (4.74)$$

where μ denote the x, y and z directions, P and q are (appropriately normalized) canonical phonon momentum and coordinate operators and v_{μ} are the sound velocities with $v_x = v_p$. As the coupling between chains is neglected, one can integrate out the perpendicular directions and consider only the phonon dynamics along a single chain. Neglecting spin-orbit coupling, the dominant coupling arises from the dependence of the exchange couplings on the distance of the atoms, $J_{ij} = J_0(R_i - R_j) \approx J_0 + a(\partial_x q)J_{sp}$. This coupling introduces contributions to H_{sp} which can, likewise, be classified into Umklapp and non-Umklapp terms, depending on whether $(\partial_x q)$ couples to an Umklapp or non-Umklapp term in H_s .

To emphasize the main effect of phononic coupling on the spin chain, it is illustrative to remind ourself of the situation in the pure spin chain *without* coupling to phonons. The memory matrix for the heat current in that case has the form

$$M_{QQ}^{\text{pure}} \sim (\Delta k)^2 \left(\frac{T}{J} \right)^{2Kn^2} e^{-\frac{v|\Delta k|}{2T}} \quad (4.75)$$

for n even, and an additional factor $(T/J)^2$ has to be included for n odd. As mentioned above (see end of section 4.1.5) we observe that this expression vanishes when $\Delta k = 0$ because the heat current commutes with the translationally invariant terms, and for finite Δk the contribution is exponentially suppressed. More precisely, for $|\Delta k| = \pi/(2a)$ and with $v \sim Ja$ the exponent becomes $\sim J/T \gg 1$.

The major effect of the coupling to phonons is, that in the exponent the fast spinon velocity is replaced by the much slower phonon velocity, leading to $e^{-v_p|\Delta k|/(2T)}$ and therefore the exponential suppression of the memory matrix is much weaker, in particular close to the Debye temperature. As in the Debye approximation the spinon velocity and the debye temperature may be related (see below), the exponent can be translated to $\sim \exp(-0.5\Theta_D/T)$. Therefore, the phonons introduce a much more efficient mechanism of scattering. The physical reason behind this effect is that the minimal energy cost of a process which involves a momentum transfer of Δk is associated with the energies $v\Delta k/2$ of the elementary excitations involved in the process (see Ref. [4]). Because in our case $v_p \sim v/20$, the phonons make momentum transfer less costly and therefore they dominate the relaxation above the spinon peak. The most dominant process has been identified to be a two

phonon process with both phonons carrying a momentum of the order of $\sim \Delta k/2$.

Let us see, how this output is generated by the memory matrix formalism. Choosing the slow modes heat current J_Q and the normalized translation operator $J_T = v(P_s + P_p)$, one obtains the diagonal memory matrix¹²

$$M_{sp} = \begin{pmatrix} M_{QQ} & 0 \\ 0 & M_{TT} \end{pmatrix} \quad (4.76)$$

where the dominant contribution to M_{QQ} stems from $n = 2, m = 1$ and $\Delta k = 0$, giving rise to a power T^3 for this contribution [4]. The translation operator component M_{TT} , however, lacks contributions with $\Delta k = 0$. This reflects the fact that the translation operator J_T conserves momentum. As argued above, Umklapp terms involving transfer of momentum between the spinons and the phonons are suppressed by an exponential on the energy scale Θ_D instead of J , and therefore they comprise the more dominant scattering mechanism. The leading contribution has been identified in [4]:

$$M_{TT} \sim T^4 \exp\left(-\frac{v_p |\Delta k|}{2T}\right), \quad (4.77)$$

with a two phonon process implying $\Delta k = G/2$, which is much smaller than M_{QQ} at temperatures below $v_p G/4 \sim 170K$. As the memory matrix is diagonal, the two components contribute separately, $\kappa \sim M_{QQ}^{-1} + M_{TT}^{-1}$, and for small temperatures thus M_{TT} dominates, leading as a result to an exponentially diverging conductivity for the clean spin chain coupled to phonons¹³. Therefore, it is necessary to include the effect of disorder and also the scattering of phonons in our considerations.

4.3.6 Result and Discussion

We are in the position to calculate the full memory matrix. We have identified all important contributions. As a lower bound for the heat conductivity we get

$$\kappa \geq \frac{1}{T} (\chi_s, \chi_p) \cdot \left[\begin{pmatrix} M_s & 0 \\ 0 & M_p \end{pmatrix} + A \begin{pmatrix} M_{TT} & 0 \\ 0 & M_{QQ} \end{pmatrix} A^T \right]^{-1} \cdot \begin{pmatrix} \chi_s \\ \chi_p \end{pmatrix} \quad (4.78)$$

¹²In Ref. [4] a 3×3 memory matrix is considered with the spin current operator as the third slow mode. However, the scattering rate of the spin current is much higher than that of the other two slow modes and consequently does not contribute to the heat current. The same applies to the scattering due to disorder, as shown in the previous section. Using this information, we omit the spin current as a slow mode right from the start.

¹³Here the scattering of phonons has been neglected.

where the transformation matrix

$$A = \begin{pmatrix} 1 & 1 \\ 1 & \gamma \end{pmatrix}^{-1}, \quad (4.79)$$

with $\gamma = (v_p/v)^2$, transforms between the bases of slow modes $\{J_s, J_p\}$ and $\{J_Q, J_T\}$.

Using $\gamma \ll 1$, we arrive at the expression

$$\begin{aligned} \kappa &\geq \frac{1}{T} \frac{\chi_p^2(M_s + M_{QQ} + \gamma^2 M_{TT}) + \chi_s^2(M_p + M_{QQ} + M_{TT})}{M_p M_s + M_p(M_{QQ} + \gamma^2 M_{TT}) + M_s(M_{QQ} + M_{TT}) + M_{QQ} M_{TT}} \quad (4.80) \\ &+ \frac{1}{T} \frac{2\chi_p \chi_s (M_{QQ} + \gamma M_{TT})}{M_p M_s + M_p(M_{QQ} + \gamma^2 M_{TT}) + M_s(M_{QQ} + M_{TT}) + M_{QQ} M_{TT}} \quad (4.81) \end{aligned}$$

This is the general expression in the presence of disorder and spin-phonon coupling. The second term is referred to as the *drag*-term. Several limits may be identified.

First, we discuss the simplest case, namely the limit where phonons do not scatter, $M_p = 0$, and the system is clean and we can set $M_s = 0$, too. This is the limit discussed in Ref. [4]. In this limit, Eq. (4.81) reduces to

$$\kappa \geq \frac{1}{T} (\chi_s + \gamma \chi_p)^2 (M_{QQ}^{-1} + M_{TT}^{-1}).$$

This reproduces the result of [4]: In the asymptotic limit $T \ll \Theta_D$, M_{TT}^{-1} is much larger, and the conductivity diverges exponentially. Physically, as momentum is conserved by the N processes, the only mechanism to lose momentum is through Umklapp scattering, which is exponentially suppressed at low temperature.

Second, we would like to identify the limits relevant to the experiment. To deal with this, we first make an obvious observation: The total heat current measured in the experiment is larger or equal to the phononic contribution (i.e. the curve one would expect for the heat conductivity without the presence of a spin chain) for all temperatures. Formally, we have $\kappa - \kappa_p > 0$, with $\kappa_p = T^{-1} \chi_p / M_p$. While it is not a priori clear that any useful information can be gained from this criterion, we shall see that its analysis leads to a better understanding of the physics behind the involved processes.

We consider two different limits. Let us take the trivial limit of no coupling, $M_{QQ} = M_{TT} = 0$, first. Then, the spin chain and the phonon subsystem carry momentum independently, and we have $\kappa = \kappa_s + \kappa_p$. Therefore, $\kappa - \kappa_p > 0$ is automatically fulfilled in the weak coupling limit.

Turning to the strong coupling limit, $M_{QQ} \gg M_p, M_s$, by calculating $\kappa - \kappa_p$ using Eq. (4.81), we arrive at the criterion

$$\frac{\chi_s(\chi_s + 2\chi_p)}{M_s} > \frac{\chi_p^2}{M_p}. \quad (4.82)$$

As all appearing quantities are positive, this provides us with two separate criteria: The full conductivity to be larger than the pure phonon part, it is sufficient, that the pure spinon conductivity be larger than the phonon conductivity,

$$\kappa_s > \kappa_p \quad (4.83)$$

or that the scattering-rate of the phonons be larger than the scattering-rate of the spinons,

$$\frac{M_p}{\chi_p} > \frac{1}{2} \frac{M_s}{\chi_s}. \quad (4.84)$$

Let us discuss the first criterion. One of the conductivities is always larger, and by symmetry of the argument, if $\kappa_p > \kappa_s$, this means that $\kappa - \kappa_s > 0$, and therefore the first criterion tells us that the smaller of the conductivities of the subsystems establishes a lower bound to the full heat conductivity,

$$\kappa \geq \min(\kappa_s, \kappa_p). \quad (4.85)$$

This relation tells us, that, no matter how strong the coupling, the conductivity is bound from below by the smaller of the conductivities. This is obvious for mechanisms which conserve momentum, e.g. M_{QQ} , as the strong coupling the coupling then simply provides a mechanism to pass momentum quickly between the systems and momentum is then relaxed according to the stronger decay mechanism, forcing the total conductivity to the smaller one of the individual subsystems. However, relation (4.85) also holds for couplings that do *not* conserve momentum, e.g. M_{TT} , which is less obvious.

More insight can be gained by considering the second criterion, (4.84), which relates the physical scattering rates to each other. Equation (4.84) tells us, that (no matter how small the heat conduction provided by the spin chain is) if the phonon scatter faster, then the spinons can not provide a more efficient mechanism of scattering, therefore the total heat conductivity is larger than the pure phononic one. We note that Eq. (4.84) was derived with the assumption that the momentum conserving mechanism M_{QQ} dominates. Considering M_{TT} , (e.g. in the regime where $M_{TT} \gg M_{QQ}$) the criterion (4.84) gets modified and becomes $\gamma M_p / \chi_p > \frac{\gamma}{2} M_s / \chi_s$. However, the exact prefactor shall not be of concern. We content ourselves with the identification of the regime $M_p / \chi_p \gg M_s / \chi_s$ as a sufficient condition for $\kappa > \kappa_p$.

Having identified these limits, which shall lead the following analysis, we turn our attention to the experimental result. The following table summarizes the contributions appearing in Eq. (4.81) that we have identified in the

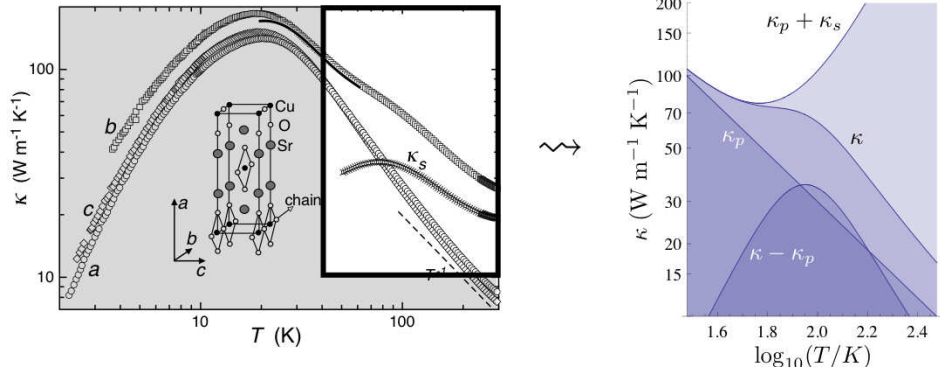


Figure 4.3: Right: Phonon heat conductivity κ_p , heat conductivity of phonons and spinons without coupling, $\kappa_p + \kappa_s$, full heat conductivity with coupling κ and full heat conductivity with the phononic contribution subtracted, $\kappa - \kappa_p$. The curves are to be compared with the experimental curves Fig. 4.1, redisplayed for direct comparison to the left. The area of interest is highlighted. The curves were obtained as described in the main text.

last sections.

$$\chi_p \sim T \quad (4.86)$$

$$\chi_s \sim T^2 \quad (4.87)$$

$$M_p \sim T^2 \quad (4.88)$$

$$M_s \sim T \quad (4.89)$$

$$M_{QQ} \sim T^3 + T^4 e^{-T^*/T} \quad (4.90)$$

$$M_{TT} \sim T^4 e^{-T^*/T} \quad (4.91)$$

The prefactors of the susceptibilities χ_p and χ_s have been determined in section 4.3.2 and all appearing constants are determined by the experiment. The prefactor of M_p is not known a priori, but can be determined by fitting κ_p to the experiment at high temperatures. We choose $\kappa_p(T = 100K) \approx 30 W m^{-1} K^{-1}$. In Fig. 4.3, we have plotted (among other) the resulting phonon heat conductivity in the region of interest. We note that we omit the low temperature region, as the interesting part of the experimental curve (where the spinon contribution is significant) resides in a temperature range where the high temperature limit to the phonon susceptibility χ_p is well suited. We remind the reader that the power of M_p has been chosen such as to account for the $\sim 1/T$ decay of the transversal (phonon) heat conductivity.

The prefactor of disorder scattering of spinons, the only contribution to M_s which we take into account, has been determined in section 4.2.5. All

appearing constants are known from experiment besides the coupling constant $g/\sqrt{2\pi a}$ appearing in front of the relevant operator, and the disorder strength. As our best guess, we chose $g/\sqrt{2\pi a} \approx J$ and let the disorder strength vary in some sensible region, $|\delta J(x)|/J = 1/1000 \cdots 1/10$, as a free parameter. Fig. 4.3 shows the conductivity with a disorder of 5% in the exchange coupling J . We observe that there is an onset of the spinon heat contribution turning to a $\sim T^2$ behavior of the conductivity, dictated by the disorder scattering of spinons. Note, that the approximation for g is crude and its exact value is not known from first principles for a generic spin chain. Therefore, this method can not be used to make a precise prediction about the strength of disorder in the spin-system. However, the *order of magnitude* for all constants should be correct, and the resulting curve (i.e. the distinct feature, the temperature at which the spinon contribution sets in) suggests that the analysis is consistent. Before turning on the coupling between spin chain and phonons, we note, that in a real measurement on a system without that coupling one would observe the phonon heat conductivity only. Namely, heat can be passed through the links to the specimen only via phonons, while spinons exist in the specimen only and can not be accessed from the outside. Therefore, coupling between spinons and phonons is crucial for the participation of the spinons in heat transport.

We turn our attention to the terms associated with the coupling of the spin chain to the phonons. The single coupling term without momentum transfer $\Delta k = 0$ appearing in M_{QQ} alone is not capable of producing a peak in the spinon contribution, as its limiting behavior is given by $1/T(T^2)^2/T^3 \sim \text{const.}$. Therefore, a term with momentum transfer $\Delta k \neq 0$ is required. Of these terms those are the most relevant for which the exponential sets in at the lowest temperature and therefore cuts off the conductivity first. In Ref. [4] the leading term has been identified and is associated with the one spinon two phonon process $n = 1 \ l = 2$ which appears (and has been included) in both M_{QQ} and M_{TT} . By tuning the (unknown) prefactor, we obtain the other two curves depicted in Fig. 4.3, one for the full heat conductivity, the other with the phonon part subtracted, as in the experimental curves measured by Sologubenko *et al.*, Fig. 4.1. As expected, the presence of the $n = 1 \ l = 2$ process leads to a suppression of the conductivity towards higher temperatures and generates a spinon peak, as observed in the experiment. The position of the peak depends sensitively on the prefactor of that term, and it has been chosen such that the position of the spinon peak is approximately where observed in the experiment. By choosing different values for the prefactor of the $\Delta k = 0$ term in M_{QQ} , one can tune the width of the spinon peak structure. A finite value always leads to a broadening of the peak, therefore the depicted curve (where the prefactor of that term has been set to zero) represents the minimal width of the spinon peak. The apparent saturation of the spinon contribution towards the highest measured temper-

atures observed in the experiment (see again Fig. 4.1) is not reproduced by our choice of the memory matrix. This may be attributed to one of several possible issues. First, the expression we used for M_{TT} $T^4 \exp(-T^*/T)$ is valid in the asymptotic limit $T \ll \Theta_D$ only. There is no reason why the power T^4 should remain the same close to or above $T^* = v_p \Delta k / 2$. (The low temperature asymptotics of the Debye-approximation, which was used to determine these expressions for the memory matrix, is good only below about $T < 0.15\Theta_D$. Above this value, considerable deviations should be expected.) In fact, the high temperature limit of this contribution ($n = 1$, $l = 2$) can be determined from Ref. [4] to be $\sim T^2$. One could argue, that in the crossover region, $T \approx \Theta_D$, one can legitimately set the power in front of the exponential to $T^{\sim 3}$, which then would be consistent with a saturation of the heat current. The second possible issue is that the process attributed to the chosen M_{TT} is quite unusual, involving the scattering of *one* spinon from one fermi point to the other and the creation of *two* phonons with equally distributed energies. While these processes have been identified to be the dominant ones in the low temperature limit, such a process can be assumed to be rare and therefore it might come with a very small prefactor. Therefore, it can be expected that, at intermediate temperatures $T \approx \Theta_D$, other Umklapp processes are more relevant, for example those with $n = 1$ and $l = 1$. As should be clear from our analysis, it is most probably possible to reconstruct every single feature of the experimental curve by accounting for other processes, providing us with additional fit parameters.

As a final step, let us identify the relevant regimes of the heat conductivity, to determine which contributions from Eq. (4.81) are the most significant. This will allow us to write down an approximation to the heat conductivity. By using the values of the fit parameters which define the curves shown in Fig. 4.3, we observe that throughout the interesting region, the scattering rate of the phonons is much larger than that of the spinons: $M_p/\chi_p \gg M_s/\chi_s$. Therefore, as argued above, the total heat conductivity is bounded from below by the phonon contribution. Furthermore, from above $T \sim 100K$ the two-phonon process contributing to M_{QQ} and¹⁴ M_{TT} starts to dominate over M_s , but remaining much smaller than M_p in the entire region. These observations are sufficient to considerably simplify the expression for the conductivity. One obtains in this limit the expression

$$\kappa = \frac{1}{T} \left(\frac{\chi_p^2}{M_p} + \frac{\chi_s^2}{M_s + M_{QQ}} \right) = \kappa_p + \frac{1}{1/\kappa_s + 1/\kappa_{sp}}, \quad (4.92)$$

¹⁴In fact, the contribution of the two-phonon Umklapp to M_{TT} may be neglected as it is suppressed by a factor $\sim \gamma$ in the conductivity, due to the structure of the transformation matrix A of Eq. (4.79).

where we have defined

$$\kappa_{sp} = \frac{1}{T} \frac{\chi_s^2}{M_{QQ}}. \quad (4.93)$$

The so-called drag-term (the mixed term in the conductivity $\sim \chi_s \chi_p$) does not contribute in this limit.

To conclude, the scattering introduced by the spin-phonon coupling is not strong enough to affect the phonon component of the heat conductivity. The scattering of the spinons by impurities and by phonons is of equal strength at the spinon peak. This result holds despite the limitations of our modeling.

The limitation concerning the spin-phonon coupling is the fact that the $\Delta k \neq 0$ terms derived in [4] are strictly valid only in the $T \ll \Theta_D$ asymptotics, as the low temperature limit of the Debye approximation has been used. As we have seen for the phonon susceptibility, this limit does probably not describe the behavior correctly at temperatures closer to Θ_D . Therefore one might question our Ansatz altogether. An analytic treatment without that approximation is cumbersome. A better account for the behavior of the conductivity above the spinon peak could be given by a numerical determination of the contributions to M_{QQ} . However, the lack of knowledge of the various coupling constants of the backscattering terms would remain a principal conceptual weakness of the presented approach, at least when it comes to fitting to the experiment and a variety of different processes contribute in an intermediary regime where it is not easy to apply selection rules based on the limiting behavior of the different contributions.

A further limitation concerns the disorder scattering. While our result predicts a quadratic increase of the spinon contribution to heat conductivity, it is hard to judge, whether the experiments show this behavior. In fact, more recent experiments on spin chain compounds have been performed by Hess *et al.* [9] in which the spinon contribution is much more pronounced. In these experiments, the spinon part shows a *linear* increase with temperature in the wide range of $\sim 100K - 300K$, rather than a quadratic one as indicated by our analysis. Such a behavior implies that the scattering length is independent of temperature. It is not possible to reproduce such a behavior with a dilute disorder calculation presented here. Therefore, at least with respect to some experiments, our description is not adequate and one probably needs to consider stronger disorder effects not accessible by the perturbative treatment presented here. It is desirable to consider the case of strong disorder to account for this effect. However, it is hard to judge whether and how such an analysis would fit into our memory matrix approach.

Appendix A

Appendices related to Chapter 1

A.1 Naive Linear Response

In this appendix we give a quick linear response derivation of the conductivity which is comprehensive, illustrative, sloppy and, above all, wrong. Nevertheless it is useful to consider it for several reasons. It gives a feeling for where different terms in the Kubo formula come from. It successfully reproduces the regular part of the conductivity while it fails to reproduce the Drude peak. Most importantly, the derivation gives us an opportunity to discuss the heat current and when it is legitimate to treat it via linear response. This shall be discussed in the second part of this appendix.

The aim of linear response theory is to evaluate the expectation value of an operator J (which in our case is some current) as a response to some (time dependent but homogeneous) external field $E(t)$. The presence of the external field leads to a perturbation in the Hamiltonian, $H'(t)$. We will not specify the dependence of the Hamiltonian on the field yet. We assume that E is switched on slowly at $t = -\infty$ and acquires its final value at $t = 0$. So we are interested in the expectation value of the current at time $t = 0$, $\langle J(0) \rangle$. However, it would be much easier to evaluate the expectation value with respect to the unperturbed Hamiltonian, i.e. at $t = -\infty$, as we know that there we can use the original thermal equilibrium Boltzmann factor of the unperturbed model. To achieve this, we have to ‘evolve back’ the current:

$$\langle J(0) \rangle = \text{tr} e^{-\beta H} U(-\infty, 0) J(0) U^\dagger(0, -\infty) \quad (\text{A.1})$$

with the time evolution operator

$$U(t_1, t_2) = T \exp(i \int_{t_1}^{t_2} dt (H + H'(t))) \quad (\text{A.2})$$

where T denotes the time ordered product. In linear order in $H'(t')$ we may use the expansion

$$U(-\infty, 0) = 1 + i \int_{-\infty}^0 dt H(t) \quad (\text{A.3})$$

and we obtain

$$\langle J(0) \rangle = -i \int_{-\infty}^0 dt \langle [J(0), H'(t)] \rangle \quad (\text{A.4})$$

for the expectation value.

Let us now assume that we are interested in the electrical current as a response to a frequency dependent external field,

$$E(t) = e^{-i\omega t} e^{\varepsilon t} E_0 \quad (\text{A.5})$$

where the factor $e^{\varepsilon t}$ with $\varepsilon \ll 1$ represents the slow switching on of the field and E_0 is the final value of the field at $t = 0$. The charge density $\rho(x, t)$ in the system feels the electric potential $U(x, t)$ induced by the external field and leads to an according term in the Hamiltonian,

$$H'(t) = \int dx \rho(x, t) U(x, t) = \int dx e^{i\omega t} e^{-\varepsilon t} U(x) \rho(x, t) \quad (\text{A.6})$$

With $E_0 = -\nabla U(x)$. Our goal is to obtain a current current correlation function and therefore it is tempting to use the continuity equation to replace the density by the current. This is exactly what we will do next, but we will do so by neglecting a boundary term, the main effect of which is that we lose the Drude weight. So let us use the continuity equation in relation (A.6) in the following manner

$$\rho(x, t) = \int_{-\infty}^t dt' \partial_{t'} \rho(x, t') = - \int_{-\infty}^t dt' \partial_x \cdot j(t') \quad (\text{A.7})$$

and partial integration in space (the boundary term from this step vanishes) delivers the current-current response function times the external field:

$$H'(t) = - \int dx e^{i\omega t} e^{-\varepsilon t} \int_{-\infty}^t dt' j(t') \cdot E_0 \quad (\text{A.8})$$

which, inserted back in Eq. (A.4), gives

$$\langle J(0) \rangle = i \int_{-\infty}^0 dt e^{i\omega t} e^{-\varepsilon t} \langle [J, \int_{-\infty}^t dt' j(t')] \rangle \quad (\text{A.9})$$

and partially integrating with respect to t (this time we keep the boundary term which gives the zero frequency offset $\chi^R(0)$) we finally arrive at

$$\langle J \rangle = \frac{i}{\omega} (\chi^R(0) - \chi^R(\omega)) \cdot E_0 \quad (\text{A.10})$$

with $\chi^R(\omega)$ defined as in appendix A.2. We readily identify the expression for the (regular part of the) conductivity, see Eq. (1.8). The reason why we do not capture the Drude weight in this calculation is the wrong replacement of the density by an integral over its time derivative, the first equality in Eq. (A.7). The correct replacement involves an additional term $\rho(x, -\infty)$ on the rhs., which leads to an additional correlation function of operators at different times, $\langle J(t=0); \rho(t=-\infty) \rangle$. This correlation function vanishes when the relaxation times are finite and contributes the Drude weight otherwise. As such correlation functions are hard to evaluate, other methods are more useful to derive expressions for the Drude weight.

As noted above, the derivation, albeit wrong, is useful to extract the expression for the heat conductivity. We only have to determine the perturbation H' induced by the presence of a small temperature gradient. The presence of a temperature gradient means that different parts of the system are at different temperatures. Heat transport is induced by the imbalance in thermal occupations of states in nearby parts of the system. The thermal balance of states is described by the Boltzmann factor. But of course the Boltzmann factor is meant to describe the full system at equilibrium. We thus should generalize the Boltzmann factor to accommodate for temperature changes across the system. More precisely, we choose $\beta = \beta(x)$ as a function of spatial position and a spatially dependent Boltzmann factor thus becomes

$$\beta H \rightarrow \int dx \beta(x) h(x) \quad (\text{A.11})$$

where $h(x)$ is the Hamiltonian density, $H = \int h(x)$. We have to assume that the temperature variation is small enough so that parts of the system can be considered to be in local thermal equilibrium, meaning that they are large enough that the notion of temperature makes sense. If thus thermal variations are small, we may locally expand, $\beta(x) = \beta + \nabla\beta \cdot x$. Thus, effectively, we may consider the temperature variations as an effective external field coupling to the energy density,

$$H \rightarrow H + H' \quad (\text{A.12})$$

$$H' = - \int dx h(x) \left(x \frac{\nabla T}{T} \right). \quad (\text{A.13})$$

with the external potential $-x \frac{\nabla T}{T}$, in analogy to equation (A.6). The calculation of the heat conductivity can thus be carried out in full analogy to the calculation presented above. As the heat conductivity is defined via the relation

$$\langle j_Q \rangle = -\kappa \nabla T, \quad (\text{A.14})$$

there is an additional factor $1/T$ in the expression for the heat conductivity in terms of the current current correlation function. (For a metal, for example, heat is transported essentially by transport of the same electrons which

carry the current. This explains the Wiedemann-Franz law, which states that the ratio of electrical conductivity to heat conductivity of a metal is proportional to temperature, which is valid whenever the Kubo formula can be applied.) The connection between heat conductivity and the formalism set up in chapter 1 can be made by simply using $\kappa(\omega) = \frac{1}{T}\sigma(\omega)$, where $\sigma(\omega) = \int_0^\infty e^{i\omega t} \langle J_Q(t) | J_Q \rangle$, according to the notation of section 1.7.

A.2 Drude Weight and the Kubo Formula

In this appendix we sketch the derivation of expression 1.12 for the Drude weight from the original Kubo formula 1.7. This relation makes it possible to identify the Drude weight with Suzuki's expression [17] and allows to use Mazur's inequality to calculate lower bounds for the Drude weight. The connection between the Drude weight and the Mazur inequality was first pointed out by Zotos in Ref. [18] and since then has been heavily applied to calculate lower bounds for the Drude weight in one-dimensional systems [18, 19, 2, 20, 21]. Despite its success, Zotos' derivation of this relation is quite restricted in that it is applicable to one dimensional systems only and requires additional assumptions. Zotos' derivation involves the introduction of a fictitious flux through the ring created by the periodic boundary conditions in the chain, and in analogy to Laughlin's argument this introduces a gauge field in the chain.

However, the connection between the Drude weight and the Mazur inequality holds in general (for any dimensions and, in the form presented here, with the only assumption of a time reversal invariant system) and can be derived via elementary manipulations from the Kubo formula 1.7. The key in the derivation is the correct use of the fluctuation-dissipation theorem. For this sake we introduce the correlation functions

$$\chi^<(t) = i\langle J(0)J(t) \rangle \quad (\text{A.15})$$

$$\chi^C(t) = \frac{1}{2}\langle [J(t), J(0)] \rangle \quad (\text{A.16})$$

$$\chi^R(t) = i\Theta(t)\langle [J(t), J(0)] \rangle \quad (\text{A.17})$$

and their Fourier transforms $\chi^<(\omega)$, $\chi^C(\omega)$ and $\chi^R(\omega)$. In terms of these, the fluctuation dissipation theorem states that

$$\chi^<(\omega)(e^{\beta\omega} - 1) = 2i\chi^C(\omega). \quad (\text{A.18})$$

To bring the Kubo formula 1.7 to the more useful form Eqs. 1.10, one has to solve for $\chi^<(\omega)$. Usually one simply divides by the factor $(e^{\beta\omega} - 1)$ which reproduces the regular part of the conductivity. To account for the Drude weight, however, it is necessary to include the possibility that $\chi^<(\omega)$ has a singularity at $\omega = 0$, or equivalently that the current does not decay,

$\lim_{t \rightarrow \pm\infty} \langle J(0)J(t) \rangle \neq 0$. This contribution would be canceled by the factor $(e^{\beta\omega} - 1)$. Thus we make the Ansatz

$$\chi^<(\omega) = 2\pi i C \delta(\omega) + 2i\mathcal{P} \frac{\chi^C(\omega)}{e^{\beta\omega} - 1}, \quad (\text{A.19})$$

where C is a constant that has to be determined independently and, as has been shown in Ref. [13], is given by

$$\beta C = \chi^T - \chi^R(\omega = 0) \quad (\text{A.20})$$

for a time-reversal invariant system. Inserting this into Eq. 1.7 one arrives at 1.8 by means of elementary transformations, using the Kramers-Kronig relations and the Fourier-space representation of the step function $\Theta(t)$.

This connection and its derivation, although quite straightforward, is hard to find in the literature, which simply means that I personally was not able to find it.

A.3 Singularities of $\sigma_{\text{reg}}(\omega)$

Throughout our analysis we assume that the regular part of the conductivity $\sigma_{\text{reg}}(\omega)$ is smooth and finite at $\omega = 0$. However, in certain situations the regular part may show a divergence, which limits the range of validity of the result of chapter 2. In this appendix we discuss possible scenarios in which such a divergence may occur.

First of all, such a divergence can not be attributed to exact conservation laws. If present, it has to stem from slow modes which need a decreasing amount of energy to be excited as $\omega \rightarrow 0$. A typical candidate for such a slow mode are phonons in a clean crystal: As the frequency of the exciting external field is reduced, phonons with lower momenta are excited for which Umklapp scattering – the only source of momentum relaxation – becomes impossible.[29] (In real systems, this effect is limited by impurities and the finite spatial extension of the lattice.) The presence of Goldstone modes generically leads to a divergence of the conductivity as $\omega \rightarrow 0$, provided that they have finite overlap with the current. Slow modes which lead to have been observed for classical systems, see c.f. [73].

As a relevant example, classical analogues of the systems we consider in this thesis (for example masses connected with anharmonic springs) show as a generic behavior anomalous long time tails and a corresponding divergence in $\sigma_{\text{reg}}(\omega)$ with a simultaneous absence of a drude peak, see Ref. [73].

One important implication on our studies is the conclusion that the methods developed are essentially useless for zero temperature calculations. However, besides the fact that $T = 0$ is impossible to realize in experiment, conductivities at $T = 0$ tend to be either infinite or zero [66]. If it is

infinite, this is often the consequence of an accumulation of low frequency slow modes.

Appendix B

Appendices related to Chapter 3

B.1 Spin Operators

In this appendix we shall review the relevant definitions of spin operators. The material can easily be found in many textbooks and we include it here for reference purposes only.

In the basis of local S^z -eigenstates, the spin operators are given by the Pauli matrices

$$S^\alpha = \frac{\hbar}{2} \sigma^\alpha \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We set $\hbar = 1$. The Pauli matrices obey the relation

$$\sigma^\alpha \sigma^\beta = \delta^{\alpha\beta} + i\varepsilon^{\alpha\beta\gamma} \sigma^\gamma$$

from which follow the commutation relations

$$[\sigma^\alpha, \sigma^\beta] = 2i\varepsilon^{\alpha\beta\gamma} \sigma^\gamma [S^\alpha, S^\beta] = i\varepsilon^{\alpha\beta\gamma} S^\gamma$$

It is sometimes convenient to introduce spin raising and lowering operators S^\pm via

$$\begin{aligned} S^+ &= S^x + iS^y & S^x &= \frac{S^+ + S^-}{2} \\ S^- &= S^x - iS^y & S^y &= \frac{S^+ - S^-}{2i} \end{aligned} \longleftrightarrow$$

The effect of S^+ in acting on a spin state is to flip it up if it is down. Then the often occurring combination $S_i^x S_j^x + S_i^y S_j^y$ becomes

$$S_i^x S_j^x + S_i^y S_j^y = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)$$

and hence describes the exchange of the spins at sites i and j .

B.2 Current operators for the XXZ model

The spin-1/2 XXZ -chain is described by the Hamiltonian

$$H = \sum_n h_n h_n = J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z)$$

where h_n is the energy density, the S_n^α being spin operators, J the spin-spin coupling constant and Δ is the anisotropy, a dimensionless parameter. The Heisenberg Model is given by $\Delta = 1$. When the range of the energy density does not exceed one lattice spacing, the heat (or thermal) current density can be defined as

$$j_n = i[h_{n-1}, h_n].$$

The local current density j_n then fulfills the continuity equation:

$$\dot{h}_n = i[H, h_n] = i[h_{n-1}, h_n] + i[h_{n+1}, h_n] = -(j_{n+1} - j_n).$$

(If the range of h_n would exceed one, this construction would not be possible in such a direct way. In the next section we introduce a more general construction scheme for the current.) The total heat current can be expressed as

$$J_{\text{th}} = \sum_n j_n$$

where j_n evaluates to

$$\begin{aligned} j_n &= iJ^2 [\delta_{n,n+1}^s, \delta_{n-1,n}^s] \\ &= J^2 (S_n^z (S_{n+1}^x S_{n-1}^y - S_{n-1}^y S_{n+1}^x) \\ &\quad + \Delta S_{n-1}^z (S_n^x S_{n+1}^y - S_{n+1}^y S_n^x) + \Delta S_{n+1}^z (S_{n-1}^x S_n^y - S_{n-1}^y S_n^x)). \end{aligned}$$

In the Heisenberg limit, $\Delta = 1$, j_n simply becomes $j_n = J^2 \mathbf{S}_{n-1} \cdot (\mathbf{S}_n \times \mathbf{S}_{n+1})$. The heat current is conserved in the XXZ -chain:

$$\dot{J}_{\text{th}} = i[H, J_{\text{th}}] = 0.$$

B.3 Implementation Notes: Frequency moments

In this appendix we outline the steps that lead to a simple and straightforward implementation of an algorithm for the calculation of frequency moments

$$\mu_p = \langle [\cdots [[J, H], \underbrace{H}_{p \times}] \cdots], J \rangle. \quad (\text{B.1})$$

As the memory function $\text{Re } \Gamma(\omega)$ is even in ω , its moments are nonvanishing for odd p only, see Eq. (3.23). By redistributing the derivatives appearing

in Eq. (B.1), we may write

$$\mu_{2n+1} = (-1)^n \langle [\cdots \underbrace{[[J, H], H] \cdots}_{n+1 \times}, \cdots \underbrace{[[J, H], H] \cdots}_{n \times}] \rangle. \quad (\text{B.2})$$

Noting that $\text{tr}[A, B] = 0$, we have to expand the Boltzmann weight in β . The high temperature limit of the moments is therefore given by

$$\mu_{2n+1} = (-1)^{n+1} \frac{1}{T} \text{tr} \left([\cdots \underbrace{[[J, H], H] \cdots}_{n+1 \times}, \cdots \underbrace{[[J, H], H] \cdots}_{n \times}] H \right). \quad (\text{B.3})$$

The Hamiltonian $H = H_0 + gH_1$, and as we are interested in the leading order $\sim g^2$ contribution to the moments only. J is the unperturbed current, and therefore $[J, H_0] = 0$, implying that the two H_1 that appear in the leading order expansion of Eq. (B.3) *have* to appear in the form $g[J, H_1]$. Therefore we can write

$$\mu_{2n+1} = (-1)^{n+1} \frac{g^2}{T} \text{tr} \left([\cdots \underbrace{[[J, H_1], H_0] \cdots}_{n \times}, \cdots \underbrace{[[J, H_1], H_0] \cdots}_{n-1 \times}] H_0 \right).$$

in leading order in g . To the trace only terms contribute which are free of spin operators, as the trace over any combination of spin operators vanishes, e.g. $\text{tr} S^\alpha = 0$ for any $\alpha = x, y, z$. Therefore we know, that from the commutator

$$[\cdots \underbrace{[[J, H_1], H_0] \cdots}_{n \times}, \cdots \underbrace{[[J, H_1], H_0] \cdots}_{n-1 \times}]$$

only terms contribute which have the structure $S_i^\alpha S_{i+1}^\alpha$ for some i , as only such terms can give a constant when multiplied by H_0 and thus have non-vanishing trace. This reduces the task of determining the moments to calculating recursively the commutators

$$L_n = \cdots \underbrace{[[J, H_1], H_0] \cdots}_{n \times} \quad (\text{B.4})$$

and to filter all terms of $[L_n, L_{n-1}]$ which have the structure $S_i^\alpha S_{i+1}^\alpha$. By using translational and rotational¹ invariance, the number of terms that have to be calculated is strongly reduced. By implementing arbitrary products of spin-operators as integers, and commutators by elementary logical operations on them, it is possible to write a very fast code. The limitation is the available memory, as the consumed memory is proportional to the number of terms appearing in L_n , which grows exponentially with n . In this way, we can calculate all moments up to μ_{27} on a contemporary desktop computer with 1GB of available memory in minutes. The resulting numerical values for the obtained moments are shown in table B.1.

¹We consider only the isotropic Heisenberg chain.

n	$\text{Im } \mu_{2n+1}/(\beta g^2)$
1	0.058594
2	0.262207
3	1.695923
4	14.115601
5	141.554512
6	1643.360378
7	21520.654747
8	312206.883681
9	4950353.427655
10	84877646.266656
11	1559847391.212904
12	30499675948.850533
13	630631274585.113403

Figure B.1: Numerical values for the high temperature expansion of the moments of the leading order memory function.

B.4 Higher Orders

In this appendix we present the calculation of the contributions to the memory function to orders J^3 and J^4 in the next-nearest neighbor coupling in the isotropic Heisenberg spin chain. As we find that the memory function vanishes to leading order in the coupling, the question arises, if it is only the second order that vanishes or if we have met a non-analytic singularity, which gives a vanishing answer to arbitrary orders in perturbation theory. The expressions derived below have been implemented numerically, and the result is shown in Fig. 3.2, which shows that the contribution of order J^4 is finite, thus excluding the latter scenario.

We have argued in the main text that for the leading order contribution it is sufficient to use the unperturbed current when calculating \dot{J} . For higher order contributions this is not obvious, and here we take into account the full heat current. The full heat current in the perturbed system obtains an additional contribution $\propto J'$, (which is determined by solving the continuity equation with the density of the perturbed Hamiltonian) and therefore \dot{J} also has a contribution $\propto J'^2$, which has to be taken into account for the higher orders.

To calculate higher order contributions to the memory function, we make use of the relation

$$M(z) = \varphi(z) + \frac{i}{z} \varphi(z) \chi^{-1} M(z) \quad (\text{B.5})$$

where $M(z)$ is the 1×1 memory matrix with the *full* heat current as the

only slow mode,

$$M(z) = \left(\dot{J}_Q \left| Q \frac{i}{z - LQ} \right| \dot{J}_Q \right) \quad (\text{B.6})$$

and $\phi(z)$ is the same expression but without the projectors,

$$\varphi(z) = \left(\dot{J}_Q \left| \frac{i}{z - L} \right| \dot{J}_Q \right). \quad (\text{B.7})$$

and $\chi = (J_Q | J_Q)$ is the generalized susceptibility. We emphasize that $\varphi(z)$ should not be confused with the approximate memory matrix $\tilde{M}(z)$ of chapter 2, as Eq. (B.7) does not use any approximations. Eq. (B.5) is a rigorous algebraic identity and holds provided only that $(\dot{J}_Q | J_Q) = 0$, which is the case as J_Q has a definite time signature.

Using the notation $\varphi(z) = \sum_n J'^n \varphi_n(z)$ for the perturbative expansion of $\varphi(z)$ in the coupling J' (in leading order we have $J'^2 \phi_2(\omega) = \tilde{M}(\omega)$ with $\tilde{M}(\omega)$ given by Eq. (2.7), or equivalently Eq. (2.5)), we begin with an expansion of the relation (B.5) in J' :

$$M(z) = J'^2 \varphi_2(z) + J'^3 \varphi_3(z) + J'^4 \left(\varphi_4(z) + \frac{i}{z} \varphi_2(z) \chi^{-1} \varphi_2(z) \right) + \mathcal{O}(\varphi^3) \quad (\text{B.8})$$

The fourth order (in J') contribution to $M(z)$ includes $\varphi_4(z)$, as well as the *counter-term* $\propto \varphi_2^2(z)$. We remind the reader, that the true perturbative series of the *full* memory matrix (including all constants of the motion) lacks any singularities $\propto \delta(\omega)$, and that a perturbative expansion of $M(z)$ of Eq. (B.6) is, for $z \neq 0$, identical to the perturbative expansion of the particular J_Q - J_Q component of the full memory matrix. Therefore, we can evaluate $\text{Re } M(0)$ (which gives a rigorous lower bound to the heat conductivity) by taking the limit $\omega \rightarrow 0$ of the expansion (B.8). The expansion may contain singularities at $z = 0$, but these can simply be dropped.

As a next step, we show that the contribution of the counter-term vanishes in our case. For this purpose, we make use of the properties of the second order contribution, $\text{Re } \varphi_2(\omega)$, which have been determined in the numeric analysis. First, $\text{Re } \varphi_2(\omega)$ behaves at least as $\propto \omega^2$ for $\omega \ll J$, and (as is clear from the numerical analysis) lacks any singular contributions at $\omega = 0$. Furthermore, $\text{Re } \phi_2(\omega)$ is an even function of frequency. We have to calculate $\lim_{\omega \rightarrow 0} \text{Re } M(\omega)$ where $M(\omega) = M(z = \omega + i0)$ from the expansion (B.8). With the Dirac identity, $i/z = \mathcal{P}i/\omega + \pi\delta(\omega)$, only the principal part is relevant. the real part of the counterterm thus becomes

$$\frac{-2}{\omega} \chi^{-1} \text{Re } \varphi_2(\omega) \text{Im } \varphi_2(\omega)$$

Due to the properties of $\text{Re } \varphi_2(\omega)$ discussed above, it is easy to show that $\text{Im } \varphi_2(\omega) \propto \omega$ at low frequencies, in particular, it has no contribution $\propto 1/\omega$.

This is most easily seen by using *Kramers-Kronig* relations. Therefore, the counterterm has to vanish as $\omega \rightarrow 0$. Therefore we have shown that, in our case, the expansion of the memory matrix to fourth order is identical to an expansion of $\varphi(\omega)$.

We next have to determine $\varphi_3(\omega)$ and $\varphi_4(\omega)$. We have to carry out the perturbation series explicitly. For this purpose, we go to imaginary time, where the expansion can be carried out most easily. We will obtain correlation functions in terms of Matsubara frequencies and the retarded correlation functions of interest are obtained by finally performing the analytic continuation to the real axis.

The real part of $M(\omega)$ of equation (B.8) can be expressed as

$$\text{Re } M(\omega) = \frac{1}{\omega\beta} \text{Im} \int_0^\beta d\tau e^{i\omega_n\tau} \left\langle T_\tau \dot{J}(\tau) \dot{J}(0) \right\rangle \Big|_{i\omega_n \rightarrow \omega + i0}.$$

We have to sort wrt. the various orders in J' : $\dot{J} = \dot{J}_1 + \dot{J}_2$ and $H = H_0 + H_1$. Define

$$M = M_2 + M_{3.1} + M_{3.2} + M_{4.1} + M_{4.2} + M_{4.3} + \mathcal{O}(J'^5)$$

where

$$M_\alpha = M_\alpha(\omega) = \frac{1}{\omega\beta} \int_0^\beta d\tau e^{i\omega_n\tau} M_\alpha(\tau) \Big|_{i\omega_n \rightarrow \omega + i0}$$

and we obtain

$$\begin{aligned} M_2(\tau) &= \left\langle T_\tau \dot{J}_1(\tau) \dot{J}_1(0) \right\rangle_0 \\ M_{3.1}(\tau) &= \left\langle T_\tau \dot{J}_1(\tau) \dot{J}_2(0) \right\rangle_0 + \left\langle T_\tau \dot{J}_2(\tau) \dot{J}_1(0) \right\rangle_0 \\ M_{3.2}(\tau) &= - \int_0^\beta d\tau' \left\langle T_\tau H_1(\tau') \dot{J}_1(\tau) \dot{J}_1(0) \right\rangle_0 \\ M_{4.1}(\tau) &= \left\langle T_\tau \dot{J}_2(\tau) \dot{J}_2(0) \right\rangle_0 \\ M_{4.2}(\tau) &= - \int_0^\beta d\tau' \left\langle T_\tau H_1(\tau') \dot{J}_1(\tau) \dot{J}_2(0) \right\rangle_0 - \int_0^\beta d\tau' \left\langle T_\tau H_1(\tau') \dot{J}_2(\tau) \dot{J}_1(0) \right\rangle_0 \\ M_{4.3}(\tau) &= \int_0^\beta d\tau' \int_0^\beta d\tau'' \left\langle T_\tau H_1(\tau') H_1(\tau'') \dot{J}_1(\tau) \dot{J}_2(0) \right\rangle_0 \end{aligned}$$

The expressions follow from an expansion of the expectation value, which depends on the perturbation J' . Using the imaginary time formalism, we

can write the expectation value as a field integral:

$$\begin{aligned}
\langle TA(\tau)B \rangle &= \frac{1}{\mathcal{Z}} \int \mathcal{D}(\bar{\psi}, \psi) T e^{-\int_0^\beta H(\tau') d\tau'} A(\tau) B \\
&= \frac{1}{\mathcal{Z}} \int \mathcal{D}(\bar{\psi}, \psi) T e^{-\int H_0 d\tau} \left(1 - \int_0^\beta d\tau' H_1(\tau') + \dots \right) A(\tau) B \\
&= \langle TA(\tau)B \rangle_0 - \int_0^\beta d\tau' \langle TH_1(\tau') A(\tau) B \rangle_0 + \dots \\
&= \langle TA(\tau)B \rangle_0 - \int_0^\tau d\tau' \langle A(\tau) H_1(\tau') B \rangle_0 - \int_\tau^\beta d\tau' \langle H_1(\tau') A(\tau) B \rangle_0
\end{aligned}$$

where the last two terms contribute to $M_{3,2}$ and $M_{4,2}$. They evaluate as

$$\begin{aligned}
&\int_0^\tau d\tau' \langle A(\tau) H_1(\tau') B \rangle_0 + \int_\tau^\beta d\tau' \langle H_1(\tau') A(\tau) B \rangle_0 \\
&= \sum_{lmn} A_{lm} H_{1mn} B_{nl} \frac{e^{-\beta E_l} e^{\Xi_{lm}\tau} (e^{\Xi_{mn}\tau} - 1)}{\Xi_{mn}} \\
&\quad + \sum_{lmn} H_{1lm} A_{mn} B_{nl} \frac{e^{-\beta E_l} e^{\Xi_{mn}\tau} (e^{\Xi_{lm}\beta} - e^{\Xi_{lm}\tau})}{\Xi_{lm}}. \\
&= \sum_{lmn} A_{lm} H_{1mn} B_{nl} \frac{e^{-\beta E_l} (e^{\Xi_{lm}\tau} - e^{\Xi_{lm}\tau})}{\Xi_{mn}} \\
&\quad + \sum_{lmn} H_{1lm} A_{mn} B_{nl} \frac{(e^{-\beta E_m} e^{\Xi_{mn}\tau} - e^{-\beta E_l} e^{\Xi_{lm}\tau})}{\Xi_{lm}}.
\end{aligned}$$

where we use the shorthand $\Xi_{mn} = E_m - E_n$. We are interested in the Fourier transform:

$$\begin{aligned}
&\int_0^\beta d\tau e^{i\omega_n\tau} \langle TA(\tau)B \rangle \Big|_{J^3} = \\
&= \sum_{lmn} A_{lm} H_{1mn} B_{nl} \frac{e^{-\beta E_l}}{\Xi_{mn}} \int_0^\beta d\tau e^{i\omega_n\tau} (e^{\Xi_{lm}\tau} - e^{\Xi_{lm}\tau}) \\
&\quad + \sum_{lmn} H_{1lm} A_{mn} B_{nl} \frac{1}{\Xi_{lm}} \int_0^\beta d\tau e^{i\omega_n\tau} (e^{-\beta E_m} e^{\Xi_{mn}\tau} - e^{-\beta E_l} e^{\Xi_{lm}\tau}) \\
&= \sum_{lmn} A_{lm} H_{1mn} B_{nl} \left(\frac{e^{-\beta E_n} - e^{-\beta E_l}}{\Xi_{mn} (i\omega_n + \Xi_{ln})} - \frac{e^{-\beta E_m} - e^{-\beta E_l}}{\Xi_{mn} (i\omega_n + \Xi_{lm})} \right) \\
&\quad + \sum_{lmn} H_{1lm} A_{mn} B_{nl} \left(\frac{e^{-\beta E_n} - e^{-\beta E_m}}{\Xi_{lm} (i\omega_n + \Xi_{mn})} - \frac{e^{-\beta E_n} - e^{-\beta E_l}}{\Xi_{lm} (i\omega_n + \Xi_{ln})} \right)
\end{aligned}$$

since we are interested in the infinite temperature limit ($T \rightarrow \infty$) we can expand the exponentials. Furthermore, we are interested in the delta function part only, which comes from first analytically continuing ($i\omega_n \rightarrow \omega + i0$)

and then applying the Dirac identity. We are left with

$$\begin{aligned}
\operatorname{Re} \varphi_{3.2}(\omega) &= \frac{1}{\omega\beta} \operatorname{Im} \sum_{lmn} A_{lm} \frac{H_{1mn}}{\Xi_{mn}} B_{nl} \left(\frac{\beta\Xi_{ln}}{\omega + i0 + \Xi_{ln}} - \frac{\beta\Xi_{lm}}{\omega + i0 + \Xi_{lm}} \right) \\
&\quad + \frac{1}{\omega\beta} \operatorname{Im} \sum_{lmn} \frac{H_{1lm}}{\Xi_{lm}} A_{mn} B_{nl} \left(\frac{\beta\Xi_{mn}}{\omega + i0 + \Xi_{mn}} - \frac{\beta\Xi_{ln}}{\omega + i0 + \Xi_{ln}} \right) \\
&= \frac{\pi}{\omega} \sum_{lmn} A_{lm} \frac{H_{1mn}}{\Xi_{mn}} B_{nl} (\delta(\omega - \Xi_{nl})\Xi_{nl} - \delta(\omega - \Xi_{ml})\Xi_{ml}) \\
&\quad + \frac{\pi}{\omega} \sum_{lmn} \frac{H_{1lm}}{\Xi_{lm}} A_{mn} B_{nl} (\delta(\omega - \Xi_{nm})\Xi_{nm} - \delta(\omega - \Xi_{nl})\Xi_{nl}) \\
&= \pi \sum_{lmn} A_{lm} \frac{H_{1mn}}{\Xi_{mn}} B_{nl} (\delta(\omega - \Xi_{nl}) - \delta(\omega - \Xi_{ml})) \\
&\quad + \pi \sum_{lmn} \frac{H_{1lm}}{\Xi_{lm}} A_{mn} B_{nl} (\delta(\omega - \Xi_{nm}) - \delta(\omega - \Xi_{nl})) \\
&= \pi \sum_{lmn} \left(A_{lm} \frac{H_{1mn}}{\Xi_{mn}} - \frac{H_{1lm}}{\Xi_{lm}} A_{mn} \right) B_{nl} \delta(\omega - \Xi_{nl}) \\
&\quad + \pi \sum_{lmn} A_{lm} \left(B_{mn} \frac{H_{1nl}}{\Xi_{nl}} - \frac{H_{1mn}}{\Xi_{mn}} B_{nl} \right) \delta(\omega - \Xi_{ml}) \\
&= \pi \sum_{lmn} A_{lm} \left(B_{mn} \frac{H_{1nl}}{\Xi_{nl}} - \frac{H_{1mn}}{\Xi_{mn}} B_{nl} \right) \delta(\omega - \Xi_{ml}) \\
&\quad + \pi \sum_{lmn} B_{lm} \left(A_{mn} \frac{H_{1nl}}{\Xi_{nl}} - \frac{H_{1mn}}{\Xi_{mn}} A_{nl} \right) \delta(\omega - \Xi_{lm})
\end{aligned}$$

and thus, taking $A = B = \dot{J}_T$ and to third order in J' :

$$\operatorname{Re} \varphi_{3.2}(\omega) = \pi \sum_{lmn} \dot{J}_{lm} \left(\dot{J}_{mn} \frac{H_{1nl}}{\Xi_{nl}} - \frac{H_{1mn}}{\Xi_{mn}} \dot{J}_{nl} \right) (\delta(\omega - \Xi_{lm}) + \delta(\omega - \Xi_{ml})).$$

$$\begin{aligned}
& \sum_{lmn} H_{1lm} \dot{J}_{mn} \dot{J}_{nl} \left(\frac{e^{-\beta E_m} - e^{-\beta E_n}}{\Xi_{lm}(i\omega_n + \Xi_{nm})} + \frac{e^{-\beta E_n} - e^{-\beta E_l}}{\Xi_{lm}(i\omega_n + \Xi_{nl})} + \right. \\
& \quad \left. - \frac{e^{-\beta E_n} - e^{-\beta E_l}}{\Xi_{lm}(i\omega_n + \Xi_{ln})} - \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\Xi_{lm}(i\omega_n + \Xi_{mn})} \right) \\
&= \sum_{lmn} \frac{H_{1lm}}{\Xi_{lm}} \dot{J}_{mn} \dot{J}_{nl} \left[(e^{-\beta E_n} - e^{-\beta E_l}) \left(\frac{1}{i\omega_n + \Xi_{nl}} - \frac{1}{i\omega_n + \Xi_{ln}} \right) \right. \\
& \quad \left. - (e^{-\beta E_m} - e^{-\beta E_n}) \left(\frac{1}{i\omega_n + \Xi_{mn}} - \frac{1}{i\omega_n + \Xi_{nm}} \right) \right] \\
&= \sum_{lmn} \frac{H_{1lm}}{\Xi_{lm}} (\dot{J}_{mn} K_{nl} - K_{mn} \dot{J}_{nl}) \\
&= \sum_{lmn} K_{lm} \left(\frac{H_{1mn}}{\Xi_{mn}} \dot{J}_{nl} - \dot{J}_{mn} \frac{H_{1nl}}{\Xi_{nl}} \right)
\end{aligned}$$

where

$$K_{lm} = \dot{J}_{lm} (e^{-\beta E_l} - e^{-\beta E_m}) \left(\frac{1}{i\omega_n + \Xi_{lm}} - \frac{1}{i\omega_n + \Xi_{ml}} \right)$$

is a matrix. The contribution to $M_{4,3}$ is evaluated in a similar fashion. We have six terms:

$$\begin{aligned}
& \int_0^\beta d\tau' \int_0^\beta d\tau'' \langle T \dot{J}(\tau) H(\tau') H(\tau'') \dot{J}(0) \rangle \\
&= \int_0^\tau d\tau' \int_0^{\tau'} d\tau'' \langle \dot{J}(\tau) H(\tau') H(\tau'') \dot{J} \rangle + \int_0^\tau d\tau' \int_{\tau'}^\tau d\tau'' \langle \dot{J}(\tau) H(\tau'') H(\tau') \dot{J} \rangle \\
&+ \int_\tau^\beta d\tau' \int_0^\tau d\tau'' \langle H(\tau') \dot{J}(\tau) H(\tau'') \dot{J} \rangle + \int_0^\tau d\tau' \int_\tau^\beta d\tau'' \langle H(\tau'') \dot{J}(\tau) H(\tau') \dot{J} \rangle \\
&+ \int_\tau^\beta d\tau' \int_\tau^{\tau'} d\tau'' \langle H(\tau') H(\tau'') \dot{J}(\tau) \dot{J} \rangle + \int_\tau^\beta d\tau' \int_{\tau'}^\beta d\tau'' \langle H(\tau'') H(\tau') \dot{J}(\tau) \dot{J} \rangle \\
&= \sum_{klmn} \dot{J}_{kl} H_{lm} H_{mn} \dot{J}_{nk} \int_0^\tau d\tau' \left(\frac{e^{\Xi_{mn}\tau'} - 1}{\Xi_{mn}} e^{\Xi_{lm}\tau'} + \frac{e^{\Xi_{lm}\tau} - e^{\Xi_{lm}\tau'}}{\Xi_{lm}} e^{\Xi_{mn}\tau'} \right) e^{\Xi_{kl}\tau} \\
&+ \sum_{klmn} H_{kl} \dot{J}_{lm} H_{mn} \dot{J}_{nk} \left(\int_\tau^\beta \frac{e^{\Xi_{mn}\tau} - 1}{\Xi_{mn}} e^{\Xi_{kl}\tau'} + \int_0^\tau \frac{e^{\beta\Xi_{kl}} - e^{\Xi_{kl}\tau}}{\Xi_{kl}} e^{\Xi_{mn}\tau'} \right) e^{\Xi_{lm}\tau} d\tau' \\
&+ \sum_{klmn} H_{kl} H_{lm} \dot{J}_{mn} \dot{J}_{nk} \int_\tau^\beta d\tau' \left(\frac{e^{\Xi_{lm}\tau'} - e^{\Xi_{lm}\tau}}{\Xi_{lm}} e^{\Xi_{kl}\tau'} + \frac{e^{\beta\Xi_{kl}} - e^{\Xi_{kl}\tau'}}{\Xi_{kl}} e^{\Xi_{lm}\tau'} \right) e^{\Xi_{mn}\tau}
\end{aligned}$$

We want to write the terms separately. We do not want to keep the matrix elements in each step, thus we omit them. They can be reinserted after the

Fourier transformation. The Fourier-transform of the $\dot{J}HH\dot{J}$ -term reads

$$\begin{aligned}
& e^{-\beta E_k} \int_0^\beta d\tau e^{i\omega_n \tau} \int_0^\tau d\tau' \left(\frac{e^{\Xi_{mn}\tau'} - 1}{\Xi_{mn}} e^{\Xi_{lm}\tau'} + \frac{e^{\Xi_{lm}\tau} - e^{\Xi_{lm}\tau'}}{\Xi_{lm}} e^{\Xi_{mn}\tau'} \right) e^{\Xi_{kl}\tau} \\
&= e^{-\beta E_k} \int_0^\beta d\tau e^{i\omega_n \tau} \left(\frac{e^{\Xi_{ln}\tau} - 1}{\Xi_{ln}\Xi_{mn}} - \frac{e^{\Xi_{lm}\tau} - 1}{\Xi_{lm}\Xi_{mn}} + \frac{e^{\Xi_{lm}\tau} (e^{\Xi_{mn}\tau} - 1)}{\Xi_{lm}\Xi_{mn}} - \frac{e^{\Xi_{ln}\tau} - 1}{\Xi_{ln}\Xi_{lm}} \right) e^{\Xi_{kl}\tau} \\
&= e^{-\beta E_k} \int_0^\beta d\tau e^{i\omega_n \tau} \left(\frac{e^{\Xi_{kn}\tau} - e^{\Xi_{kl}\tau}}{\Xi_{ln}\Xi_{mn}} - \frac{e^{\Xi_{km}\tau} - e^{\Xi_{kl}\tau}}{\Xi_{lm}\Xi_{mn}} + \frac{e^{\Xi_{kn}\tau} - e^{\Xi_{km}\tau}}{\Xi_{lm}\Xi_{mn}} - \frac{e^{\Xi_{kn}\tau} - e^{\Xi_{kl}\tau}}{\Xi_{ln}\Xi_{lm}} \right) \\
&= \frac{e^{-\beta E_n} - e^{-\beta E_k}}{i\omega_n - \Xi_{nk}} \frac{\Xi_{ln}\Xi_{mn}}{e^{-\beta E_l} - e^{-\beta E_k}} - \frac{e^{-\beta E_l} - e^{-\beta E_k}}{i\omega_n - \Xi_{lk}} \frac{\Xi_{ln}\Xi_{mn}}{e^{-\beta E_n} - e^{-\beta E_k}} - \frac{e^{-\beta E_m} - e^{-\beta E_k}}{i\omega_n - \Xi_{mk}} \frac{\Xi_{lm}\Xi_{mn}}{e^{-\beta E_n} - e^{-\beta E_k}} \\
&\quad + \frac{e^{-\beta E_n} - e^{-\beta E_k}}{i\omega_n - \Xi_{nk}} \frac{\Xi_{lm}\Xi_{mn}}{e^{-\beta E_n} - e^{-\beta E_k}} + \frac{e^{-\beta E_l} - e^{-\beta E_k}}{i\omega_n - \Xi_{lk}} \frac{\Xi_{lm}\Xi_{mn}}{e^{-\beta E_l} - e^{-\beta E_k}} - \frac{e^{-\beta E_m} - e^{-\beta E_k}}{i\omega_n - \Xi_{mk}} \frac{\Xi_{lm}\Xi_{mn}}{e^{-\beta E_l} - e^{-\beta E_k}} \\
&\quad - \frac{e^{-\beta E_n} - e^{-\beta E_k}}{i\omega_n - \Xi_{nk}} \frac{\Xi_{ln}\Xi_{lm}}{e^{-\beta E_l} - e^{-\beta E_k}} + \frac{e^{-\beta E_l} - e^{-\beta E_k}}{i\omega_n - \Xi_{lk}} \frac{\Xi_{ln}\Xi_{lm}}{e^{-\beta E_l} - e^{-\beta E_k}}
\end{aligned}$$

That of the second term ($H\dot{J}H\dot{J}$)

$$\begin{aligned}
& e^{-\beta E_k} \int_0^\beta d\tau e^{i\omega_n \tau} \left(\int_\tau^\beta d\tau' \frac{e^{\Xi_{mn}\tau'} - 1}{\Xi_{mn}} e^{\Xi_{kl}\tau'} + \int_0^\tau d\tau' \frac{e^{\beta\Xi_{kl}} - e^{\Xi_{kl}\tau'}}{\Xi_{kl}} e^{\Xi_{mn}\tau'} \right) e^{\Xi_{lm}\tau} \\
&= 2e^{-\beta E_k} \int_0^\beta d\tau e^{i\omega_n \tau} \frac{(e^{\beta\Xi_{kl}} - e^{\Xi_{kl}\tau}) (e^{\Xi_{mn}\tau} - 1)}{\Xi_{kl}\Xi_{mn}} e^{\Xi_{lm}\tau} \\
&= \frac{2}{\Xi_{kl}\Xi_{mn}} \int_0^\beta d\tau e^{i\omega_n \tau} \left(e^{-\beta E_l} (e^{\Xi_{ln}\tau} - e^{\Xi_{lm}\tau}) - e^{-\beta E_k} (e^{\Xi_{kn}\tau} - e^{\Xi_{km}\tau}) \right) \\
&= \frac{2}{\Xi_{kl}\Xi_{mn}} \left(\frac{e^{-\beta E_n} - e^{-\beta E_l}}{i\omega_n - \Xi_{nl}} - \frac{e^{-\beta E_m} - e^{-\beta E_l}}{i\omega_n - \Xi_{ml}} - \frac{e^{-\beta E_n} - e^{-\beta E_k}}{i\omega_n - \Xi_{nk}} + \frac{e^{-\beta E_m} - e^{-\beta E_k}}{i\omega_n - \Xi_{mk}} \right)
\end{aligned}$$

and finally the third term. After a right-rotation of the third term it becomes completely symmetric to the first one. Each term occurs once again but with the negative energy-difference of the frequency and a global minus sign. To cope with the rest of the calculation, we introduce some notation. Writing

$$\tilde{A}_{kl} = \frac{A_{kl}}{\Xi_{kl}} (1 - \delta_{\Xi_{kl}}) = \frac{A_{kl}}{E_k - E_l} (1 - \delta_{E_k, E_l})$$

and

$$\Delta_{kl} = \left(e^{-\beta E_l} - e^{-\beta E_k} \right) \left(\frac{1}{i\omega_n - \Xi_{lk}} - \frac{1}{i\omega_n - \Xi_{kl}} \right) \quad (\text{B.9})$$

and

$$(\bar{A})_{kl} = \Delta_{kl} A_{kl}$$

we can omit the indices. For example, the very first contribution to the $\dot{J}HH\dot{J}$ term together with the corresponding contribution to the $HH\dot{J}\dot{J}$

term may be written as

$$\sum_{klmn} \dot{J}_{kl} H_{lm} H_{mn} \dot{J}_{nk} \left(\frac{e^{-\beta E_n} - e^{-\beta E_k}}{(i\omega_n - \Xi_{nk}) \Xi_{ln} \Xi_{mn}} + \frac{e^{-\beta E_k} - e^{-\beta E_n}}{(i\omega_n - \Xi_{kn}) \Xi_{ln} \Xi_{mn}} \right) = \text{tr } \widetilde{J H \tilde{H} \bar{J}}.$$

Proceeding this way, we also can write the rest of the terms. We find

$$\text{tr} \left(\widetilde{J H \tilde{H} \bar{J}} - \bar{J} \widetilde{H \tilde{H} J} - \overline{J \tilde{H} \tilde{H} J} + \overline{J \tilde{H} \tilde{H} J} + \widetilde{J \tilde{H} \tilde{H} \bar{J}} - \overline{J \tilde{H} \tilde{H} J} - \widetilde{J \tilde{H} \tilde{H} \bar{J}} + \overline{J \tilde{H} \tilde{H} J} \right)$$

for the $\widetilde{J H \tilde{H} \bar{J}}$ - together with the $\overline{H H \tilde{H} \tilde{H}}$ -term, whereas, after some regrouping of the terms, the $\overline{J H \tilde{H} \tilde{H} J}$ -term becomes

$$\text{tr} \left(\overline{J \tilde{H} \tilde{H} J} - 2 \overline{J \tilde{H} \tilde{H} J} + \overline{J \tilde{H} \tilde{H} J} \right).$$

After some further regrouping we arrive at the simple expression

$$\text{tr} \left(\overline{J} \left[\dot{J}, \left[\widetilde{H, \tilde{H}} \right] \right] + \overline{J} \left[\tilde{H}, \left[\tilde{H}, \dot{J} \right] \right] + \left[\tilde{H}, \dot{J} \right] \left[\tilde{H}, \dot{J} \right] \right). \quad (\text{B.10})$$

Now we can perform the high temperature limit and the analytic continuation $i\omega_n \rightarrow \omega + i0$. Both of these procedures concern only the factor Δ_{kl} of equation (B.9). For high temperatures $e^{-\beta E_l} - e^{-\beta E_k} = \beta(E_k - E_l) = \beta \Xi_{kl}$. Furthermore, since we are interested in the imaginary part only, we can use the Dirac identity and express the terms by means of Dirac delta functions:

$$\text{Im} \frac{1}{\omega + i0 - \Xi_{kl}} = -\pi \delta(\omega - \Xi_{kl}).$$

Hence the prefactors from the temperature expansion can be transformed into $\pm\beta\omega$. We arrive at the replacement rule

$$\Delta_{kl} \rightarrow \pi\beta\omega (\delta(\omega - \Xi_{kl}) + \delta(\omega - \Xi_{lk})).$$

Since what we want to calculate has the structure

$$\text{Re } M_{4,3}(\omega) = \frac{1}{\beta\omega} \text{Im} \int_0^\beta d\tau e^{i\omega_n \tau} \int_0^\beta d\tau' \int_0^\beta d\tau'' \left\langle T_\tau H(\tau') H(\tau'') \dot{J}(\tau) \dot{J}(0) \right\rangle \Big|_{i\omega_n \rightarrow \omega + i0},$$

the replacement rule

$$\Delta_{kl} \rightarrow \pi\delta(\omega - \Xi_{kl}) + \pi\delta(\omega - \Xi_{lk})$$

applied to equation (B.10) leads to the correct result for $\text{Re } M_{4,3}(\omega)$.

This completes the derivation of the third and fourth order contributions to the memory matrix. The results can straightforwardly be implemented to numerically evaluate these contributions. As a result, the third order contribution vanishes at zero frequency for the Heisenberg case (as it must, if the second order vanishes), but the fourth order is finite, see Fig. 3.2. This excludes the possibility that the heat conductivity in the isotropic Heisenberg spin chain has an essential singularity of the nnn-perturbation J' , and shows that the heat conductivity behaves as $\propto 1/J'^4$.

Appendix C

Appendices related to Chapter 4

C.1 Commutators

In this appendix we demonstrate how contractions can be carried out for arbitrary functions of the bosonic fields. For simple polynomials of the fields, all we need is the canonicity identity

$$[\phi(x), \Pi(x')] = i\delta(x - x')$$

and the relation

$$[AB, C] = A[B, C] + [A, C]B.$$

For other functions we can use that commutators act as derivations,

$$[A, f(B)] = [A, B]f'(B)$$

which is valid whenever $[[A, B], B] = 0$. This in our case is generally true since $[A, B]$ will be a c-number. This gives us all tools that we need to calculate the commutators. As an example, we calculate the following two

commutators:

$$\begin{aligned}
& \int dx' [\Pi(x) \partial_x \phi(x), (\partial_{x'} \phi)^2(x')] \\
&= \int dx' [\Pi(x), (\partial_{x'} \phi)^2(x')] \partial_x \phi(x) \\
&= 2 \int dx' [\Pi(x), \partial_{x'} \phi(x')] \partial_{x'} \phi(x') \partial_x \phi(x) \\
&= 2 \int dx' \partial_{x'} [\Pi(x), \phi(x')] \partial_{x'} \phi(x') \partial_x \phi(x) \\
&= -2i \int dx' (\partial_{x'} \delta(x - x')) \partial_{x'} \phi(x') \partial_x \phi(x) \\
&= 2i \partial_x^2 \phi(x) \partial_x \phi(x) \\
&= i \partial_x (\partial_x \phi(x))^2
\end{aligned}$$

and

$$\begin{aligned}
& \int dx' [\Pi(x) \partial_x \phi(x), (\Pi(x'))^2] \\
&= \int dx' \Pi(x) [\partial_x \phi(x), (\Pi(x'))^2] \\
&= 2 \int dx' \Pi(x) \partial_x [\phi(x), \Pi(x')] \Pi(x') \\
&= 2i \int dx' \Pi(x) \partial_x \delta(x - x') \Pi(x') \\
&= 2i \Pi(x) \partial_x \Pi(x) \\
&= i \partial_x (\Pi(x))^2
\end{aligned}$$

Other commutators are calculated in full analogy.

C.2 Contractions

In this appendix we demonstrate how one can perform contractions of various functions of the fields. The correlation functions

$$\langle \phi(x, t) \phi(0, 0) \rangle_0 = G_\phi(x, t)$$

and

$$\langle \theta(x, t) \theta(0, 0) \rangle_0 = G_\theta(x, t)$$

where $\partial_x \theta(x) = \pi \Pi(x)$ are known. Using Wicks theorem (we are dealing with a Gaussian theory) we are able to calculate the contractions, e.g.

$$\langle \phi^2(\xi) \phi^2(0) \rangle_0 = \langle \phi^2(\xi) \rangle_0 \langle \phi^2(0) \rangle_0 + 2 (\langle \phi(\xi) \phi(0) \rangle_0)^2 = G_\phi^2(0) + 2G_\phi^2(\xi)$$

To deal with the derivatives, we note that

$$\langle \partial_x^k \phi(x, t) \phi(0, 0) \rangle_0 = \partial_x^k G_\phi(x, t)$$

and furthermore

$$\langle \phi(x, t) \partial_x^k \phi(0, 0) \rangle_0 = \langle \phi(0, 0) \partial_x^k \phi(-x, -t) \rangle_0 = (-\partial_x)^k G_\phi(x, t).$$

More generally

$$\langle \partial_x^k \phi(x, t) \partial_x^l \phi(0, 0) \rangle_0 = (-1)^l \partial_x^{k+l} G_\phi(x, t)$$

All correlation functions that are simple products of the fields and derivatives thereof can be treated in this manner. The correlation functions in which the bosonic fields appear in the exponent are slightly more complicated to evaluate. The recipe is described and used in Ref. [4]. The only combination that appears in our context can be readily given:

$$\left\langle e^{i2n\phi(x)} \times e^{-i2n\phi(x')} \right\rangle_0 = e^{4n^2 G_\phi(x-x')}.$$

We furthermore note that due to the symmetry properties of the propagators one has $G^{(2n+1)}(0, t) = 0$ and $\tilde{G}^{(2n)}(0, t) = 0$ where the number in parentheses in the superscript denotes derivation with respect to the spatial variable.

C.3 Momentum Susceptibility of Phonons

The generalized susceptibility of the phonon translation operator appearing in the memory matrix expression of heat conductivity is given by the correlation function

$$\chi_p = \frac{1}{V} \langle \langle P_{\text{ph}}; P_{\text{ph}} \rangle \rangle_{\omega=0}$$

where the momentum operator is

$$P_{\text{ph}} = \sum_k k a_k^\dagger a_k.$$

The evaluation happens via the associated correlation function

$$\chi_p(\omega) = i \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [P_{\text{ph}}(t), P_{\text{ph}}(t')] \rangle,$$

or, in Matsubara-language:

$$\chi_p(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau P_{\text{ph}}(\tau), P_{\text{ph}}(0) \rangle.$$

We are interested in the value of this correlation function at $\omega = 0$. In leading order, we may take the unperturbed Hamiltonian to average over, which is given by

$$H = \sum_k \varepsilon_k a_k^\dagger a_k.$$

In imaginary time we have the simple expressions $a_k^\dagger(\tau) = e^{\tau\varepsilon_k} a_k^\dagger$ and $a_k(\tau) = e^{-\tau\varepsilon_k} a_k$ for the time dependence of the operators, such that

$$P_{\text{ph}}(\tau) = \sum_k k a_k^\dagger(\tau) a_k(\tau) = \sum_k k a_k^\dagger a_k$$

is independent of τ . Thus the integral over τ simply gives β :

$$\chi_p = \frac{\beta}{V} \langle P_{\text{ph}} P_{\text{ph}} \rangle$$

i.e. the square of the expectation value of the square of the translation operator. We thus can average directly. With Wick's theorem we get

$$\begin{aligned} V\chi_p &= \beta \sum_{k,k'} k k' \langle a_k^\dagger a_k a_{k'}^\dagger a_{k'} \rangle \\ &= \beta \sum_{k,k'} k k' \left(\langle a_k^\dagger a_k \rangle \langle a_{k'}^\dagger a_{k'} \rangle + \langle a_k^\dagger a_{k'} \rangle \langle a_{k'}^\dagger a_k \rangle - \langle a_k^\dagger a_k \rangle + \langle a_{k'}^\dagger a_{k'} \rangle \delta_{kk'} \right) \\ &= \beta \sum_{k,k'} k k' \left(n_B(\varepsilon_k) n_B(\varepsilon_{k'}) + \delta_{kk'} n_B(\varepsilon_k)^2 - n_B(\varepsilon_k) + n_B(\varepsilon_k) \delta_{kk'} \right) \\ &= \beta \left(\sum_k k n_B(\varepsilon_k) \right)^2 + \beta \sum_k k^2 n_B(\varepsilon_k)^2 - \beta \left(\sum_k k n_B(\varepsilon_k) \right) \underbrace{\sum_{k'} k'}_{=0} + \beta \sum_k k^2 n_B(\varepsilon_k) \end{aligned}$$

where we have used $\langle a_k^\dagger a_{k'} \rangle = \delta_{k,k'} n_B(\varepsilon_k)$ and $n_B(\varepsilon_k) = (e^{\beta\varepsilon_k} - 1)^{-1}$ is the usual Bose distribution function. The first term vanishes since the integrand in the sum is odd in k . Thus we are left with

$$\chi_p = \frac{\beta}{V} \sum_k k^2 n_B(\varepsilon_k) (n_B(\varepsilon_k) + 1) = -\frac{1}{V} \sum_k k^2 \frac{\partial n_B(\varepsilon_k)}{\partial \varepsilon_k}$$

Now we replace the summation by an integration,

$$\sum_k \rightarrow V \int \frac{d^d k}{(2\pi)^d}.$$

Using the Debye-approximation, $\varepsilon_k = c|k|$ for $c|k| < \Theta_D$, we have

$$\chi_p = \frac{\beta \Omega_d}{(2\pi)^d} \int_0^{\Theta_D/c} dk k^{d-1} \frac{e^{\beta c k} k^2}{(e^{\beta c k} - 1)^2} = \frac{\Omega_d}{(2\pi)^d c^{2+d}} \left(\int_0^{\Theta_D/T} dy \frac{e^y y^{1+d}}{(e^y - 1)^2} \right) T^{1+d}$$

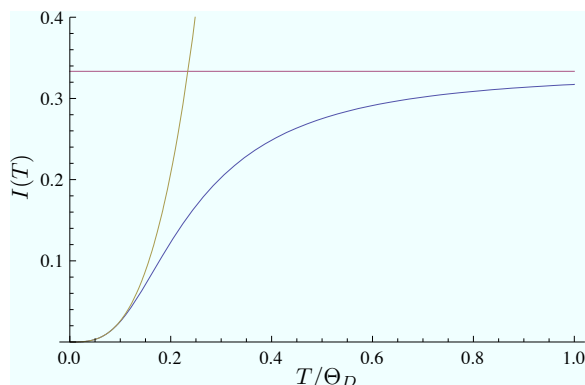


Figure C.1: The shown curves are proportional to χ_p/T and the low and high temperature approximations to it, respectively.

Here Ω_d is the volume of the d -dimensional unit sphere. The limiting behavior of the susceptibility therefore is $4\pi^4/15$ for $T \ll \Theta_D$ and $1/3(\Theta_D/T)^3$ for $T \gg \Theta_D$. Therefore, we get

$$\chi_p = \begin{cases} \frac{2\pi^2}{15c^5} T^4 & \text{for } T \ll \Theta_D \\ \frac{\Theta_D^3}{6\pi^2 c^5} T & \text{for } T \gg \Theta_D \end{cases} \quad (\text{C.1})$$

The curve associated with the integral

$$I(T) = \int_0^{\Theta_D/T} dy \frac{e^y y^4}{(e^y - 1)^2} (T/\Theta_D)^3 \quad (\text{C.2})$$

appearing in the expression for χ_p and the corresponding approximations to it are depicted in Fig. C.1. We observe that the low temperature approximation is only good up to about $0.15\Theta_D$, deviating from the Debye approximation already at $0.2\Theta_D$ by 50%. On the other hand, the high temperature approximation has the same deviation at about $0.25\Theta_D$ and captures the right order of magnitude for all temperatures above.

C.4 Finite Range Disorder

The objective of this appendix is to analyze how disorder scattering is affected by choosing a finite range disorder potential instead of the delta-correlated disorder used so far. I.e., we want to repeat the calculations of the memory matrix with the disorder being correlated according to:

$$\overline{h(x)} = 0 \quad \overline{h(x)h(x')} = \frac{D}{\sqrt{2\pi}l_D} \exp\left(-\frac{(x-x')^2}{2l_D^2}\right)$$

with l_D denoting the disorder range. Such a correlation may be expected if the impurity potential acts not at the single point it is located at, but rather affects its surrounding environment which is within a distance l_D . The assumption of a smeared out effect of a single impurity is probably more physical than the singular expression we have worked with so far, which has been chosen such only because it reduces calculational effort. Obviously, the limit $l_D \rightarrow 0$ reproduces the delta-correlated disorder, while a finite l_D introduces a new length-scale to the problem. The physically probably most relevant values are where l_D is a few lattice spacings, $l_D \gtrsim a$.

The major effect of the finite-width disorder is, that the two integrations over the space coordinates now do not reduce to the value of the correlators at zero distance. Instead of

$$\frac{1}{L} \int dx \int dx' \delta(x - x') f(x - x') = f(0)$$

we now have

$$\begin{aligned} \frac{1}{\sqrt{2\pi}l_D L} \int dx \int dx' \exp\left(-\frac{(x_1 - x_2)^2}{2l_D^2}\right) f(x_1 - x_2) \\ = \frac{1}{\sqrt{2\pi}l_D} \int d\Delta x \exp\left(-\frac{x^2}{2l_D^2}\right) f(x). \end{aligned}$$

Therefore, we will need to consider the contribution Δk_{nm} which so far could simply be neglected in connection with disorder. It will turn out, that contributions to the memory matrix coming from the ‘Umklapp’ terms with finite Δk are exponentially suppressed, as the smeared out disorder potential in combination with the spatial oscillation tends to average out the effect of the impurities. The results for $\Delta k = 0$ are, however, unchanged.

For $\Delta k \neq 0$, it is hard to carry out the space integration after the disorder averaging for general values of the disorder length l_D analytically. However, it is possible use a saddle point approximation in the limit $l_D \gg a$. As an example, we calculate the QQ memory matrix element associated with the disorder induced fluctuation in the Umklapp coupling constant g_{nm}^U for odd n . By carrying out the disorder average, we are left with the integral (here we avoid constant prefactors which are inessential for our argument)

$$I = \frac{-i}{\sqrt{2\pi}l_D} \int dt \int dx \quad t \quad e^{-x^2/(2l_D^2)} e^{i\Delta k x} G_\phi^{(2)}(x, t) e^{4n^2 G_\phi(x, t)}$$

with the kernel

$$\begin{aligned} G_\phi^{(2)}(x, t) e^{4n^2 G_\phi(x, t)} = \\ \frac{K\tau^2}{2} (\tau a)^{2n^2 K} \text{sh}^{-2-n^2 K} \tau(x - vt + ia) \text{sh}^{-n^2 K} \tau(x + vt - ia). \end{aligned}$$

Upon changing the variables to $s = \tau(x + vt)$ and $s' = \tau(x - vt)$ we get $dt dx = \frac{1}{\tau^2 v} ds ds'$ and defining $f(s, s') = -(s+s')^2/(8\tau^2 l_D^2) + i\Delta k(s+s')/(2\tau)$ we have

$$I = \frac{-i}{\sqrt{2\pi} l_D \tau v^2} (\tau a)^{2n^2 K} \int ds ds' (s - s') e^{f(s, s')} \text{sh}^{-2-n^2 K}(s' + i\tau a) \text{sh}^{-n^2 K}(s - i\tau a).$$

We perform the s' -integration first. The single saddle-point of $f(s, s')$ is given by $s'_0 = -s + i2\Delta k\tau l^2$ and $f''(s, s'_0) = -1/(4k^2 l_D^2)$ is always real. Saddle-point integration leads to

$$I = \frac{-i}{v^2} (\tau a)^{2n^2 K} e^{-\frac{\Delta k^2 l_D^2}{2}} \int ds (s - 2i\tau\Delta k l_D^2) \times \\ \times \text{sh}^{-2-n^2 K}(-s + i\tau(a + 2\Delta k\tau l_D^2)) \text{sh}^{-n^2 K}(s - i\tau a)$$

Using the limit $\tau a \ll 1$, or, equivalently, $T \ll J$, we can approximate this as

$$I = \frac{-in^2 K}{v^2} (\tau a)^{2n^2 K} e^{-\frac{\Delta k^2 l_D^2}{2}} \int ds s (i \text{sh}(s - i\tau a))^{-2-2n^2 K}$$

which leads us back to the memory matrix result already derived in the main text. As a final result, the memory matrix averaged over a disorder potential of width l_D is related to the earlier result, the memory matrix averaged over a local, delta-correlated disorder is given by the simple relation

$$M^{l_D} = \exp\left(-\frac{\Delta k^2 l_D^2}{2}\right) M^{l_D=0}.$$

Therefore, the contributions with finite $\Delta k \neq 0$ are exponentially suppressed, with an exponential factor of the order $\sim -(l_D/a)^2$, which is what we intended to show. Clearly, the limit $l_D \rightarrow 0$ is reproduced correctly.

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Köln, den 20. September 2007

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