Transport in quasi one-dimensional spin-1/2 systems

F. Heidrich-Meisner^{1, a}, A. Honecker², and W. Brenig³

Abstract. We present numerical results for the spin and thermal conductivity of one-dimensional (1D) quantum spin systems. We contrast the properties of integrable models such as the spin-1/2 XXZ chain against nonintegrable ones such as frustrated and dimerized chains. The thermal conductivity of the XXZ chain is ballistic at finite temperatures, while in the nonintegrable models, this quantity is argued to vanish. For the case of frustrated and dimerized chains, we discuss the frequency dependence of the transport coefficients. Finally, we give an overview over related theoretical work on intrinsic and extrinsic scattering mechanisms of quasi-1D spin systems.

1 Introduction

Quantum magnetism in 1D is a successful example for a fruitful interplay between theory and experiment. On the one hand, many bulk materials exist that almost perfectly realize 1D spin models (see [1,2] for a review) and on the other hand, powerful theoretical methods such as bosonization [3], the Bethe ansatz [4], or the density-matrix renormalization group method [5] are available. Often, excellent agreement between theoretical predictions and experiments has been found as far as ground-state properties, excitation spectra, thermodynamic or optical properties are concerned (see [1,6]). The understanding of transport properties is of great importance for the interpretation of transport or NMR measurements (see, e.g., Refs. [7]). Substantial progress has been made in the past years, but the understanding is still incomplete, especially for systems involving many coupled degrees of freedom such as spins, orbitals, and phonons. Theoretically, the topic of transport in 1D quantum magnets is challenging. First, several experiments demand for a more complete theoretical picture as will be outlined below, and second, transport theory often requires the computation of non-trivial correlation functions [8]. Third, transport is closely related to relaxation and non-equilibrium phenomena and thus connects to the rapidly evolving field of non-equilibrium physics of strongly correlated electron systems.

In particular, the discovery of the *colossal* magnetic heat transport in spin ladder materials such as $(Sr,Ca,La)_{14}Cu_{24}O_{41}$, where the magnetic contribution to the total thermal conductivity κ exceeds the phonon part substantially [9–11], has sparked interest in transport properties of quasi-1D spin models. Often, a magnetic mean-free path is defined within a Boltzmann type of description [9,10] used to analyze the experimental data, which in the case of spin ladders can be of the order of several hundred lattice constants [10]. This observation – originally suggested to reflect ballistic transport properties of pure spin ladders [12] – is not yet completely understood.

¹ Materials Sciences and Technology Division, Oak Ridge National Laboratory, Tennessee 37831, and Department of Physics, University of Tennessee, Knoxville, Tennessee 37996, USA

 $^{^2\,}$ Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany

³ Technische Universität Braunschweig, Institut f
ür Theoretische Physik, Mendelssohnstrasse 3, 38106 Braunschweig, Germany

^a e-mail: fheidric@utk.edu

Several other spin-1/2 chain materials (see, e.g., [13,14]) and 2D cuprate antiferromagnets [15, 16] possess similar thermal transport properties, although typically the values measured for the magnetic contribution are much smaller. A very interesting aspect is the strong magnetic field dependence observed in some 2D [15,17] and 1D materials [18,19]. Not all materials that exhibit a strong dependence of κ on magnetic field are actually believed to have a significant contribution to κ from magnetic excitations. Nevertheless, the possibility of tuning the thermal current through magnetic fields is appealing and may even allow to design functional devices such as spin valves [15]. We refer the reader to a recent review [20] and the article by C. Hess in this volume for more details on the experimental developments.

Much theoretical work has focused on intrinsic transport properties of spin systems, addressing intriguing questions such as the different transport properties of integrable as compared to nonintegrable ones. While in the remainder of this article, we restrict the discussion to the application of linear response theory – i.e., Kubo formulae – to spin and thermal transport of quasi-1D spin-1/2 systems as derived in Refs. [8,21], we note that alternative approaches such as master-equation techniques incorporating a modeling of heat baths have been pursued for quantum systems [22–24]. Moreover, while widely used, the derivation of Kubo formulae for heat transport may be questioned, as strictly speaking, no analogue to the voltage or magnetization gradients driving electrical and spin currents exists in the case of thermal transport. We refer the reader to recent work on this issue [24-27]. For brevity, we also concentrate on spin-1/2 systems and refer to the literature for more details on Haldane systems [28]. Note, though, that due to similar low-energy properties [29], the transport behavior of gapped quantum systems such as spin ladders and spin-1 chains can be expected to be generic at low temperatures. Analogous questions, i.e., the properties of integrable vs nonintegrable systems, the validity of Fourier's law, and the modeling of heat baths are timely subjects in the study of transport of classical systems (see Ref. [30] for a review).

In linear response theory, ballistic transport is defined by the existence of a finite Drude weight D [31,32], which is the zero-frequency contribution to the real part of the conductivity:

$$\operatorname{Re} \kappa[\sigma](\omega) = D_{\operatorname{th}[s]}\delta(\omega) + \kappa[\sigma]_{\operatorname{reg}}(\omega), \qquad (1)$$

where κ denotes the thermal and σ the spin conductivity. $\delta(\omega)$ is a δ -function and $\kappa[\sigma]_{reg}(\omega)$ is assumed to be regular at $\omega = 0$. Generally, the transport coefficients are computed from current-current correlation functions:

$$\kappa[\sigma](\omega) = -\frac{\beta^r}{N} \int_0^\infty dt \, e^{i(\omega+i0^+)t} \int_0^\beta d\tau \langle j_{\rm th[s]} \, j_{\rm th[s]}(t+i\tau) \rangle \,. \tag{2}$$

Here and in all succeeding equations, r = 0 for spin transport (labeled by 's') and r = 1 for thermal transport (labeled by 'th'). $\beta = 1/T$ is the inverse temperature and $\langle . \rangle$ denotes the thermodynamic expectation value. A finite Drude weight implies a divergent dc conductivity. If D vanishes, then either a finite dc conductivity $\sigma_{dc} = \lim_{\omega \to 0} \sigma_{reg}(\omega)$ can result, or, if $\sigma_{reg}(\omega)$ exhibits an anomalous frequency dependence for $\omega \to 0$, σ_{dc} may still diverge [33]. Note that here, we mainly consider finite temperatures, while the Drude weight was original introduced by Kohn to characterize a metal at T = 0 [31,32].

Trivially, if the respective current operator commutes with the Hamiltonian, the Drude weight is finite at any temperature. It has long been known that the energy current operator of the spin-1/2 XXZ chain is a conserved quantity [34], but only later, a deeper connection between the existence of finite Drude weights at finite temperatures and the *integrability* of a model system has been made [35].

As a main objective of this paper, we wish to summarize recent theoretical progress, concentrating on one-dimensional systems and their intrinsic spin and heat transport properties (see also Refs. [33,36] for recent reviews). We will contrast the properties of integrable systems such as the spin-1/2 XXZ chain discussed in Sec. 2 against nonintegrable ones. As an example for the latter class of systems, we present numerical results for the spin and thermal conductivity of the frustrated and dimerized spin-1/2 chain in Sec. 3. With respect to the experimental findings, obviously, both *intrinsic* as well as *extrinsic* scattering processes are of relevance. Recent theoretical results on extrinsic scattering channels are summarized in Sec. 4.

2 Transport properties of the *XXZ* chain

We now turn to the nearest-neighbor spin-1/2 XXZ chain. The Hamiltonian is:

$$H_{XXZ} = \sum_{l} h_{l} = J \sum_{l} \left[\frac{1}{2} (S_{l}^{+} S_{l+1}^{-} + h.c.) + \Delta S_{l}^{z} S_{l+1}^{z} \right].$$
(3)

We set J = 1 in the following and periodic boundary conditions are imposed throughout this work. The current operators corresponding to the local energy density $d_l = h_l$ defined in Eq. (3) and local spin density $d_l = S_l^z$ are obtained from the equations of continuity:

$$j_{\text{th}[s],l+1} - j_{\text{th}[s],l} = -i[H, d_{\text{th}[s],l}] \quad \Rightarrow \quad j_{\text{th}[s]} = i \sum_{l=1}^{N} [h_{l-1}, d_l].$$
 (4)

It turns out that the energy current of the spin-1/2 XXZ chain is a nontrivial conserved quantity of this integrable model [35].¹ Hence in the case of thermal transport, $\text{Re}\kappa(\omega) = D_{\text{th}}\delta(\omega)$ for any exchange anisotropy Δ of this model. Although the spin current is not in general conserved in the case of the spin-1/2 XXZ chain, it has nevertheless been conjectured that D_{s} should be finite at T > 0 in the case of integrable models, but vanish in the case of nonintegrable ones [37,38]. While we will argue in Sec. 3 that this picture seems to be correct for the massive phases of nonintegrable 1D spin models, some counterexamples have been proposed in the literature [39,40].

2.1 The thermal and the spin Drude weight at zero magnetic field

As for the Drude weights of the spin-1/2 XXZ chain, the following picture has emerged: the thermal transport is ballistic for any exchange anisotropy and at all non-zero temperatures. Its dependence on T and Δ has been studied by means of Bethe-ansatz (BA) techniques [41, 42], exact diagonalization (ED) [12,43,44], and with mean-field theory [43,45]. An example is shown in Fig. 1(a), where we display ED data for the thermal Drude weight of the XXZ chain at $\Delta = 1$ vs temperature [43], in comparison with BA results from Ref. [41]. Note that numerically, the Drude weight can be computed from [35]

$$D_{\rm th[s]}(T) = \frac{\pi \beta^{r+1}}{Z N} \sum_{\substack{m,n \\ E_m = E_n}} e^{-E_n/T} |\langle m | j_{\rm th[s]} | n \rangle|^2.$$
(5)

Here, $|n\rangle$ and E_n are eigenstates and -energies of H, respectively, and $Z = \sum_n e^{-E_n/T}$ denotes the partition function. Using system sizes as large as N = 20, the ED agrees with BA down to temperatures of $T/J \sim 0.25$, which can be improved by employing extrapolation methods [43].

Spin transport in the XXZ chain is a more involved problem as $[H, j_s] \neq 0$, and has been the objective of many studies [35, 44, 45, 38, 46–61]. While the spin Drude weight at T = 0 is known exactly [62], for the massless regime $|\Delta| < 1$, where agreement exists that $D_s(T > 0) > 0$, several BA calculations arrive at contradicting results for the temperature dependence [49, 57, 63]. The same holds for the question whether $D_s(T > 0)$ is finite or not at the SU(2) symmetric point $\Delta = 1$. We refer the reader to Refs. [36, 57] for a discussion of this issue and the conceptual problems that BA approaches face. Recent numerical studies are consistent with $D_s(T > 0) > 0$ [44, 51, 61]. We illustrate this in Fig. 1(b) and (c) where we show ED results for $D_s(T > 0) > 0$ as a function of temperature in Fig. 1(b) and a finite-size scaling analysis of the leading residue $C_s = \lim_{T\to\infty} [T \cdot D_s]$ in Fig. 1(c). Within numerical precision and under the assumption that $C_s \propto 1/N$ does not change at very large N, the extrapolation results in finite values for $|\Delta| \leq 1$. We refer to Ref. [44] for a detailed discussion of the finite-size scaling and to Refs. [44, 50, 56] for recent work on the massive, antiferromagnetic regime $\Delta > 1$. Numerical results for the ferromagnetic phase $\Delta \leq -1$ can be found in Ref. [43]. The frequency dependence of the regular part of the spin conductivity has numerically been studied in Refs. [38, 48, 56, 64].

¹ Trivial conserved quantities are, e.g., the total energy.



Fig. 1. Spin-1/2 XXZ chain. (a): Thermal Drude weight, ED (dashed lines: even N, dot-dashed lines: odd N; see [43]) vs BA results (solid line, [41]) at $\Delta = 1$. (b): Spin Drude weight as a function of temperature and for several system sizes at $\Delta = 1$. (c) Finite-size scaling at high temperatures: $C_{\rm s} = \lim_{T\to\infty} [T \cdot D_{\rm s}]$ for $\Delta = 0, 0.5, 0.6, 1, 1.5$ (from [44], with additional data for N = 20 at $\Delta = 1$).

2.2 Finite magnetic fields

In the presence of magnetic fields $H_Z = -h \sum_i S_i^z$, the energy current $j_{\rm th}$ and the spin current $j_{\rm s}$ couple since particle-hole symmetry is broken and hence $\langle j_{\rm th} j_{\rm s} \rangle \neq 0$ [35].² This gives rise to magnetothermal effects, similar to the Seebeck effect of conduction electrons [8]. Transport in the XXZ chain in the presence of magnetic fields has been studied theoretically in [65–68], focusing on the magnetothermal effect and the thermomagnetic power. To describe transport, now a 2 × 2 matrix description is necessary [8,65,66]:

$$\begin{pmatrix} J_1 \\ J_2 \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} \nabla h \\ -\nabla T \end{pmatrix}, \tag{6}$$

where ∇h and ∇T are the gradient in field and temperature, respectively.³ The conservation of j_{th} is sufficient to show that all four Drude weights D_{ij} corresponding to the transport coefficients L_{ij} are finite at all temperatures [35]. Then, assuming the condition of zero magnetization current flow, the thermal Drude weight K_{th} is obtained as

$$K_{\rm th}(h,T) = D_{22}(h,T) - \frac{D_{12}^2(h,T)}{T D_{11}(h,T)},$$
(7)

where now the magnetothermal correction $D_{12}^2(h,T)/[T D_{11}(h,T)]$ contributes as well. Some of the main results of our work Ref. [66] are (i) a reduction of $K_{\rm th}(h,T)$ due to the magnetothermal correction and (ii) expressions for the leading contributions to $K_{\rm th}(h,T)$ at low temperatures. The latter has been obtained from mean-field theory and bosonization. In the gapless phase of the XXZ chain (see, e.g., [69] for details on the phase diagram), $K_{\rm th}(h,T) \propto T$, but at the quantum critical line separating the gapless from the ferromagnetic regime, we find $K_{\rm th}(h,T) =$ $AT^{3/2}$ with A independent of the exchange anisotropy Δ . Note that $K_{\rm th}(h,T)$ has not been calculated yet by means of BA since $D_{\rm s}(h,T)$ escapes an analytical treatment [57,67]. Meanfield theory, as outlined in Refs. [43,44,66], proves useful as it provides a quantitatively good approximation to the thermal Drude weight both in zero [43] and finite magnetic fields [66].

In most cuprate based spin chain and ladder materials, exchange couplings are of the order of 1000K [1,2] hence little effects of a magnetic field on the thermal conductivity have been observed. In a recent experiment, the thermal conductivity of copper pyrazine dinitrate has been studied [19]. Since $J \sim 10.3K$ [70], a significant field dependence is found at low temperatures. The analysis of the experimental data employing the mean-field theory description of Ref. [66] yields a constant mean-free path. The origin of this result especially at the quantum critical line remains to be elucidated. Magnetothermal effects do not seem to be present in this material.

 $^{^{2}}$ We invoke the notion of particle hole symmetry as 1D spin models can be mapped onto spinless fermions with local interactions using the Jordan-Wigner transformation [8].

³ Note that $J_1 = j_s$ and $J_2 = j_{th} - hj_s$ and therefore, $D_s = D_{11}$.



Fig. 2. (a): Regular part of the thermal conductivity $\kappa_{\rm reg}(\omega)$ for a frustrated chain with $\alpha = 0.2$ [N = 18 sites; T/J = 1, 2 (circles, triangles)]. (b): Finite-size scaling of the thermal Drude weight in the high-temperature limit: $C_{\rm th} = \lim_{T \to \infty} [T^2 D_{\rm th}]$ for $\alpha = 0.1, 0.2, 0.35, 1$ (circles, squares, diamonds, triangles) for $N = 8, 10, \ldots, 20$ sites (see also Ref. [44]). (c): Integrated spectral weight $I_{\rm th}$ for $\alpha = 0.2$ and T/J = 0.5, 1, 2. (d): $\kappa_{\rm reg}(\omega)$ as a function of frequency ω for $\alpha = 1$ [N = 18, 20]. (e): Integrated spectral weight vs frequency at T/J = 0.3, 1, 5 ((d),(e): reproduced from Ref. [72]).

3 Transport properties of nonintegrable systems

While originally conjectured to exhibit diffusive transport properties [37,38,71], upon the experimental observation of large thermal conductivities in spin ladder, nonintegrable models have been discussed controversially in the literature [12,40,43,44,46,51,54,60,61,72–76]. As of now, many studies point at a vanishing of both Drude weights [40,43,44,61,72,77,78] in massive phases of nonintegrable models, including spin ladders. The massless regime of the frustrated chain remains a controversial issue [40,44]. Here we illustrate some numerical results for the finite-size scaling of the Drude weights [44] taking the example of the frustrated and dimerized chain and in particular, we also discuss the frequency dependence of the transport coefficients.

The Hamiltonian of the dimerized and frustrated spin-1/2 chain is:

$$H = \sum_{l=1}^{N} h_l = J \sum_{l=1}^{N} \left[\lambda_l \mathbf{S}_l \cdot \mathbf{S}_{l+1} + \alpha \mathbf{S}_l \cdot \mathbf{S}_{l+2} \right];$$
(8)

where α parameterizes the frustration and dimerization is introduced through $\lambda_l = 1(\lambda)$ for an even(odd) site index l ($\lambda \leq 1$). The current operators derive from Eq. (4) [43]. The regular part of $\kappa[\sigma](\omega)$ appearing in Eq. (1) can be written as:

$$\kappa[\sigma]_{\rm reg}(\omega) = \frac{\pi \beta^r}{ZN} \frac{1 - e^{-\beta\omega}}{\omega} \sum_{\substack{m,n\\ E_m \neq E_n}} e^{-E_n/T} |\langle m|j_{\rm th[s]}|n\rangle|^2 \,\delta(\omega - (E_m - E_n))\,. \tag{9}$$

3.1 Frustrated chain

As a result of preceding studies of the finite-size scaling of the thermal Drude weight [44], we concluded that no indications for a finite Drude weight are evident from the system sizes accessible by ED. This result is illustrated in Fig. 2(b), where we show the leading coefficient of an expansion of the thermal Drude weight $D_{\rm th}(T)$ in powers of 1/T, i.e., $C_{\rm th} = \lim_{T\to\infty} [T^2 D_{\rm th}(T)]$, as a function of system size (including new data for N = 20 as compared to Ref. [44]). The decrease of $C_{\rm th}$ with N is evident for all α as soon as the system size N becomes large enough (see Ref. [44] for details). The same picture arises for spin transport [44].

Let us mention the main features of $\operatorname{Re} \kappa(\omega)$ as found for the case of $\alpha = 1$, i.e., in the massive regime, shown in Fig. 2(d) [72]: (i) $\kappa_{\operatorname{reg}}(\omega)$ is a broad, featureless function extending up to frequencies $\omega/J \leq 4$; (ii) at T/J = 1 and N = 20, the thermal Drude weight only gives a small contribution to the total weight of less than 3%.

We now proceed by a discussion of the frequency dependence of the thermal conductivity of frustrated chains in the massless regime, i.e., $\alpha \leq 0.241$ [79]. Our numerical results for $\kappa_{\rm reg}(\omega)$



Fig. 3. Dimerized chain with $\lambda = 0.1$. (a): Regular part of the thermal conductivity as a function of frequency ω (N = 18 sites; T/J = 0.3, 0.4, 0.5; solid, dotted, dashed line). (b): Integrated weight $I_{\rm th}$ vs ω for T/J = 0.2, 0.5, 1, 2. Inset of (a): Integrated weight $I_{\rm th}(\omega)$ for $\omega/J = 0.5$ as a function of temperature. (c): Regular part of the spin conductivity vs ω (N = 18 sites; T/J = 0.4, 0.5, 1; solid, dotted, dashed line). (d): Integrated weight $I_{\rm s}$ vs ω for T/J = 0.4, 0.5, 1, 2. Inset of (c): Enlarged view of the low-frequency region of panel (c). Vertical, dotted lines mark the position of the spin gap.

and $\alpha = 0.2$ are shown in Fig. 2(a) for N = 18 sites and T/J = 1, 2. $\kappa_{\rm reg}(\omega)$ consists of a narrow peak centered around $\omega = 0$, extending up to $\omega/J \lesssim 0.05$. This is reflected in the integrated spectral weight $I_{\rm th}(\omega) = \int_0^{\omega} d\omega' \operatorname{Re}\kappa(\omega')$, depicted in Fig. 2(c). As this quantity also includes the contribution from the Drude weight, the figure reveals that the thermal Drude weight on the system sizes considered here amounts to more than 50% of the total spectral weight. This observation is in stark contrast to the behavior of $\kappa(\omega)$ in the massive regime on chains of a comparable length as summarized above. While on the one hand, the analysis of the finite-frequency properties of κ for $\alpha > 0.241$ supports the conclusion of a vanishing Drude weight, the question arises on the other hand whether the conclusion of $D_{\rm th} \to 0$ needs to be reconsidered in the massless regime.

From the numerical data, it is difficult to establish a definitive conclusion about the thermodynamic limit from small system sizes as far as current-current correlation functions are concerned. Still, no substantial differences are found between the massless and the massive regime concerning the finite-size scaling of the thermal Drude weight [44], the common feature being a monotonic decrease of $D_{\rm th}$ with system size N for N large enough. Moreover, bosonization studies on general grounds predict a vanishing Drude weight for thermal transport, irrespective of the presence of a gap [43,44,71,77]. In a recent work [78], Jung et al. have shown that, to first order in α , the commutator $[H, j_{\rm th}]$ between the Hamiltonian and the energy current operator vanishes, preserving the exact conservation of the energy current operator of the nearest-neighbor XXZ chain. While this feature explains the peculiar behavior of $\kappa(\omega)$ for small system sizes as observed here, a vanishing of the Drude weight can still be expected in the thermodynamic limit where all terms of $[H, j_{\rm th}]$ in powers of α become relevant and cause a finite dc conductivity. The results of a quantum Monte-Carlo (QMC) study, however, seem to indicate that in massless phases of nonintegrable models, finite Drude weights may exist [40]. Note though that the interpretation of Monte-Carlo data at finite frequencies is quite involved as an analytic continuation from Matsubara to real frequencies needs to be performed [39,40, 51].

In summary, the peculiar feature of $\kappa(\omega)$ of frustrated chains in the massless regime, i.e. $\alpha < 0.241$, as found for the system sizes accessible numerically, is that most spectral weight is found in the Drude weight, while the regular part consists of a narrow peak around $\omega = 0$ only.

3.2 The dimerized chain

We next address finite-frequency transport properties of the dimerized chain ($\alpha = 0$). In the following, we choose $\lambda = 0.1$, i.e., we focus on the limit of strong dimerization $\lambda \ll 1$. To first order in λ , the dispersion relation of the elementary triplet excitation is described by $\epsilon_k/J = 1 + (\lambda/2) \cos(k)$ [80], where k denotes the momentum. The spin gap G is quite large and roughly given by G/J = 0.95, while triplet-triplet interactions are suppressed by decreasing λ . One may therefore on the one hand expect both the spin and heat conductivity to be small due to the large spin gap, but on the other hand, the transport properties should be well approximated by considering a weakly interacting gas of hardcore bosons [81], which may, as a future project, allow for a comparison between numerical and analytical results.

Our numerical results for the conductivities $\kappa(\omega)$ and $\sigma(\omega)$ are presented in Figs. 3(a) and 3(c), respectively. The computations were performed for N = 18 sites, $\lambda = 0.1$, and several finite temperatures as listed in the figure's caption. The distinctive features of both conductivities visible in Figs. 3(a) and 3(c) are: (i) Significant spectral weight is only found around $\omega = 0$ and in a high-frequency peak located around $\omega/J \gtrsim 0.95$, which corresponds to the spin gap. (ii) While the low frequency peak (including the Drude weight) contains a large fraction of the total weight in the case of the thermal conductivity, the spectral weight of the spin conductivity is mainly concentrated in the high-frequency peak. The latter is illustrated in Figs. 3(b) and 3(d), showing the integrated spectral weight $I_{\text{th}[s]}(\omega)/I_0$, where I_0 is the full spectral weight of $\kappa[\sigma](\omega)$. The low-frequency peak is present in $\sigma(\omega)$ as well. The inset and the main panel of Fig. 3(c) show that the low-frequency peak extends up to $\omega/J \sim 0.1$, which corresponds to the width of the one-triplet band.

Furthermore, by integrating the low-frequency peak in $\kappa_{\rm reg}(\omega)$ over ω up to $\omega/J \approx 0.5$ yielding $I_{\rm reg}(\omega/J = 0.5)$, we find that this quantity is independent of system size within numerical precision. $I_{\rm th}(\omega/J = 0.5)$ is plotted in the inset of Fig. 3(a) for N = 16 and N = 18sites. Hence, a significant redistribution of spectral weight as the system size increases is not expected. One further observes a maximum in $I_{\rm th}(\omega/J = 0.5)$ at roughly $T/J \sim 0.35$ and a $1/T^2$ -dependence at high temperatures.

In summary, both models exhibit an intriguing behavior of the frequency dependence of both the spin and thermal conductivity that deserves further investigations.

4 Extrinsic scattering

As mentioned in the introduction, and as is evident form the phenomenological analysis of experimental data for spin ladder [9–11,83,82] as well as spin chain materials [13,14,84,85], it is important to include external scattering processes to arrive at a realistic theory of thermal transport in quasi 1D magnetic materials. For instance, doping with nonmagnetic impurities in $(Sr,Ca,La)_{14}Cu_{24}O_{41}$ [82] – substitution of Zn for Cu – has been found to result in a suppression of the thermal conductivity linear in the Zn content. Mobile charge carriers effectively suppress the magnon thermal transport in spin ladder systems [83]. As heat transport via magnetic systems in a material requires the heat to be transferred from the lattice to the spin system, inevitably, spin-phonon scattering needs to be modeled by theory.

First studies have addressed the thermal conductivity of spin-phonon coupled spin chains [77,86–88] as well as spin ladders [89]. Some of these works [77,89] start from effective field theories and describe transport within the Memory-matrix formalism [90,91] by first identifying the slowest decaying modes, following the spirit of Ref. [71]. These then determine the long-time behavior of current-current correlation functions. For the case of spin chains, an exponentially large thermal conductivity $\kappa_{\text{total}} \propto \exp(a \Theta/2T)$ is predicted [77], where Θ is the Debye temperature. A peculiar result of the Boltzmann theory of Refs. [86,87] is the constant spin thermal conductivity at high temperatures. For spin ladders, Ref. [89] highlights the relevance of spin-phonon drag terms contributing to the total thermal conductivity, with a rich interplay of energy scales influencing the low-temperature behavior. A direct comparison of these results with experiments, however, needs to be done in future, in particular, as disorder may be of relevance in the structurally disordered spin ladder compounds (Sr,Ca,La)₁₄Cu₂₄O₄₁

[9,10,89]. Finally, note that spin phonon coupling has also been studied in the context of spin transport in the spin-1/2 chain by means of QMC [92].

Note that via the Jordan-Wigner transformation Heisenberg type of models can be mapped onto spinless fermions [8], the transport properties of which have extensively been studied in the context of localization [93]. We just mention an incomplete list of recent, closely related works addressing Heisenberg chains [94–99], spin ladders [73], or effective low-energy models [86,87,100]. Interestingly, some works seem to indicate that the dc spin conductivity may be finite for interacting systems in the case of off-diagonal disorder [95,96]. Also, even if the dc spin conductivity vanishes, the same is not necessarily true for thermal transport as energy can still be transfered over a weak link [100].

Finally, only results from a mean-field theory are available for the thermal conductivity of doped spin ladders in the literature [101]. Transport properties of 1D t-J and Hubbard models have widely been investigated (see, e.g., Ref. [33] for an overview), and it is beyond the scope of this work to discuss the charge and spin transport of these systems. Their thermal transport properties have, however, not been studied sufficiently [102]. Note that the Hubbard model, being integrable, is expected to exhibit ballistic thermal transport, which also holds for the supersymmetric point of the t-J model [35].

5 Summary

We may conclude that the intrinsic thermal transport properties of the spin-1/2 XXZ chain in zero and finite longitudinal fields are well understood. The spin transport of this model still poses some challenges to theorists, such as an analytical calculation of the spin Drude weight of the spin-1/2 Heisenberg chain. As for nonintegrable systems and within linear response theory, it seems that generically, ballistic transport in the sense of finite Drude weights is not realized. Rather, the relevant information is encoded in the frequency dependence of the conductivities. The challenge to computational scientists is to devise algorithms that can simulate low temperature regimes. Analytical approaches face the problem that effective field-theories of nonintegrable models are typically integrable, with diverging transport coefficients. Hence, the definition of a low-energy theory that describes transport accurately is a nontrivial task.

Promising results with respect to the interpretation of experiments have been obtained from first studies incorporating phonons or disorder, but a consistent picture has not emerged yet.

Highly interesting and potentially new physics is expected from both experiments and novel theoretical methods such as the time-dependent density matrix renormalization group method [103] that investigate transport and relaxation of strongly-correlated electron systems away from equilibrium.

Acknowledgments This work has been possible only through collaborations and discussions with B. Büchner, D.C. Cabra, and C. Hess, which we gratefully acknowledge. We would also like to thank N. Andrei, J. Gemmer, C. Gros, P. Jung, A. Klümper, T. Lorenz, K. Louis, M. Michel, A. Rosch, A. Sologubenko, and X. Zotos for fruitful discussions.

References

- 1. E. Dagotto, Rep. Prog. Phys. 62 (1999) 1525.
- D. C. Johnston, M. Troyer, S. Miyahara, D. Lidsky, K. Ueda, M. Azuma, Z. Hiroi, M. Takano, M. Isobe, Y. Ueda, M. A. Korotin, V. I. Anisimov, A. V. Mahajan, and L. L. Miller, condmat/0001147 (unpublished); D. C. Johnston, R. K. Kremer, M. Troyer, X. Wang, A. Klümper, S. L. Bud'ko, A. F. Panchula, and P. C. Canfield, Phys. Rev. B **61** (2000) 9558.
- H. Schulz, in: Correlated Fermions and Transport in Mesoscopic Systems, edited by T. Martin, G. Montambaux, and J. Tran Thanh Van, Editions Frontières, Gif-sur-Yvette, 1996.
- 4. H. Bethe, Z. Phys. 71 (1931) 205; A. Klümper, Lect. Notes Phys. 645 (2004) 349.
- 5. S. R. White, Phys. Rev. Lett. 69 (1992) 2863; U. Schollwöck, Rev. Mod. Phys. 77 (2005) 259.
- 6. U. Schollwöck, J. Richter, D. Farnell, and R. Bishop, editors, *Quantum Magnetism*, volume 645 of *Lecture Notes in Physics*, Springer, Berlin Heidelberg New York, 2004.

- M. Takigawa, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **76** (1996) 4612;
 K. Thurber, A. Hunt, T. Imai, and F. Chou, Phys. Rev. Lett. **87** (2001) 247202.
- 8. G. D. Mahan, Many-Particle Physics, Plenum Press, New York London, 1990.
- A. V. Sologubenko, K. Gianno, H. R. Ott, U. Ammerahl, and A. Revcolevschi, Phys. Rev. Lett. 84 (2000) 2714.
- C. Hess, C. Baumann, U. Ammerahl, B. Büchner, F. Heidrich-Meisner, W. Brenig, and A. Revcolevschi, Phys. Rev. B 64 (2001) 184305.
- K. Kudo, S. Ishikawa, T. Noji, T. Adachi, Y. Koike, K. Maki, S. Tsuji, and K. Kumagai, J. Phys. Soc. Jpn. 70 (2001) 437.
- 12. J. V. Alvarez and C. Gros, Phys. Rev. Lett. 89 (2002) 156603.
- A. V. Sologubenko, K. Gianno, H. R. Ott, A. Vietkine, and A. Revcolevschi, Phys. Rev. B 64 (2001) 054412; A. V. Sologubenko, E. Felder, K. Gianno, H. R. Ott, A. Vietkine, and A. Revcolevschi, Phys. Rev. B 62 (2000) R6108.
- C. Hess, H. ElHaes, A. Waske, B. Büchner, C. Sekar, G. Krabbes, F. Heidrich-Meisner, and W. Brenig, Phys. Rev. Lett. 98 (2007) 027201.
- B. C. Sales, M. D. Lumsden, S. E. Nagler, D. Mandrus, and R. Jin, Phys. Rev. Lett. 88 (2002) 095901; B. C. Sales, R. Jin, and D. Mandrus, cond-mat/0401154.
- X. F. Sun, S. Komiya, and Y. Ando, Phys. Rev. B 67 (2003) 184512; M. Hofmann, T. Lorenz, K. Berggold, M. Grüninger, A. Freimuth, G. S. Uhrig, and E. Brück, Phys. Rev. B 67 (2003) 184502; R. Jin, Y. Onose, Y. Tokura, D. Mandrus, P. Dai, and B. C. Sales, Phys. Rev. Lett. 91 (2003) 146601; C. Hess, B. Büchner, U. Ammerahl, L. Colonescu, F. Heidrich-Meisner, W. Brenig, and A. Revcolevschi, Phys. Rev. Lett. 90 (2003) 197002.
- 17. M. Hofmann, T. Lorenz, G. S. Uhrig, H. Kierspel, O. Zabara, A. Freimuth, H. Kageyama, and Y. Ueda, Phys. Rev. Lett. 87 (2001) 047202.
- Y. Ando, J. Takeya, D. L. Sisson, S. G. Doettinger, I. Tanaka, R. S. Feigelson, and A. Kapitulnik, Phys. Rev. B 58 (1998) R2913; J. Takeya, I. Tsukada, Y. Ando, T. Masuda, and K. Uchinokura, Phys. Rev. B 62 (2000) R9260; J. Takeya, I. Tsukada, Y. Ando, T. Masuda, K. Uchinokura, I. Tanaka, R. S. Feigelson, and A. Kapitulnik, Phys. Rev. B 63 (2001) 214407.
- A. V. Sologubenko, K. Berggold, T. Lorenz, A. Rosch, E. Shimshoni, M. D. Phillips, and M. M. Turnbull, Phys. Rev. Lett. 98 (2007) 107201.
- 20. A. V. Sologubenko, T. Lorenz, H. R. Ott, and A. Freimuth, J. Low Temp. Phys. 147 (2007) 387.
- 21. J. M. Luttinger, Phys. Rev. 135 (1964) A1505; B. Shastry, Phys. Rev. B 73 (2006) 085117.
- K. Saito, S. Takesue, and S. Miyashita, Phys. Rev. E 54 (1996) 2404; K. Saito, Europhys. Lett. 61 (2002) 34; K. Saito and S. Miyashita, J. Phys. Soc. Jpn. 71 (2002) 2485.
- 23. C. Meja-Monasterio, T. Prosen, and G. Casati, Europhys. Lett. 72 (2006) 520.
- 24. M. Michel, M. Hartmann, J. Gemmer, and G. Mahler, Eur. Phys. J B 34 (2003) 325.
- 25. M. Michel, J. Gemmer, and G. Mahler, Eur. Phys. J B 42 (2004) 555.
- 26. M. Michel, G. Mahler, and J. Gemmer, Phys. Rev. Lett. 95 (2005) 180602.
- 27. J. Gemmer, R. Steinigeweg, and M. Michel, Phys. Rev. B 73 (2006) 104302.
- S. Sachdev and K. Damle, Phys. Rev. Lett. **78** (1997) 943; K. Damle and S. Sachdev, Phys. Rev. B **57** (1998) 8307; S. Fujimoto, J. Phys. Soc. Jpn. **68** (1999) 2810; J. Karadamoglou and X. Zotos, Phys. Rev. Lett. **93** (2004) 177203.
- K. Hida, Phys. Rev. B 45 (1992) 2207; S. R. White, Phys. Rev. B 53 (1996) 52; A. Kolezhuk and H. Mikeska, Phys. Rev. B 56 (1997) R11380.
- 30. S. Lepri, R. Livi, and A. Politi, Phys. Rep. 377 (2003) 1.
- 31. W. Kohn, Phys. Rev 133 (1964) A171.
- 32. D. J. Scalapino, S. R. White, and S. Zhang, Phys. Rev. B 47 (1993) 7995.
- 33. X. Zotos and P. Prelovšek, *in: Strong Interactions in Low Dimensions*, chapter 11, Physics and Chemistry of Materials with Low-Dimensional Structures, Kluwer Academic Publishers, 2004.
- 34. T. Niemeyer and H. van Vianen, Phys. Lett. **34A** (1971) 401.
- 35. X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B 55 (1997) 11029.
- 36. X. Zotos, J. Phys. Soc. Jpn. Suppl. **74** (2005) 173.
- 37. H. Castella, X. Zotos, and P. Prelovšek, Phys. Rev. Lett. 74 (1995) 972.
- 38. X. Zotos and P. Prelovšek, Phys. Rev. B **53** (1996) 983.
- 39. S. Kirchner, H. G. Evertz, and W. Hanke, Phys. Rev. B 59 (1999) 1825.
- 40. D. Heidarian and S. Sorella, Phys. Rev. B **75** (2007) 241104(R).
- 41. A. Klümper and K. Sakai, J. Phys. A **35** (2002) 2173.
- 42. K. Sakai and A. Klümper, J. Phys. A 36 (2003) 11617.
- 43. F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Phys. Rev. B 66 (2002) 140406(R).

- F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Phys. Rev. B 68 (2003) 134436;
 J. Mag. Mag. Mat. 272-276 (2004) 890; Phys. Rev. Lett. 92 (2004) 069703.
- 45. P. Lou, W.-C. Wu, and M.-C. Chang, Phys. Rev. B 70 (2004) 064405.
- 46. B. N. Narozhny, A. J. Millis, and N. Andrei, Phys. Rev. B 58 (1998) R2921.
- 47. K. Fabricius and B. M. McCoy, Phys. Rev. B 57 (1998) 8340.
- 48. F. Naef and X. Zotos, J. Phys. C 10 (1998) L183.
- 49. X. Zotos, Phys. Rev. Lett. 82 (1999) 1764.
- N. M. R. Peres, P. D. Sacramento, D. K. Campbell, and J. M. P. Carmelo, Phys. Rev. B 59 (1999) 7382; S.-J. Gu, V. M. Pereira, and N. M. R. Peres, Phys. Rev. B 66 (2002) 235108.
- 51. J. V. Alvarez and C. Gros, Phys. Rev. Lett. 88 (2002) 077203; Phys. Rev. B 66 (2002) 094403.
- 52. S. Fujimoto and N. Kawakami, Phys. Rev. Lett. 90 (2003) 197202.
- M. W. Long, P. Prelovšek, S. ElShawish, J. Karadamoglou, and X. Zotos, Phys. Rev. B 68 (2003) 235106.
- 54. D. A. Rabson, B. N. Narozhny, and A. J. Millis, Phys. Rev. B 69 (2004) 054403.
- 55. N. Laflorencie and H. Rieger, Eur. Phys. J. B 40 (2004) 201.
- 56. P. Prelovšek, S. ElShawish, X. Zotos, and M. W. Long, Phys. Rev. B 70 (2004) 205129.
- 57. J. Benz, T. Fukui, A. Klümper, and C. Scheeren, J. Phys. Soc. Jpn. Suppl. 74 (2005) 181.
- 58. D. Gobert, C. Kollath, U. Schollwöck, and G. Schütz, Phys. Rev. E **71** (2005) 036102.
- 59. J. Sirker, Phys. Rev. B 73 (2006) 224424.
- 60. S. Mukerjee, V. Oganesyan, and D. Huse, Phys. Rev. B 73 (2006) 035113.
- 61. S. Mukerjee and B. S. Shastry, arXiv:0705.3791.
- 62. B. Shastry and B. Sutherland, Phys. Rev. Lett. 65 (1990) 243.
- 63. Z. Qiu-Lan and G. Shi-Jian, Chinese Physics Letters 24 (2007) 1354.
- 64. F. Heidrich-Meisner, Transport properties of low-dimensional quantum spin systems, Ph.D. thesis, Technische Universität Braunschweig, http://opus.tu-bs.de/opus/volltexte/2005/712/, 2005.
- 65. K. Louis and C. Gros, Phys. Rev. B 67 (2003) 224410.
- 66. F. Heidrich-Meisner, A. Honecker, and W. Brenig, Phys. Rev. B 71 (2005) 184415.
- 67. K. Sakai and A. Klümper, J. Phys. Soc. Jpn. Suppl. 74 (2005) 74.
- 68. S. Furukawa, D. Ikeda, and K. Sakai, J. Phys. Soc. Jpn. **74** (2005) 3241.
- 69. D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. B 58 (1998) 6241.
- 70. P. R. Hammar, M. B. Stone, D. H. Reich, C. Broholm, P. J. Gibson, M. M. Turnbull, C. P. Landee, and M. Oshikawa, Phys. Rev. B 59 (1999) 1008.
- 71. A. Rosch and N. Andrei, Phys. Rev. Lett. 85 (2000) 1092.
- 72. F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Physica B 359-361 (2005) 1394.
- 73. E. Orignac, R. Chitra, and R. Citro, Phys. Rev. B 67 (2003) 134426.
- 74. K. Saito, Phys. Rev. B 67 (2003) 064410.
- 75. X. Zotos, Phys. Rev. Lett. 92 (2004) 067202.
- 76. T. Sakai and S. Yamamoto, J. Phys. Soc. Jpn. Suppl. 74 (2005) 191.
- 77. E. Shimshoni, N. Andrei, and A. Rosch, Phys. Rev. B 68 (2003) 104401.
- 78. P. Jung, R. W. Helmes, and A. Rosch, Phys. Rev. Lett. 96 (2005) 067202.
- 79. K. Nomura and K. Okamoto, J. Phys. Soc. Jpn. 62 (1993) 1123.
- 80. A. B. Harris, Phys. Rev. B 7 (1973) 3166; G. S. Uhrig, Phys. Rev. Lett. 79 (1997) 163.
- 81. S. Sachdev and R.N. Bhatt, Phys. Rev. B 41 (1990) 9323.
- C. Hess, P. Ribeiro, B. Büchner, H. ElHaes, G. Roth, U. Ammerahl, and A. Revcolevschi, Phys. Rev. B 73 (2006) 104407.
- C. Hess, H. ElHaes, B. Büchner, U. Ammerahl, M. Hücker, and A. Revcolevschi, Phys. Rev. Lett. 93 (2004) 027005; C. Hess, C. Baumann, and B. Büchner, J. Mag. Mat. 290-291 (2005) 322.
- 84. A. V. Sologubenko, H. R. Ott, G. Dhalenne, and A. Revcolevschi, Europhys. Lett. 62 (2003) 540.
- P. Ribeiro, C. Hess, P. Reutler, G. Roth, and B. Büchner, J. Mag. Mag. Mat. 290-291 (2005) 334.
- 86. A. V. Rozhkov and A. L. Chernyshev, Phys. Rev. Lett. 94 (2005) 087201.
- 87. A. L. Chernyshev and A. V. Rozhkov, Phys. Rev. B 72 (2005) 104423.
- 88. K. Louis and P. Prelovšek and X. Zotos, Phys. Rev. B 74 (2006) 235118.
- 89. E. Boulat, P. Mehta, N. Andrei, E. Shimshoni, and A. Rosch, Phys. Rev. B 76 (2007) 214411.
- D. Forster, Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions, Addison-Wesley Publishing, Reading, Massachusetts, 1990.
- 91. P. Jung and A. Rosch, Phys. Rev. B 75 (2007) 245104.
- 92. K. Louis and X. Zotos, Phys. Rev. B 72 (2005) 214415.

- 93. B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56 (1993) 1469.
- 94. G. Bouzerar, D. Poilblanc, and G. Montambaux, Phys. Rev. B 49 (1994) 8258.
- 95. K. Damle, O. Motrunich, and D. A. Huse, Phys. Rev. B 84 (2000) 003434.
- 96. O. Motrunich, K. Damle, and D. A. Huse, Phys. Rev. B 63 (2001) 134424.
- 97. T. M. R. Byrnes, R. J. Bursill, H.-P. Eckle, C. J. Hamer, and A. W. Sandvik, Phys. Rev. B 66 (2002) 195313.
- 98. F. C. Dias, I. R. Pimentel, and M. Henkel, Phys. Rev. B 73, (2005) 075109.
- 99. F. Heidrich-Meisner, Physica B **378** (2006) 299.
- 100. C. I. Kane and M. P. A. Fisher, Phys. Rev. Lett. 76 (1996) 3192.
- 101. J. Qin, S. Feng, F. Yuan, and W. Y. Chen, Phys. Lett. A 335 (2005) 477.
- 102. M.R. Peterson, S. Mukerjee, B.S. Shastry, and J.O. Haerter, Phys. Rev. B 76 (2007) 125110.
- 103. S. R. White and A. E. Feiguin, Phys. Rev. Lett. 93 (2004) 076401; A. Daley, C. Kollath, U. Schollwöck, and G. Vidal, J. Stat. Mech.: Theory Exp. (2004) P04005; K. Al-Hassanieh, A. Feiguin, J. Riera, C. Büsser, and E. Dagotto, Phys. Rev. B 73 (2006) 195304; G. Schneider and P. Schmitteckert, cond-mat/0601389.