Spin and magnetothermal transport in the $S = 1/2$ XXZ chain

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We present a temperature and magnetic field dependence study of the spin Drude weight and of magnetothermal corrections to the thermal conductivity of the spin $S = 1/2$ integrable Heisenberg chain, extending an earlier analysis using the Bethe ansatz method. We critically discuss the low temperature, weak magnetic field behavior, the effect of magnetothermal corrections in the vicinity of the critical fields and in particular their role in recent thermal conductivity experiments of 1D quantum magnets.

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Thermal transport by magnetic excitations is a research domain of actual interest where theoretical concepts are confronted and converge with state of the art experiments. The synthesis of high quality quasi-one dimensional quantum magnets allows the study of magnetic thermal conduction in spin liquids states, gapped and exotic topological excitation systems [1]. It is also amusing that prototype models used in the description of these systems, as the spin 1/2 Heisenberg model, turn out to be totally unconventional, exhibiting ballistic transport at all temperatures due to the underlying integrability of the model [2].

So far most thermal conductivity experiments are done on cuprates compounds, e.g. Sr_2CuO_3, $SrCuO_2$ or the ladder $Sr_{14}Cu_{24}O_{41}$ materials, where the magnetic exchange constant J is of the order of 2'000 K and thus a magnetic field, is not expected to play a significant role. Only a few experiments in low J (of the order of 10K) compounds exist [3–5] that pose the problem of magnetothermal corrections in thermal transport.

Several intriguing phenomena in which the interplay of spin and heat play a crucial role have been suggested [6, 8, 9]. In analogy to the thermoelectric Seebeck effect in electronic conductors the thermomagnetic Seebeck effect should arise in the presence of a temperature gradient and a magnetic field in electronic insulators. In spin systems a current of magnetic moments should flow in the presence of magnetic field H and a temperature gradient ∇T along the chain. Theoretically the problem in the Heisenberg spin - 1/2 chain has been adressed by mean-field methods plus relaxation time approximation[7] and a combination of numerical exact diagonalization as well as Bethe ansatz techniques[8, 9].

Within linear response theory the spin and energy current operators are defined from the continuity equation for the density of the conserved local spin component S_n^z and local energy correspondingly. For the Heisenberg chain,

$$\mathcal{H} = \sum_{n=1}^{N} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta\ S_n^z S_{n+2}^z) + H\ S_n^z\,, \quad (1)$$

where $S_i^\alpha = \frac{\sigma_i^\alpha}{2}$ are the Pauli spin operators with components $\alpha = \{x, y, z\}$. The continuity equations lead to the spin $\mathcal{J}_s = J\sum_n (S_n^x S_{n+1}^y - S_n^y S_{n+1}^x)$, energy $\mathcal{J}_E = J^2 \sum_n \mathbf{S}_n \cdot (\mathbf{S}_{n-1} \times \mathbf{S}'_{n+1})$ ($\mathbf{S}'_n = (S_n^x, S_n^y, \Delta S_n^z)$) and heat $\mathcal{J}_Q = \mathcal{J}_E + H\mathcal{J}_s$ current operators[2, 10]. $\mathcal{J}_Q$ and $\mathcal{J}_S$ are related to the gradients of magnetic field ∇H and temperature ∇T by the transport coefficients C_{ij} [10] :

$$\begin{pmatrix} \mathcal{J}_Q \\ \mathcal{J}_s \end{pmatrix} = \begin{pmatrix} C_{QQ} & C_{Qs} \\ C_{sQ} & C_{ss} \end{pmatrix} \begin{pmatrix} -\nabla T \\ \nabla H \end{pmatrix}, \quad (2)$$

where $C_{QQ} = \kappa_{QQ}$ ($C_{ss} = \sigma_{ss}$) is the heat (spin) conductivity. The coefficients C_{ij} correspond to time–dependent current–current correlation functions and it is straightforward to see that due to Onsager's relations [10], $C_{sQ} = \beta C_{Qs}$. The real part of $C_{ij}(\omega)$ can be decomposed into a δ function at $\omega = 0$ and a regular part:

$$\mathrm{Re}(C_{ij}(\omega)) = 2\pi D_{ij}\delta(\omega) + C_{ij}^{\mathrm{reg}}(\omega)\,. \quad (3)$$

Unconventional ballistic behaviour in the sense of non decaying currents is signalled by a finite Drude weight $D_{th,s}$ implying a divergent conductivity. The integrability of a model characterized by the existence of nontrivial local conservation laws is directly related to the existence of finite Drude weights at all temperatures [2]. To start with, it is well established that the energy current operator $\mathcal{J}_E$ of the $S = 1/2$ *XXZ* model coincides with the first nontrivial conserved quantity [11], the currents do not decay and the long time asymptotic of the energy current–current dynamic correlations is finite, implying a finite D_{th} at any temperature which has been evaluated using Bethe ansatz techniques [12].

Concerning the spin transport the situation is more involved as the spin current does not commute with the Hamiltonian. Nevertheless, it was shown [2] using an inequality proposed by Mazur and Suzuki [13] that for several quantum integrable systems D_{ss} is bounded by the thermodynamic overlap of the current operator with at least one conserved quantity. Unfortunately, for the Hamiltonian of the $S = 1/2$ model all local conservation laws are invariant under spin inversion, whereas the spin current operator $\mathcal{J}_s$ is odd giving no useful bound at zero magnetic field. The existence of a finite D_{ss} at finite T, as found by a BA approach[14, 15] has proven to be a delicate theoretical question for the zero magnetic field case.

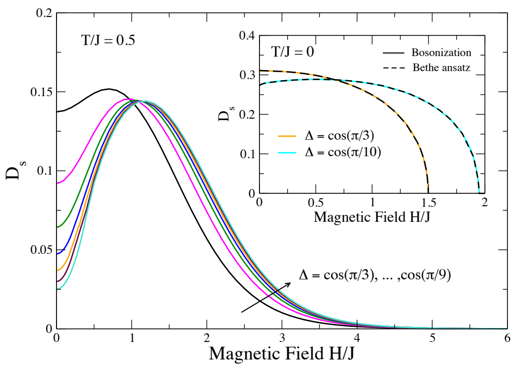

Figure 1. (Color online) Magnetic field dependence of D_{ss} at $T/J = 0.5$ and several values of the anisotropy parameter Δ. The inset depicts the magnetic field dependence of D_{ss} at $T = 0$ and two values of the anisotropy parameter $\Delta = \cos(\pi/3), \cos(\pi/10)$. Solid lines correspond to results obtained from bosonization and dashed lines from Bethe ansatz.

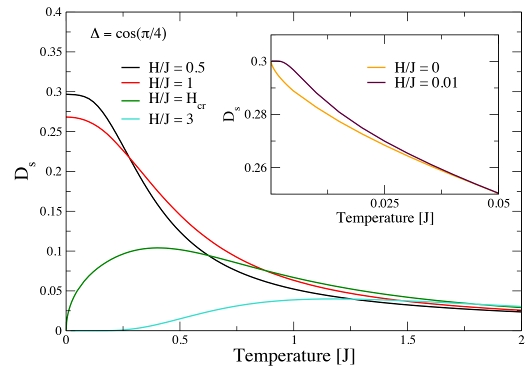

Figure 2. (Color online) Temperature dependence of D_{ss} for $\Delta = \cos(\pi/4)$ and various magnetic fields. The inset depicts the $H = 0$ power–law behaviour of D_{ss} at low temperatures given by Eq.(6). The presence of small magnetic field $H/J = 0.01$ suffices to destroy this critical behavior.

Not until recently was an improved Mazur bound was obtained [16] using a different approach based on deriving a whole family of almost conserved quasilocal conservation laws for an open XXZ chain up to boundary terms. It turns out that the quasilocal operator, with different symmetry properties than the local ones, has a finite overlap with $\mathcal{J}_s$ providing a nonzero lower bound for the spin Drude weight. This important result was later extended to the XXZ chain with periodic boundary conditions, where a family of exactly conserved quasilocal operators was constructed [17, 18].

In the scope of these recent advances in this Letter we adress the calculation of the spin Drude weight D_{ss} in the presence of magnetic field. The calculation relies on a generalization of the approach proposed in Ref. [14] at zero magnetic field. The presence of magnetic field results in some changes to the Bethe ansatz equations [19] but the overall analysis is essentially the same. The knowledge of $D_{ss}(T, H)$ also allows for the calculation of the thermal Drude weight K_{th} and intriguing magnetothermal phenomena that arise due to the coupling of the energy and spin currents [6].

A certain simplification of the Bethe ansatz equations for the massless regime $0 \le \Delta \le 1$ is provided under the parametrization $\Delta = \cos(\pi/\nu)$, ν integer. The main results of this approach are that in the gapless regime $0 \le \Delta \le 1$, $D_{ss}(T, H = 0)$ is nonzero with power–law behaviour at low temperatures as:

$$D_{ss}(T, H = 0) = D_{ss}(T = 0, H = 0) - cons.T^{\alpha}, \quad (4)$$

$\alpha = \frac{2}{\nu-1}$, while in the high temperature limit $\beta \to 0$ the spin Drude weight behaves like $D_{ss}(T, H = 0) = \beta C(\Delta)$ [15], where $C(\Delta)$ equals:

$$C(\Delta) = \frac{\frac{\pi}{\nu} - \frac{1}{2}\sin(2\frac{\pi}{\nu})}{16\frac{\pi}{\nu}}\,. \quad (5)$$

a result coinciding with the improved bound [16] at $\Delta = \cos(\pi/\nu)$.

At zero temperature the calculation of the magnetic field dependence of the spin Drude weight is feasible by considering the low–energy effective Hamiltonian of the *XXZ* model using abelian bosonization. Within the Luttinger Liquid description, the spin Drude weight is expressed as $D_{ss} = u(\Delta, H)K(\Delta, H)$, where the Fermi velocity $u(\Delta, H)$ and the so-called Luttinger parameter $K(\Delta, H)$ depend on both the magnetic field H and anisotropy parameter Δ. For $H = 0$ they can be found in closed form [20], while at finite magnetic field, both parameters can be computed exactly from the Bethe ansatz solution [21].

We now turn our attention to the magnetic field dependence of D_{ss} at finite temperature. In Fig. 1 we depict D_{ss} as a function of magnetic field H for $T/J = 0.5$ and various values of the anisotropy Δ. The inset depicts the $D_{ss}(H)$ curve at $T = 0$, calculated using the Luttinger Liquid description and the Bethe ansatz technique. The lines are indistinguishable providing a test of the Bethe ansatz calculation. We also find, as expected, that $D_{ss}(H)$ vanishes for $H > H_{cr} = J(1+\cos(\pi/\nu))$, as the system enters its massive phase.

Among the facts that become apparent from Fig. 1 are the following: (i) At small magnetic fields the spin Drude weight goes like $D_{ss} \simeq AH^2$, a behaviour that is significantly different from the one at $T = 0$. (ii) Upon increase of the magnetic field, D_{ss} increases until it reaches a maximum and then it exponentially goes to zero. In the vicinity of H_{cr}, D_{ss} is a smooth function of H that is in direct contrast with the $T = 0$ result. (iii) Upon increase of Δ, starting from $\Delta = 1/2$ and approaching the isotropic point $\Delta = 1$, the spin Drude weight seems to converge to a limiting behavior that remains unaffected as one further increases Δ. Already at $\Delta = \cos(\pi/9)$ and for magnetic fields $H/J \gtrsim 0.5$, D_{ss} has approached its limiting behaviour. This is not true for small magnetic fields $H/J \lesssim 0.5$, where such a convergence should not be ex-

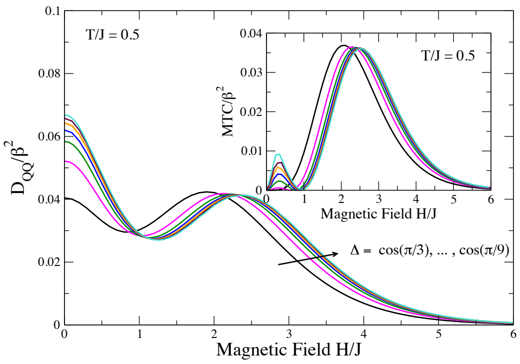

Figure 3. (Color online) Magnetic field dependence of heat Drude weight D_{QQ} at $\Delta = \cos(\pi/8)$ and several values of temperature T. The inset depicts the magnetic field dependence of MTC term at the same Δ.

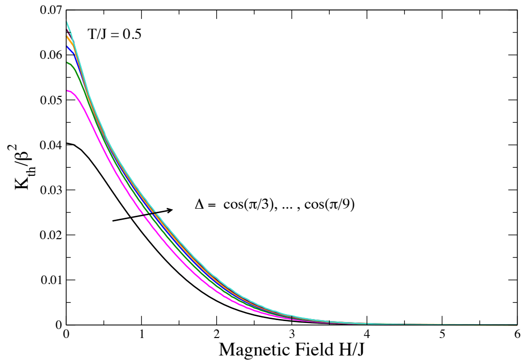

Figure 4. (Color online) Magnetic field dependence of thermal Drude weight K_{th} at $\Delta = \cos(\pi/8)$ and several values of temperature T.

pected. The $D_{ss}(H = 0)$ value strongly depends on Δ and goes to zero as $\Delta \to 1$ [14].

The temperature dependence of the spin Drude weight is also studied for four typical magnetic fields and $\Delta = \cos(\pi/4)$ and the main features are depicted in Fig. 2. At $H < H_{cr}$ the system is at its gapless phase, D_{ss} is finite at small temperatures and decreases like:

$$D_{ss}(T) \simeq D_{ss}(0) - Ae^{-H/T}T^{\gamma(H,\Delta)}\,, \tag{6}$$

provided that A is constant and the exponent γ depends on both H and Δ. At elevated temperatures, the $D_{ss}(T)$ curve vanishes exponentially. The low T behaviour is in contrast with the $H = 0$ results [14] as the power–law of Eq.(4), attributed to enhanced half-filling Umklapp scattering, is attenuated at $T < H$. At $H = H_{cr}$ the system enters its gapped regime and D_{ss} vanishes at $T = 0$. Nevertheless, D_{ss} becomes finite upon a small increase of temperature, exhibiting a $\sqrt{T}$ critical behaviour at low T. The curve increases with T until it reaches a maximum and then drops exponentially. Finally, in the gapped $H > H_{cr}$ regime we notice that at low T Drude weight is zero, it is exponentially activated upon increase of T and vanishes after taking a maximum. This behaviour is summarized in Fig. 2. Also note that in the high temperature limit, spin Drude weight behaves like $D_{ss}(T) = \beta C(\Delta)$, where $C(\Delta)$ is given by Eq.(5).

To relate correlation functions C_{ij} to experimentally accessible quantities we note that the spin conductivity σ measured under the condition of $\nabla T = 0$ is equal to $\sigma(\omega) = C_{SS}(\omega)$ and the thermal conductivity under the assumption of vanishing spin current $\mathcal{J}_s = 0$, which is relevant to certain experimental setups, is redefined as follows:

$$\kappa(\omega) = C_{QQ}(\omega) - \beta\frac{C^2_{Qs}(\omega)}{C_{ss}(\omega)}\,, \tag{7}$$

where the second term is usually called the magnetothermal correction. Such a term originates from the coupling of the heat and spin currents in the presence of magnetic field [6–8] and is absent when $H = 0$. In the case of ballistic transport, the thermal conductivity K_{th} is found by combining Eqs.(7) and (3):

$$K_{th} = D_{QQ} - \beta\frac{D^2_{Qs}}{D_{ss}}\,. \tag{8}$$

The first term D_{QQ} corresponds to the heat conductivity, while the second term is the magnetothermal correction $MTC = \beta\frac{D^2_{Qs}}{D_{ss}}$. We should stress, in view of experiments[3–5], that this relation holds assuming the same relaxation rates for spin and energy transport. It becomes apparent that D_{QQ} and K_{th} are the main quantities which play central role in the study of thermal conductivity in the $S = 1/2$ *XXZ* chain. The thermal Drude weight K_{th} is the result of a combination of two competing terms, the D_{QQ} and MTC term and for a complete picture of the thermal transport of the model all three terms need to be explored. One can decompose the heat Drude weight D_{QQ} in terms of the energy and spin contribution, which yields:

$$D_{QQ} = D_{EE} + 2\beta HD_{Es} + \beta H^2 D_{ss}\,. \tag{9}$$

Similarly the MTC term, and consequently the K_{th} term, can be decomposed in terms of D_{EE}, D_{Es} and D_{ss}. The D_{EE} and D_{Es} at finite temperatures have been calculated by Sakai and Klümper [8] using a lattice path integral formulation, where a quantum transfer matrix (QTM) in the imaginary time is introduced. This method produces all relevant correlations by solving two nonlinear integral equations at arbitrary magnetic fields and temperatures.

Let us begin by considering the magnetic field dependence of the various quantities. In Fig. 3 we depict the heat Drude weight D_{QQ} as a function of H for various values of T and $\Delta = \cos(\pi/8)$. An important fact of Fig. 3 is that $D_{QQ}(H)$ exhibits a pronounced nonmonotonic behaviour as a function of H. At small magnetic fields it decreases quadratically and then it rises again creating a peak before it vanishes at large magnetic fields.

Next, we consider the behaviour of the MTC term as a function of H as illustrated in the inset of Fig. 3 for several T's

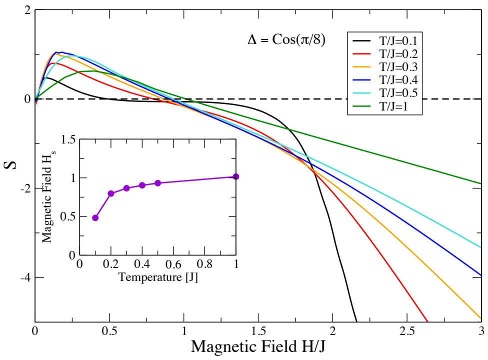

Figure 5. (Color online)Thermal Seebeck coefficient S for $\Delta = \cos(\pi/8)$ and several values of T as a function of H. The inset depicts the magnetic field H_s at which S changes sign, as a function of T.

and $\Delta = \cos(\pi/8)$. As expected, the MTC term is exactly zero at $H = 0$, but becomes finite at finite H, where it develops two peaks with the second being more dominant than the first. The MTC term turns out to be significant and should be taken into account for a complete description of thermal transport.

The resulting behaviour of the total thermal Drude weight K_{th}, as a sum of two competing terms, is summarised in Fig. 4, where it is plotted as a function of H for different temperatures. Fig. 4 allows for two major observations: (i) the thermal Drude weight turns out to be a smooth function of magnetic field with no peaks observed as a function of H. The inclusion of the MTC term results in an overall suppression of K_{th} and the cancellation of the nonmonotonic peaked behaviour of D_{QQ}. For all considered temperatures the MTC and D_{QQ} terms develop a peak located exactly at the same field; the subtraction of these two terms results a K_{th} that is a smooth function of H. This finding is consistent with a numerical study of the thermal transport in the $S = 1/2$ *XXZ* chain in the presence of a magnetic field [7] based on exact diagonalization of a finite chain. (ii) As in the case of $D_{QQ}(H)$ and MTC the thermal Drude weight $K_{th}(H)$ is approaching a limiting behaviour in the $H/J \gtrsim 0.25$ region as $\Delta \to 1$. In general the Δ dependence of D_{QQ}, MTC and K_{th} is minor with qualitatively the same H features.

Considering magnetothermal effects using Eq.(2) the magnetic Seebeck coefficient S under the condition of zero spin current $\mathcal{J}_s = 0$ and for ballistic transport is given by,

$$S = \frac{\nabla H}{\nabla T} = \frac{C_{sQ}}{C_{ss}} = \frac{D_{sQ}}{D_{ss}}\,. \tag{10}$$

Here we take advantage of Bethe ansatz technique to calculate S as a function of H for various temperatures in the thermodynamic limit. In Fig.5 we depict the magnetic field dependence of S for $\Delta = \cos(\pi/8)$ and several values of T. We note that at small magnetic fields S is positive, while at a certain magnetic field H_s it changes sign and remains negative. In Ref. [9] it was suggested that the sign of S is a criterion to clarify the types of carriers; a positive (negative) S implies that the spin and heat are dominantly carried by carriers with up (down) spin. Upon increase of T the structure of S changes, but at any T there is a single H_s at which the Seebeck coefficient changes sign (see inset in Fig. 5).

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