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

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Abstract. We present a temperature and magnetic field dependence study of spin transport and magnetothermal corrections to the thermal conductivity in the spin $S = 1/2$ easy-plane Heisenberg chain, extending an earlier analysis based on 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 field and their role in recent thermal conductivity experiments in 1D quantum magnets.

Keywords: quantum transport in one-dimension, thermodynamic Bethe Ansatz
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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 gapless, gapped, spin liquid, with topological excitations states [1]. It is also amusing that prototype models used in the description of these systems, as the $S = 1/2$ 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 materials as the Sr$_2$CuO$_3$, SrCuO$_2$ or the ladder Sr$_{14}$Cu$_{24}$O$_{41}$ cuprate compounds, where the magnetic exchange constant $J$ is of the order of 2000 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 10 K) compounds exist [3–5] that pose the problem of magnetothermal corrections in thermal transport.

In experiments, the measured thermal conductivity includes contributions from all itinerant particles or quasi-particles, such as charge carriers, spin excitations, phonons. In the case of insulators the study of thermal transport as a function of magnetic field is particularly attractive, as the magnetic field provides a handle to separate the field-independent phononic contribution from the total measured thermal conductivity [3], confronting subtle theoretical analysis to experiments. Furthermore, several intriguing phenomena in which the interplay of spin and heat transport play a crucial role have been suggested [6–9]. In analogy to the thermoelectric effect in electronic conductors a spin-Seebeck effect should arise in the presence of a temperature gradient in electronic insulators. Over the last few years, a great deal of experimental work has demonstrated such a generation of spin currents in a variety of (anti) ferro-magnetic insulating materials [10] attracting interest to the novel field of spin-caloritronics [11].

In addition, one important aspect of thermal transport as a function of magnetic field is the behavior of the various transport quantities close to the critical field $H_{cr}$, that corresponds to a quantum critical point (QCP). The presence of a QCP can significantly affect the thermodynamic properties of a quantum magnet, such as the magnetization or specific heat. However, new insights on the QCPs could be provided by the thermal and spin transport and consequently by the thermomagnetic coefficients.

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

$$
\mathcal{H} = \sum_{n=1}^{N} J(S^x_n S^x_{n+1} + S^y_n S^y_{n+1} + \Delta S^z_n S^z_{n+1}) - H S^z_n,
$$

For a very partial reference list to this rapidly developing field, [10].

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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 $\mathcal{J}_S = J \sum_n (S_n^x S_{n+1}^x - S_n^y S_{n+1}^y)$, energy $\mathcal{J}_E = J^2 \sum_n S_n \cdot (S_{n-1} \times S_{n+1})$ and heat $\mathcal{J}_Q = \mathcal{J}_E - H \mathcal{J}_S$ current operators [2, 12]. $\mathcal{J}_Q$ and $\mathcal{J}_S$ are related to the gradients of magnetic field $\nabla H$ and temperature $\nabla T$ by the transport coefficients $C_\eta$ [12]:

$$
\begin{pmatrix}
\mathcal{J}_Q \\
\mathcal{J}_S 
\end{pmatrix} = 
\begin{pmatrix}
C_{QQ} & C_{Q\eta} \\
C_{S\eta} & C_{SS} 
\end{pmatrix}
\begin{pmatrix}
-\nabla T \\
\nabla H 
\end{pmatrix},
$$

(2)

where $C_{QQ} = \kappa_{QQ}$ ($C_{SS} = \sigma_{SS}$) is the heat (spin) conductivity. The coefficients $C_\eta$ correspond to time-dependent current–current correlation functions and it is straightforward to see that due to the Onsager’s relations [12], $C_{SQ} = \beta C_{QS}$. The real part of $C_\eta(\omega)$ can be decomposed into a $\delta$-function at $\omega = 0$ and a regular part:

$$
\text{Re}(C_\eta(\omega)) = 2\pi D_\eta \delta(\omega) + C_{\eta reg}(\omega).
$$

(3)

Unconventional ballistic behavior in the sense of non decaying currents is signalled by a finite Drude weight $D_{QQ, SS}$ 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 [13], the currents do not decay and the long time asymptotic of the energy current–current dynamic correlations is finite, implying a finite $D_{EE}$ at any temperature which has been evaluated by a quantum transfer matrix technique [14].

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 [15], 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 Bethe Ansatz (BA) approach [16, 17] has proven to be a delicate theoretical question for the zero magnetic field case. Not until recently, an improved Mazur bound was obtained [18] using a different approach based on deriving a whole family of almost conserved quasi-local 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 [19, 20].

In light of these recent advances, we address in this paper 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 [16] at zero magnetic field. The presence of a magnetic field results in some changes to the Bethe ansatz equations [21], 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 magnetothermal phenomena that arise.
due to the coupling of the energy and spin currents [6]. Theoretically, the problem of transport in the Heisenberg $S = 1/2$ chain has been addressed by mean-field methods plus a relaxation time approximation [22], a combination of numerical exact diagonalization as well as BA techniques [7, 8].

A certain simplification of the Bethe ansatz equations in the massless regime $0 \leq \Delta \leq 1$ is provided under the parametrization $\Delta = \cos(\pi \nu)$, with integer $\nu$. The main results of this approach are that, in the gapless regime $0 \leq \Delta \leq 1$, $D_{SS}(T, H = 0)$ is non-zero with power-law behavior at low temperatures as:

$$\alpha = \frac{2}{\nu - 1}; \text{ in the high temperature limit } \beta \to 0 \text{ the spin Drude weight behaves like } D_{SS}(T, H = 0) = \beta C(\Delta)$$

$$C(\Delta) = \frac{1}{16} \left[ 1 - \frac{\sin(\frac{2\pi}{\nu})}{\frac{2\pi}{\nu}} \right],$$

a result interestingly coincident with the improved lower bound at $\Delta = \cos(\pi \nu)$ [18].

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 $\Delta$. For $H = 0$ they can be found in closed form [23], while at finite magnetic field, both parameters can be computed exactly from the Bethe ansatz solution [24].

We now turn our attention to the magnetic field dependence of $D_{SS}$ at finite temperature. In figure 1 we depict $D_{SS}$ as a function of magnetic field $H$ for $T/J = 0.5$.

Figure 1. Magnetic field dependence of $D_{SS}$ at $T/J = 0.5$ and several values of the anisotropy parameter $\Delta$. 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.
and various values of the anisotropy $\Delta$. The inset depicts the $D_{SS}(H)$ curve at $T = 0$, calculated using the Luttinger liquid description and the Bethe Ansatz method. The lines are indistinguishable providing a test of the BA calculation. We also find, as expected, that $D_{SS}(H)$ vanishes for $H > H_{cr} = J(1 + \Delta)$, as the system enters its massive phase. The facts that become apparent from figure 1 are the following: (i) at small magnetic fields the spin Drude weight goes like $D_{SS} \propto \sqrt{H}$, a behavior that is significantly different from the one at $T = 0$. (ii) Upon increasing 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 increasing $\Delta$, starting from $\Delta = 1/2$, approaching the isotropic point $\Delta = 1$ and for magnetic fields $H/J \gtrsim 0.5$, $D_{SS}$ seems to converge to a limiting behavior. This is not true for small magnetic fields $H/J \lesssim 0.5$, where such a convergence should not be expected. The $D_{SS}(H = 0)$ value strongly depends on $\Delta$ and goes to zero as $\Delta \to 1$ [16].

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

$$D_{SS}(T, H) - D_{SS}(T, 0) \sim -e^{-H/T^\gamma(H, \Delta)},$$

where the exponent $\gamma$ depends on both $H$ and $\Delta$. At elevated temperatures, the $D_{SS}(T)$ curve vanishes as $1/T$. As shown in the inset of figure 2, the low $T$ behavior is in contrast to the $H = 0$ results [16] as the power-law of equation (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, it becomes finite upon a small increase of temperature, exhibiting a $\sqrt{T}$ critical behavior at low $T$. The curve increases with $T$ until it reaches a maximum and then drops as $1/T$. Finally, in the gapped $H > H_{cr}$ regime we notice that at low $T$ the Drude weight is exponentially activated upon increasing $T$ and vanishes after a maximum. This behavior is summarized

Figure 2. Temperature dependence of $D_{SS}$ for $\Delta = \cos(\pi/4)$ and various magnetic fields. The inset depicts the $H = 0$ power-law behavior of $D_{SS}$ at low temperatures given by equation (6). The presence of small magnetic field $H/J = 0.01$ suffices to destroy this singular behavior.
in figure 2. Also note that in the high temperature limit, the spin Drude weight behaves like \( D_{SS}(T) = \beta C(\Delta) \), where \( C(\Delta) \) is given by equation (5).

Interesting conclusions can be drawn by a comparison to the special case of \( \Delta = 0 \) (XY) model, where both the spin and thermal currents are conserved and exact results can be found using the Jordan–Wigner transformation \([8]\). The majority of features of \( D_{SS} \) presented here for the \( 0 < \Delta < 1 \) model are also realized for the \( \Delta = 0 \) case. Nonetheless, one should emphasize that the power-law behavior of equation (4) is absent in the XY model.

Now, with the novel input of \( D_{SS} \) from the Bethe ansatz analysis above, we can address the evaluation of thermal conductivity and magnetothermal coefficients. To relate the correlation functions \( C_{ij} \) to experimentally accessible quantities we note that the spin conductivity \( \sigma \) measured under the condition of \( \nabla T = 0 \) is equal to \( \sigma(\omega) = C_{SS}(\omega) \). Furthermore, the thermal conductivity under the assumption of vanishing spin current \( J_{S} = 0 \), which is relevant to certain experimental setups, is redefined as follows:

\[
\kappa(\omega) = C_{QQ}(\omega) - \beta \frac{C_{QS}^{2}(\omega)}{C_{SS}(\omega)},
\]

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 a magnetic field \([6, 7, 22]\) and is absent when \( H = 0 \). In the case of ballistic transport, the thermal conductivity \( K_{th} \) is found by combining equations (7) and (3):

\[
K_{th} = D_{QQ} - \beta \frac{D_{QS}^{2}}{D_{SS}}.
\]

The first term \( D_{QQ} \) corresponds to the heat conductivity, while the second term is the magnetothermal correction \( MTC = \beta \frac{D_{QS}^{2}}{D_{SS}} \). We should stress, in view of experiments \([3–5]\), that this relation holds only when we assume the same relaxation rates for the magnetization and energy transport, \( C_{ij} \sim D_{ij}\tau \) \([6]\), an assumption deserving further study as it is not generally valid when inelastic processes are present \([25]\).

It becomes apparent that \( D_{QQ} \) and \( K_{th} \) are the main quantities which play a 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 evaluated. One can decompose the heat Drude weight \( D_{QQ} \) in terms of the energy and spin contribution, which yields:

\[
D_{QQ} = D_{EE} - 2\beta HD_{ES} + \beta H^{2}D_{SS}.
\]

Similarly, MTC and consequently \( K_{th} \), can be decomposed in terms of \( D_{EE}, D_{ES} \) and \( D_{SS} \). As the energy current \( J_{E} \) commutes with the Hamiltonian, the \( D_{EE} = \beta^{2} \langle J_{E}^{2} \rangle \) and \( D_{ES} = \beta \langle J_{E} J_{S} \rangle \) (\( \langle \ldots \rangle \) is a thermal average) terms have been calculated by Sakai and Klümper \([7]\) using a quantum transfer matrix method. 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 figure 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 figure 3 is that $D_{QQ}(H)$ exhibits a pronounced nonmonotonic behavior 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. This peak structure, reminiscent of the behavior of the specific heat which exhibits a double peak in the vicinity of the critical field at low temperatures [26], cannot be explained using a simple picture and is a signature of the strong correlations in the system.

Next, we consider the behavior of the MTC term as a function of $H$ as illustrated in the inset of figure 3 for several $T$’s 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 two peaks can be understood by the nonmonotonic behavior of $D_{QS}$ that changes sign at a certain magnetic field and as it appears as a square in the MTC, it results to a two peak structure. The change of sign can be interpreted as a change of the sign of carriers as we discuss below in the context of the Seebeck coefficient. The MTC term turns out to be significant in equation (8) and should be taken into account in a complete theoretical description of magnetothermal transport.

The resulting behavior of the total thermal Drude weight $K_{th}$, as a sum of two competing terms, is summarised in figure 4, where it is plotted as a function of $H$ for different temperatures. Figure 4 allows for two major observations: (i) at $T/J \gtrsim 0.3$ 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 behavior of $D_{QQ}$. At higher temperatures the MTC and $D_{QQ}$ terms develop a peak located exactly at the same field; the subtraction of these two terms results at 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 [22] based on exact diagonalization of a finite chain.
Concerning thermal conductivity experiments [3–5] in a magnetic field, although not conclusive, it seems that the rather featureless field dependence indicated in figure 4 (at $T/J \geq 0.1$) is not observed but rather the nonmonotonic one shown in figure 3. The absence of magnetothermal corrections was attributed to the nonconservation of total magnetization due to spin–orbit scattering [27] and supported by a mean field approximation in the relaxation time approximation [3]. But it could also be due to vastly different relaxation times for magnetization and energy transport [25]. If $C_0 \sim D_0 \tau_0$ [6] and $\tau_0 \gg \tau_{QS}^2 T SS$ then the MTC term would give a negligible contribution.

Finally, considering magnetothermal effects using equation (2), the magnetic Seebeck coefficient $S$ under the condition of zero spin current $J_S = 0$, ballistic transport and equal relaxation times, is given by,

Figure 4. Magnetic field dependence of thermal Drude weight $K_{th}$ at $\Delta = \cos(\pi/8)$ and several values of temperature $T$. Vertical dotted line denotes the position of $H_{cr}$.

Figure 5. 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 $T$. 
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$$S = \frac{\nabla H}{\nabla T} = \frac{C_{SQ}}{C_{SS}} = \frac{D_{SQ}}{D_{SS}} = \beta \frac{D_{ES}}{D_{SS}} - \beta H. \quad (10)$$

Here we take advantage of the Bethe ansatz technique to calculate $S$ as a function of $H$ at various temperatures in the thermodynamic limit. In figure 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 [7, 8], the low temperature behavior ($T \ll H$) of $S$ was analyzed without directly evaluating $D_{SS}$. It was suggested that the sign of $S$ is a criterion to distinguish the types of carriers, a positive (negative) $S$ implying that the spin and heat are dominantly carried by carriers with up (down) spin. Upon increasing $T$ 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 figure 5). The change of carrier sign is a well-known effect due to strong correlations in electronic systems [28, 29] and indeed in the XY model, $\Delta = 0$, (equivalent to non-interacting spinless fermions) there is no sign change as a function of magnetic field (or particle density).

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