Diverging magnetothermal response in the one-dimensional Heisenberg chain

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(Dated: March 22, 2022)

A current of magnetic moments will flow in the spin-1/2 Heisenberg chain in the presence of an external magnetic field \( B \) and a temperature gradient \( \Delta T \) along the chain. We show that this magnetothermal effect is strictly infinite for the integrable Heisenberg-model in one dimension. We set-up the response formalism and derive several new generalized Einstein relations for this magnetothermal effect which vanishes in the absence of an external magnetic field. We estimate the size of the magnetothermal response by exact diagonalization and Quantum Monte Carlo and make contact with recent transport measurements for the one-dimensional Heisenberg compound \( \text{Sr}_2\text{CuO}_3 \).

PACS numbers: 75.30.Gw,75.10.Jm,78.30.-j

I. INTRODUCTION

The nature of magnetic and thermal transport in magnetic insulators with reduced dimensions is a long standing problem. Huber, in one of the first works on the subject,\textsuperscript{3,4} evaluated the thermal conductivity \( \kappa(T) \) for the Heisenberg-chain with an equation-of-motion approximation and found a finite \( \kappa(T) \), a result which is, by now, known to be wrong. A few years later, Niemeijer and van Vianen calculated \( \kappa(T) \) in the case \( J_z = 0 \) using the Jordan-Wigner transform and found a diverging result.\textsuperscript{3} It has been shown recently,\textsuperscript{5} that the energy-current operator commutes with the Hamiltonian for the spin-1/2 Heisenberg chain. The thermal conductivity is consequently infinite for this model. The intriguing question, “under which circumstances does an interacting quantum-system show an infinite thermal conductivity”, is being intensively studied theoretically\textsuperscript{5,6,7,8} motivated, in part, by new experimental findings.

An anomalous large magnetic contribution to \( \kappa \) has been observed for the spin-ladder system \( \text{Sr}_{14-x}\text{Ca}_x\text{Cu}_2\text{O}_{11} \) and \( \text{Ca}_9\text{La}_3\text{Cu}_2\text{O}_{11} \),\textsuperscript{9} raising the possibility of ballistic magnetic transport limited only by residual spin-phonon and impurity scattering. Large energy-relaxation times have been found in recent experimental\textsuperscript{10} and theoretical\textsuperscript{11} studies of the thermal conductivity for the quasi-one dimensional spin-chain compounds \( \text{SrCuO}_2 \) and \( \text{Sr}_2\text{CuO}_3 \), consistent with \( ^{17}\text{O} \) NMR studies.\textsuperscript{10}

It is known\textsuperscript{11,12} that there is no magnetothermal effect in the Heisenberg chain since the magnetic-current operator is a pseudo-vector. This can be seen by a simple symmetry argument in the standard setting, when we consider only a temperature gradient along the sample. A non-zero magnetothermal effect would yield a magnetization along an arbitrary quantization axis. But because of the isotropic conditions there is no preferred direction along which such a magnetization might occur, the effect vanishes consequently.

The situation is, however, different if there is an external magnetic field.\textsuperscript{13} A temperature gradient will now cause a magnetization current with a magnetization vector parallel to the field, see Fig. 1. This magnetothermal effect can be considered the generalization to magnetic systems of the Seebeck effect occurring in normal conductors. It is diverging for the isolated Heisenberg chain, leading to a finite non-zero ‘magnetothermal Drude weight’. In this paper we discuss magnetothermal effects in spin chains, i.e., we examine how the magnetic and thermal currents couple to external sources.

In Sec. II we will discuss the differences in between the thermomagnetic effects found in normal metals and the magnetothermal response we study here for magnetic insulators. In Sec. III \textsuperscript{14} and in Sec. IV we set-up the formalism for the magnetic and energy current operators in the presence of an external magnetic field and for the correlation and response-functions, respectively.

In Sec. VII we evaluate the magnetothermal response for the xy-chain via a Jordan-Wigner transformation and derive and discuss several generalized Einstein relations in Sec. VIII. In Sec. IX we derive and discuss a new exact magnetothermal Einstein relation.

We present in Sec. X numerical results obtained from Quantum-Monte-Carlo Simulations and exact-diagonalization studies. Finally, we discuss the size of the magnetothermal effect expected for \( \text{Sr}_2\text{CuO}_3 \) together with a dimensional analysis in Sec. XI.

II. THERMOMAGNETIC AND MAGNETOTHERMAL RESPONSE

In a conventional solid there is normally a variety of ways in which external parameters (e.g., current density \( j \), temperature gradient and magnetic field \( B \)) couple to the voltage \( \nabla \mu \) and the thermal current \( j_E \) leading to numerous thermoelectric and thermomagnetic effects. A phenomenological equation which gives full account of all these effects would look as (see, e.g., Ref. 12)

\[
\begin{pmatrix}
-\nabla \mu \\
\quad j_E
\end{pmatrix} = \begin{pmatrix}
\rho & Q \\
\Pi & -\kappa
\end{pmatrix} + \begin{pmatrix}
R & N \\
E\kappa & L\kappa
\end{pmatrix} B \times \begin{pmatrix}
\quad j \\
\nabla T
\end{pmatrix}.
\]
\( (\mathbf{B} \times \mathbf{E}) \) is understood to be applied to both components separately. \( \rho \) is the resistivity, \( \kappa \) the thermal conductivity, and the other coefficients describe the Seebeck- (Q), Peltier- (\( P \)), Hall- (\( R \)), Nernst- (\( N \)), Ettingshausen- (\( E \)), and Righi-Leduc-effect (\( L \)). The latter four effects are called thermomagnetic – for obvious reason – and are not to be confounded with the effects which are to be discussed in this paper which we denote \textit{magnetothermal effects}. One should note that in magnetic systems the magnetic field corresponds to the chemical potential, leaving no analogues for the entries of the second matrix.

Following Ref.\[12\] we write the dependence of the current densities \( j_M \) (particle) and \( j_E \) (energy) on external sources (field \( \nabla B = -\nabla \mu \) and temperature gradient \( \nabla T \)) in the following manner

\[
\begin{pmatrix}
  j_M \\
j_E
\end{pmatrix} = \begin{pmatrix}
  \hat{L}_{MM} & \hat{L}_{ME} \\
  \hat{L}_{EM} & \hat{L}_{EE}
\end{pmatrix} \begin{pmatrix}
  \nabla B \\
  -\nabla T
\end{pmatrix}.
\tag{1}
\]

We deviate from the standard notation by indexing the components of the tensor by \( M \) and \( E \) rather than 1 and 2. The notation with \( M \) as particle index and \( E \) as chemical potential borrows from spin systems, this article’s chief case of interest. Eq.\[11\] may therefore be used as a reference for both electrical and magnetic systems.] Normally, the two off-diagonal components governing the Seebeck and Peltier effect are not independent but related via the \textit{Onsager relation}. Here, with the given choice of external forces, it reads (where \( T \) denotes temperature)

\[
T \hat{L}_{ME} = \hat{L}_{EM}.
\tag{2}
\]

To compute the response functions \( \hat{L}_{ij} \) we use the standard Kubo-formula\[2,6,13,14\] which yields for the Heisenberg model generally an \( L \)-Tensor with infinite components, i.e., a delta function times a weight-factor. These weight-factors will be denoted by the entries of the \( L \)-Tensor \( L_{ij} \) (without \( \hat{\cdot} \)-accent). Normally, one has an additional finite contribution – the regular part – which will turn out to be zero for all but the MM-component. We assume that due to some – so far unaccounted – scattering processes with external degrees of freedoms (like phonons or impurities) the infinite peak broadens, and the coefficients (we consider only the real part) may be replaced according to (cf., e.g., Ref.\[14\])

\[
\hat{L}_{ij} (\omega) = L_{ij} \pi \delta (\omega) \rightarrow \frac{L_{ij} \tau}{1 + (\omega \tau)^2}
\tag{3}
\]

with \( i,j \in \{M,E\} \) and a finite relaxation time \( \tau \) – for simplicity, a possible dependence on \( i \) and \( j \) shall be neglected.

**III. CURRENT OPERATORS**

In this article, we discuss the analogue of the thermoelectric effect in spin-chains. The Hamiltonian is the standard \( xxz \)-chain,

\[
H_n = J_z (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J_z S_n^z S_{n+1}^z + \mu_B BS_n^z.
\tag{4}
\]

\( \mu_B \) is the Bohr magneton and the lattice spacing will be denoted by \( c \); the \( S_n \) are supposed to be dimensionless.

Instead of the electrical current we consider the magnetic current\[15\]

\[
J_M = i \mu_B \frac{e}{\hbar} \frac{c^2}{2} \sum_n \left[ S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+ \right]
\tag{5}
\]

where we have defined the magnetic polarization \( P_M = \mu_B \sum_n n S_n^z \), which is possible only for chains with open boundary conditions (OBC).

For the energy current\[2,3\] we have equivalently

\[
\frac{\hbar}{c} J_E = i \sum_n \left[ h_n, h_{n+1} \right] = \frac{B}{c} J_M + \sum_n \tilde{S}_n \cdot (S_{n+1} \times \tilde{S}_{n+2})
\]

\[
= \frac{B}{c} J_M + \sum_n \det \left[ S_n S_{n+1} S_{n+2} \right] = i \left[ H, P_E \right],
\tag{6}
\]

where we have used \( S_n = (S_n^x, S_n^y, S_n^z) \) and the definition \( \tilde{S}_n = (J_z S_n^x, J_y S_n^y, J_z S_n^z) \). In the following we will denote with \( j_i = J_i / \text{Vol}, \ i \in \{M,E\} \) the respective current densities. Here \( \text{Vol} = c N \) is the one-dimensional volume, where \( c \) is the lattice constant and \( N \) the number of sites.

The energy polarization \( P_E = \sum_n n h_n \) entering Eq.\[10\] for OBC represents a temperature gradient, and, as is well known\[16\] entails always a magnetic polarization \( P_M \), which stems from the chemical potential-term (magnetic-field-term). To see this we insert a site-dependent (linear)

\[
\beta = \beta (n) = \beta + n e \nabla \beta
\]

into the thermodynamical expectation value\[11\] The Boltzmann-factor can be rewritten as follows:

\[
\exp \left( -\sum_n \beta (n) h_n \right) = \exp \left[ -\frac{\beta}{\tilde{\beta}} \left( H + \frac{e c \nabla \beta}{\tilde{\beta}} \sum_n n h_n \right) \right] = \exp \left[ -\frac{\beta}{\tilde{\beta}} (H + F c P_E) \right]
\tag{7}
\]

where \( F = \nabla \beta / \tilde{\beta} = -\nabla (\nabla T) / T \). This motivates the use of \( P_E \) to model a temperature gradient.

**IV. CORRELATION FUNCTIONS**

Setting up the notation for the response theory we define with\[15,17\]

\[
\Lambda (AB) (z) \equiv \frac{i}{\hbar} \int_0^\infty e^{izt} \langle [A(t), B] \rangle \ dt
\tag{8}
\]
the retarded Green’s function of two operators $A$ and $B$. In our case $A$ and $B$ will be mostly current operators; we therefore introduce the notation $\Lambda(J,J_0) = \Lambda_{ij}$. $\Lambda(AB)(z)$ vanishes when one of the operators is a constant of motion and commutes with the Boltzmann-factor: by the cyclic property of the trace one has in this case $\langle AB \rangle = \langle BA \rangle$.

The energy-current operator $J_E$ commutes with the Hamiltonian in the absence of an external magnetic field $B$. Using Eq. (6) we have $\Lambda_{ME} = \Lambda_{EM} = B\Lambda_{MM}$ and $\Lambda_{EE} = B^2\Lambda_{MM}$.

The isothermal susceptibility is given by

$$\chi^T(AB) \equiv \int_0^\beta \langle \Delta A(\tau)\Delta B \rangle d\tau,$$

with $\Delta A = A - \langle A \rangle$ and $\Delta B = B - \langle B \rangle$. It takes the usual form $\chi^T(AB) = \beta\langle \Delta A\Delta B \rangle$ when one of the operators is a constant of motion. The generalized Drude weight (which is used, e.g., in Ref. 4) is defined by

$$\langle AB \rangle = \lim_{z \to 0} (-iz) \int_0^\infty e^{itz}\langle \Delta A(t)\Delta B \rangle dt.$$  

These three correlation functions are not independent, comparing the respective eigenstates-representation, e.g., $Z\Lambda(AB)(0) = \sum_{E_n\neq E_k} \Delta \Lambda_{nk} \Delta B_{kn} (e^{-\beta E_n} - e^{-\beta E_k}) / (E_n - E_k)$, where $Z$ is the partition function, one finds

$$\beta \langle AB \rangle + \Lambda(AB)(0) = \chi^T(AB).$$  

Under open boundary conditions, when the relations $J_i = i\hbar [H, P_j]$ are valid, we can express the isothermal susceptibility, Eq. (9), as a static expectation value. Note, however, that the value of the susceptibility is independent of the boundary conditions in the thermodynamic limit: $\chi^{T, OBC}(J,J) = \chi^{T, PBC}(J,J)$.

### V. MAGNETOTHERMAL COEFFICIENTS

We now discuss the general recipe for the computation of the entries of the $L$-Tensor, appearing in Eq. (3).

We assume a perturbation in the form of a polarization, (cf., e.g., Ref. 13) i.e., we add to the Hamiltonian a term $e\nabla B \cdot P_M$ with $P_M := \mu_B \sum_n n S_n^z$ and compute the response of the current density operator to obtain the MM-component. (A different but equivalent approach is given in Ref. 14.) To compute the remaining entries of the $L$-Tensor, we replace the magnetic by the energy current density (in the second row) and/or substitute $P_E := \sum_n nh_n$ for $P_M$ – as well as $e\nabla T$ for $e\nabla B$ – and add a factor $k_B\beta$ (in the second column). [One should compare this procedure with Eq. (7).]

The linear response theory gives the following contribution to $L_{ij}$

$$(k_B\beta)^{-1} \int_0^\infty e^{itz} \langle [j_i, P_j(-t)] \rangle dt$$

where $\beta^M := \beta$, $\beta^E := \beta^2$, etc., and $j_i = J_i/\text{Vol}$ (see Sec. III). Integration by parts yields for the above expression

$$\lim_{z \to 0} (k_B\beta)^{-1} \int_0^\infty e^{itz} \langle [j_i(t), J_j] \rangle dt.$$

One should note that $\Lambda_{ij}(0) = 0$ if one of the currents commutes with the Hamiltonian, and consequently there is no regular part. The factor $(-iz)^{-1}$ accounts for the delta-function in the zero-frequency limit and we have

$$L_{ij} = (k_B\beta)^{-1} \left\{ \frac{ie}{\hbar} \langle [j_i, P_j] \rangle - \Lambda_{ij}(0) \right\}.$$  

It is also possible to express this result by the correlation function defined in Eq. (10) using Eqs. (11) and (12):

$$L_{ij} = (k_B\beta)^{-1} \left\{ \frac{ie}{\hbar} \langle [j_i, P_j] \rangle - \Lambda_{ij}(0) \right\}.$$  

From Eq. (13) follows the well-known result for the magnetic Drude weight $L_{MM} = \langle -T_{MM} \rangle \hbar - \Lambda_{MM}$, where $T_{MM} = -i\langle [j_M, P_M] \rangle$ is the kinetic energy per site – apart from a prefactor. In view of Eq. (14) we define the generalized kinetic energy

$$T_{ij} = -i\langle [j_i(B = 0), P_j(B = 0)] \rangle.$$  

Here, one should note a particularity produced by the twofold rôle played by the operator $P_E$ in the xxz-chain: it not only describes thermal response but also acts as a 'boost'-operator for the constants of motion. Hence, $J_E$ as well as $T_{EE}$ are constants of motion.

Taking into account that $J_E$ commutes with the Hamiltonian for $B = 0$ and using Eqs. (3) and (13) we have

$$L_{EM} = \frac{ie}{\hbar} \langle [j_E, P_M] \rangle - B\Lambda_{MM}$$

$$= \frac{ie}{\hbar} \langle [j_E(B = 0), P_M] \rangle + B \left\{ \frac{ie}{\hbar} \langle [j_M, P_M] \rangle - \Lambda_{MM} \right\}$$

$$= (-T_{EM}) \frac{e}{\hbar} + B\Lambda_{MM}$$

and at finite B: $hL_{EE}/(ck_B\beta) = \{i\langle [j_E(B = 0) + B\Lambda_{MM}] \rangle - B^2\Lambda_{MM} \} = B(-T_{ME}) + B(-T_{EM}) - B^2(T_{MM}) + h\Lambda_{MM}/c$.

The generalized kinetic energy $T_{EM} = -i\langle [j_E, P_M] \rangle$-perturbation in the form of a polarization, (cf., e.g., Ref. 13) i.e., we add to the Hamiltonian a term $e\nabla B \cdot P_M$ with $P_M := \mu_B \sum_n n S_n^z$ and compute the response of the current density operator to obtain the MM-component. (A different but equivalent approach is given in Ref. 14.) To compute the remaining entries of the $L$-Tensor, we replace the magnetic by the energy current density (in the second row) and/or substitute $P_E := \sum_n nh_n$ for $P_M$ – as well as $e\nabla T$ for $e\nabla B$ – and add a factor $k_B\beta$ (in the second column). [One should compare this procedure with Eq. (7).]
pearing in Eq. (16) is given by (in units \(\mu_B c/\hbar\))

\[
T_{EM} = \frac{-i}{\text{Vol}} \sum_n \left( n \epsilon_{\alpha \beta \gamma} \left[ \hat{S}_n^\alpha, S_{n+1}^\beta \right] S_{n+1}^\gamma + \text{cycl.} \right)
\]

\[
= \sum_n \left\{ n \hat{S}_n \times (S_{n+1} \times S_{n+2}) + \text{cycl.} \right\}_{z} / \text{Vol}
\]

\[
= \frac{1}{\text{Vol}} \sum_n \left\{ \hat{S}_{n+2} \times (\hat{S}_n \times S_{n+1}) - \hat{S}_n \times (\hat{S}_{n+1} \times S_{n+2}) \right\}_{z}
\]

\[
= \frac{J_z^2}{\text{Vol}} \sum_n \left\{ -S_n^z S_{n+1}^z S_n^{-1, z}_{n+1} - S_n^{-1, z} S_{n+1}^z S_n^{+1, z} + S_n^{+1, z} S_{n+1}^{-1, z} S_n^z + S_n^z S_{n+1}^{+1, z} S_n^{-1, z} \right\}
\]

\[
\text{at (in units } \mu_B c/\hbar) \]

\[
T_{ME} = -i [J_M, P_E]
\]

\[
= \frac{-i}{\text{Vol}} \sum_n \left( n \left[ \hat{S}_n \times S_{n+1}, \hat{S}_n \cdot S_{n+1} \right] + \right)
\]

\[
\text{(n+1)} \hat{S}_n \times \left( S_{n+1}, S_{n+1} \cdot \hat{S}_n \right) + \right)
\]

\[
n \left[ \hat{S}_{n+1}, \hat{S}_n \cdot S_{n+1} \right] \times S_{n+2} \right)_{z}
\]

\[
= \sum_n \left( n/2 J_z^2 (S_n - S_{n+1}) - (n+1) \hat{S}_n \times (S_{n+1} \times S_{n+2}) \right)
\]

\[
- n \hat{S}_{n+2} \times (\hat{S}_n \times S_{n+1}) \right)_{z} / \text{Vol}
\]

\[
= \sum_n J_z^2 / 2 \left\{ -S_n^z S_{n+1}^z S_n^{-1, z}_{n+1} - S_n^{-1, z} S_{n+1}^z S_n^{+1, z} + \right.
\]

\[
\left. (n+1) J_z / J_z (S_n^z S_{n+1}^z S_n^{-1, z}_{n+1} + S_n^{-1, z} S_{n+1}^z S_n^{+1, z}) + \right)
\]

\[
M / \mu_B - S_0^z \cdot \text{Vol}/c \right) / \text{Vol},
\]

which differs apparently from \( T_{EM} \). This does not contradict the Onsager relation because we find that \( \langle T_{ME} \rangle = \langle T_{EM} \rangle \) still holds. This may be seen by first using Eqs. (15) and (16):

\[
\langle T_{ME} \rangle - \langle T_{EM} \rangle = \frac{c}{\hbar} \left\langle \left[ [H, P_M], P_E \right] - \left[ [H, P_E], P_M \right] \right\rangle
\]

then adding a term which is zero by the cyclic property of the trace:

\[
= \frac{c}{\hbar} \left\langle \left[ [H, P_M], P_E \right] + \left[ [P_M, P_E], H \right] + \left[ [P_E, H], P_M \right] \right\rangle.
\]

That this final expression is zero is just Jacobi’s identity. Here it should be emphasized that \( \langle T_{ME} \rangle \) has non-negligible contributions from the boundary, and is — unlike \( \langle T_{EM} \rangle \) — sensitive to a change from PBC to OBC.

VI. JORDAN-WIGNER TRANSFORM AND FREE FERMION MODEL

For our spin Hamiltonian all quantities may easily be calculated when \( J_z = 0 \) via the Jordan-Wigner mapping to a free fermion system. Under this condition the Hamiltonian is straightforwardly diagonalized by a Fourier transform with eigenvalues \( \cos k \) (setting \( J_y = 1 \)) following the Fermi-Dirac distribution \( \langle n_k \rangle = \langle c_k c_k \rangle = \left[ 1 + \exp(\beta \cos k) \right]^{-1} \). The Drude weight entering (18) is given simply by

\[
-L_{MM} = \langle T_{MM} \rangle / c/\hbar = \int \cos k(n_k) dk / (2 \pi c)(\mu_B c/\hbar)^2.
\]

At the same time \( T_{EM} \) simplifies to (again in units \( \mu_B c/\hbar \)):

\[
T_{EM} = \frac{1}{\text{Vol}} \sum_n \left\{ -S_n^z S_{n+1}^z S_n^{-1, z}_{n+1} - S_n^{-1, z} S_{n+1}^z S_n^{+1, z} \right\}
\]

\[
= - \int \frac{dk}{2 \pi c} \cos(2k) n_k.
\]
Following (18) we need to compute the right-hand side in units $\mu_0^2 e^2/h$

$$\langle (-\beta M)(-T_{EM}) \rangle = \frac{-\beta}{\text{Vol}} \sum_{k,q} \cos(2k) \left\langle n_k \left( n_q - \frac{1}{2} \right) \right\rangle.$$ 

$$\langle n_k n_q \rangle = \langle n_k \rangle \langle n_q \rangle$$ holds for $k \neq q$, $n_k^2 = n_k$ and $\sum_{k,q} \cos(2k) \langle n_k \rangle \langle n_q \rangle = 0$. We find:

$$\langle (-\beta M)(-T_{EM}) \rangle = \frac{\beta}{\text{Vol}} \sum_k [-\cos(2k)] \left[ \langle n_k \rangle - \langle n_k \rangle \right]$$

$$= -\beta \int \frac{dk}{2\pi c} \frac{\cos(2k)}{4 \cosh^2 [\beta \cos(k)/2]} \quad (20)$$

This result can be related with the temperature-derivative of the kinetic energy,

$$\langle T_{EM}(-\beta M) \rangle = \frac{d}{dT} \left[ T\langle -T_{EM} \rangle \right], \quad (21)$$

where $T_{MM}$ for the xy-Model is defined above. The relation (21) is easily verified using a partial integration.

VII. EINSTEIN RELATIONS

Let us recapitulate Einstein’s relation for diffusive transport in a metal: In a closed system the diffusive current $j_D = -D \nabla n$, driven by a gradient in the particle density $n$, and the electrical current driven by an external potential, $j = \sigma E$, add to zero: $j_D = -j$. This condition yields Einstein’s famous relation:

$$\frac{\dot{\sigma}}{D} = \frac{\nabla n}{E}. \quad (22)$$

Here, in the case of a magnetic system, we are not interested in a variation of the electron particle density, but in a change in internal energy or magnetization. Hence, we replace $n(x) \to A_n$, where $A_n$ is either $h_n$ or $\mu_B S_n^z$. Furthermore, the currents are not driven by a field $E$, but by a polarization $P_F = \sum_n n F_n$ (times the lattice constant $c$), for a conserved $F$: $[F, H] = 0$. In our case the operator $F$ is either the magnetization or the internal energy.

We will also assume that there is diffusive transport for both the magnetization and the energy current. Thereby, we are led to the following definitions of the corresponding diffusion coefficients

$$j_M \equiv \dot{D}_{MM} \nabla M \quad j_E \equiv \dot{D}_{EE} \nabla E$$

where $M$ and $E$ are the magnetization and internal energy.

Generalized Einstein relations can be derived using static response of $\nabla A_n := (A_{n+1} - A_n)c$ to a perturbation $cP_F$, where $c$ is the lattice constant along the chain:

$$\nabla n/E \to \sum_n \chi^T(\nabla A_n c P_F)/\text{Vol},$$

where we perform a volume average. (This becomes mandatory because we consider the response to the current density rather than to the current at a fixed site.) Using the linearity of the isothermal susceptibility we find (by a discrete version of an integration by parts):

$$c \chi^T(\nabla A_n | P_F) = \sum_m \left\{ \chi^T[A_{n+1}(m F_m)] - \chi^T[A_n(m F_m)] \right\}$$

$$= \sum_m \left[ (m + 1) \chi^T(A_n F_m) - m \chi^T(A_n F_m) \right]$$

$$= \sum_m \chi^T(A_n F_m)$$

and with the volume average on both sides

$$\sum_n c \chi^T(\nabla A_n | P_F)/\text{Vol} = \beta \langle \Delta A \Delta F \rangle/\text{Vol}. \quad (23)$$

We rewrite (24) for the case of magnetothermal response, $j_M \equiv \dot{L}_{ME} \nabla T = \dot{D}_{MM} \nabla M \equiv -j_d$, and find

$$\dot{L}_{ME} \quad \dot{D}_{MM} = \frac{\chi^T \nabla M}{\beta E} \quad = \frac{k_B}{k_B T (\nabla T/T)} \quad (24)$$

$$= k_B \beta \chi^T(\nabla M | P_F) = \frac{k_B \beta^2}{\text{Vol}} (\Delta M \Delta H),$$

where we have assumed equal relaxation times $\tau$ for $\dot{L}_{ME} = \tau \dot{L}_{ME}$ and the magnetization diffusion: $\dot{D}_{MM} = \tau \dot{D}_{MM}$. (This assumption was only made for simplicity. At least, to our knowledge there is no reason why the relaxation times should equal each other. However, the assumption is natural as in both cases the finite relaxation time comes from the fact that magnons lose momentum, and the physical processes responsible for that should be in both cases the same.) Eq. (21) leads to

$$\frac{L_{ME}}{D_{MM}} = \frac{k_B \beta^2}{\text{Vol}} (\Delta M \Delta H) \approx B \frac{d}{dT} \frac{k_B \beta^2}{\text{Vol}} (\Delta M \Delta H)$$

$$= \frac{B k_B \beta^3}{\text{Vol}} (\Delta M \Delta M) - \frac{B k_B \beta^3}{\text{Vol}} (\Delta M^2 \Delta H) \quad (25)$$

for small magnetic fields $B$, the structure of this equation is similar to Eq. (18). The first term of the right-hand-side of Eq. (25) is just $B \chi/T$, where $\chi = \beta (\Delta M^2)/\text{Vol}$ is the magnetic susceptibility. The second term of the right-hand-side of Eq. (25) simplifies to

$$\frac{B k_B \beta^3}{\text{Vol}} \frac{d}{dT} (\Delta M \Delta M) = \frac{B k_B \beta^3}{\text{Vol}} \frac{d}{dT} \chi = -\frac{B}{T} \frac{d}{dT} [T \chi]$$

We therefore find the new relation:

$$\frac{L_{ME}}{D_{MM}} = \frac{B}{T} \chi - \frac{B}{T} \frac{d}{dT} [T \chi] = -\frac{B}{T} \frac{d}{dT} \chi. \quad (26)$$

Classically, the diffusion constant is $\dot{D} = v^2 \tau$, where $v$ is the velocity of the elementary excitations, here the magnon velocity. This leads at low-temperatures to a temperature-independent diffusion coefficient $D =$
\( \hat{D}/\tau = v^2 \) and via (26) to vanishing magnetothermal response for \( T \to 0 \), whenever \( \chi(T) \) becomes constant for \( T \to 0 \). Setting \( A = M \) and \( F = M \) in the general Einstein relation yields\(^{11,14} \)

\[ L_{MM}/D_{MM} = \chi, \quad (27) \]

and with the choice \( A = H = F \) one may obtain\(^{11} \) an analogous relation: \( L_{EE}/D_{EE} = c_v \).

We will now introduce a formula which we believe to be approximately valid at small \( T \). As stated above, the diffusion constant is known not to vary much near \( T = 0 \). Because of our restriction to low \( T \) we assume a temperature-independent diffusion coefficient \( D_{MM} \) (see discussion above). Then we can rewrite (27) as

\[ \frac{d}{dT} L_{MM} = \frac{d}{dT} \langle \chi D_{MM} \rangle \approx D_{MM} \frac{d}{dT} \chi. \]

Inserting this expression into (26) we obtain

\[ (-L_{ME}) = B \frac{d}{dT} L_{MM}. \quad (28) \]

In the case of free fermions this is just the result of Eq. (26). In the case of a finite interaction it seems to be correct in the limit \( T \to 0 \) if we use data from Ref. 21.

We provide tests of this relation in section IX.

**VIII. AN EXACT EINSTEIN EQUATION**

In Sec. VII we did set-up several versions of generalized Einstein relations appropriate for magnetothermal response. Those relations may be viewed as a link between the dynamical and static response theory, as they connect corresponding correlation functions by introducing diffusion constants.

Upon closer examination of the right-hand sides of the Einstein relations like (27) - namely, \( \chi, c_v \) and \( d\chi/dT \) - we find that these are static expectation values of products of \( \Delta M \)- and \( \Delta H \)-operators which could be generated by derivatives. Hence, it is an easy task to establish functional relations between the static correlations, e.g.,

\[ T^2 \frac{d^2}{dB^2} c_v = \frac{d}{dT} \left[ T^2 \frac{d}{dT}(\langle T\chi \rangle) \right]. \]

An intriguing question is, whether the analogous equations obtained by switching between static and dynamical responses - \( \chi \leftrightarrow L_{MM} \), etc. - could also be valid. For one of these relations, Eq. (28), the range of validity is confined to the low temperature regime unless \( J_z = 0 \). (A detailed discussion follows in Sec. IX) One reason for the failure could be the fact that in this particular case one of the correlation functions does not reduce to a thermodynamical expectation value. We therefore focus on a relation between the thermal and magnetothermal response coefficients - both mere thermal expectation values. We claim that the relation

\[ T^2 \frac{d^2}{dB^2} (-T_{EE}) = \frac{d}{dT} \left[ T^2 \langle T_{EM}(-\beta M) \rangle \right] \quad (29) \]

is exact. The proof is provided in the appendix. This equation could be useful to derive an analytical solution for the magnetothermal response.

The arguments of the proof rely mainly on the fact that one of the currents is a constant of motion. It is by the same line of arguments possible to show that Eq. (29) is exact in the case where \( [H, M] = 0 \). Unfortunately, this is a very restricting constraint; only the xy-model and the Haldane-Shastry Hamiltonian\(^{20} \) meet the requirement.

**IX. NUMERICAL RESULTS**

In the free fermion case \( L_{EM} \) is easily accessible by a simple evaluation of the analytic expression (29) and a corresponding one for \( L_{MM} = -\langle T_{MM} \rangle \), using (18). If \( J_z \neq 0 \) we have to compute a mere thermal expectation value in order to obtain \( T_{EM} \), a task which is tractable to Monte-Carlo-simulations. Here, we use the stochastic series expansion (SSE), which is a Taylor expansion based Monte-Carlo-method\(^{21} \).

We assume a Hamiltonian of the form \( H = \sum_n J_n h_n \), we may write the partition function \( Z = \sum \alpha \prod_{m=1}^\infty h_{\phi_m(i)} h_{\phi_m(i)}^\dagger \) where the sum runs over all numbers \( m \), all functions \( \phi_m : \{1, \ldots, m\} \to \mathbb{N} \), and \( S^z \)-eigenbasis-states \( \alpha \). The SSE-program now samples the products of operators appearing in this expression of \( Z \) with their relative weight factors.

Normally, with MC-methods it is problematic to measure operators which are not diagonal in the \( S^z \)-eigenbasis. But with SSE another class of operators is easily accessible: Following a standard procedure in statistical mechanics, we have \( \langle h_n \rangle = (\partial h_n Z)/Z \). For the SSE this means that we can measure any operator \( h_n \) appearing in the Hamiltonian simply by counting how often it appears in the products sampled by our SSE-program (and dividing by \( J_n \)). So it is fairly easy to measure sums of products of parts of the Hamiltonian as \( S^z_n S^z_{n+1}, S^-_n S^z_{n+1} \) or \( S^z_n S^z_{n+1} \). To make use of this fact in the given context, it is expedient to find an expression for \( T_{EM} \) which consists only of terms appearing in the Hamiltonian. Here we present one \( (T_{EM}) \) in units \( \mu_{BC}/h \):

\[ T_{EM} = \frac{-i h}{\mu_{BC}} \sum_n \{ \langle j_n, h_{n+1} \rangle + \langle h_n, j_{n+1} \rangle \}/\text{Vol} \]

\[ = \sum_n \frac{1}{2} \left[ J_z^2 \left[ S^-_n S^-_{n+1} - S^+_n S^-_{n+1}, S^+_n S^z_{n+1} + S^-_n S^z_{n+1} \right] \right. \]

\[ + J_x^2 \left[ S^-_n S^-_{n+1} - S^+_n S^-_{n+1}, S^+_n S^z_{n+1} \right] \]

\[ + J_x J_z \left[ S^+_n S^-_{n+1} - S^-_n S^+_n, S^z_n S^z_{n+1} - S^z_{n+1} S^z_{n+2} \right] \]

\[ + J_z^2 \left[ S^z_n S^z_{n+1}, S^+_n S^-_{n+2} - S^+_n S^z_{n+2} \right] /\text{Vol}, \]

which then allows to access the magnetothermal coefficient by the SSE.

The Drude weight - which is the other input in Eq. (18) - may in principle be calculated by the Bethe-Ansatz
method. This was attempted by several authors, but their calculations are still under discussion and so far there are no reliable results. We therefore use exact-diagonalization to obtain data for the Drude-peak. This has clearly the disadvantage that we cannot make any statements about the low-temperature behavior. However, by using QMC for much faster with system size than the Drude weight, the partition function in temperature for various interaction strengths. The data for \( J_z \neq 0 \) are obtained by MC-simulations and in Fig. (3) by formula Eq. (28) and Eq. (13).

The MC-results in Fig. 2 are clearly not good enough to determine exactly the \( T \approx 0 \) value. However, for \( J_z = J_x \) the data seems to extrapolate to 0.25, which is the Bethe-Ansatz result for the dimensionless Drude weight for the isotropic Heisenberg chain. This result would imply a vanishing magnetothermal response for \( T \to 0 \) and via a \( T \)-derivative of the Drude weight, in contrast to previous results.

In Fig. 3 we present a comparison (at low \( T \)) between the MC-results for \( \langle (-\beta M)T_{EM} \rangle \) and the results from equation (28), where we have used Bethe-Ansatz results (because of the finite size gap exact diagonalization provides here no alternative) from Ref. 24 – which we prefer to Ref. 22 because it is in agreement with Ref. 23 – for the temperature-dependent Drude weight \( L_{MM} \). The agreement is very good for \( T < 0.2 \). As a consequence we may deduce from Eq. (28) that \( \langle (-\beta M)T_{EM} \rangle = L_{MM} \hbar/c \) at \( T = 0 \), the linear magnetothermal effect as given by Eq. (15) vanishes consequently for \( T \to 0 \).

The results for \( L_{EM} \) and the thermopower (the prime denotes a derivative with respect to the magnetic field \( B \)) \( Q'_M = L'_{ME}/L_{MM} \) are presented in Fig. 4 and Fig. 5 respectively. Here we use exact-diagonalization, because for the computation of the Drude weight QMC-methods normally fail at higher \( T \). (The standard procedure is to extrapolate from the Matsubara frequencies to \( \omega = 0 \) as attempted in Ref. 14. This procedure becomes soon unstable if \( T \) – and hence the spacing of the Matsubara frequencies – grows.) We use exact-diagonalization for the computation of \( \langle T_{EM} \rangle \) as well. Since \( \langle T_{EM} \rangle \) converges much faster with system size than the Drude weight, the finite size error is determined by the Drude weight, so using QMC for \( \langle T_{EM} \rangle \) alone would not give better results. On the contrary, if we used MC-data we would introduce the statistical error. For the Drude peak we use Eq. (14) with \( \langle (j_i j_j) \rangle = \sum_{E_n = E_{1n}} \langle n | j_i | k \rangle \langle k | j_j | n \rangle e^{-\beta E_n} / Z \) (\( Z \) is again the partition function) for \( \langle T_{EM} \rangle \) we simply use the expression in Eq. (17). The use of these expressions makes it possible for us to exploit translational symmetry which allows us to consider slightly larger systems than in Ref. 24 (namely, up to 18 sites).

Because of the resulting finite size gap we can only discuss the high-\( T \) regime. (In the xy-model we find a vanishing thermopower at \( T = 0 \) with a linear power-law.)

For small \( J_z \) we find a maximum at intermediate temperatures which decreases and is shifted to higher \( T \) as we increase \( J_z \).

At higher \( J_z \) the convergence becomes slower, so we cannot make any precise statements about the transport coefficients. However, in Fig. 4 and Fig. 5 the curves decrease with system size (for \( T \) sufficiently large). This behavior can be confirmed for all systems sizes, our curves provide an upper bound to the exact results. But this would imply a reversion of the effect (negative thermopower). While at \( J_z = 0 \) the effect is always positive – apart from a reversion due to the finite size gap, one finds \( Q'_M \leq 0 \) for a certain \( T \)-interval if \( J_z \) is large enough. Because of the slow convergence it is impossible for us to predict the precise location of this interval. Here one should emphasize that our conclusions were drawn from the inspection of relatively small systems, so we cannot really exclude that the observed reversion is only due to finite size effects.

However, we see the reason for this reversion in the fact that the magnetothermal coefficient consists of two summands \( \text{see Eq. (15)} \) which turn out to have opposite signs. These behave very differently under a change of the distance between neighbor sites, and \( J_z \) does not decay so much, such that it becomes the dominating part.

X. SIZE OF THE MAGNETOTHERMAL EFFECT

Based on Eqs. (1) and (30) and using the low \( B \) approximation in Eq. (18) we present in this section estimates of the size of the magnetic Seebeck effect.

A. Dimensional analysis

As we are considering effects linear in the magnetic field \( B \) we use \( t \) as a shorthand for \( \frac{\partial}{\partial B} \). Using \( [J_M] = [\mu_B] \text{m/s} \) and \( E \) = Wm (compare Eq. 5 and 6) and \( [J_{M/E}] = [J_{M/E}] / \text{m} \) we may decompose the response coefficients into dimension-full and dimension-less quantities:

\[
L'_{ME} = \frac{k_B \mu_B c}{\hbar} (J_x \beta)^3 L'_{ME} \quad (30)
\]

\[
L'_{EM} = \frac{J_z \mu_B c}{\hbar} (J_x \beta)^2 L'_{EM} \quad (31)
\]

where \( \beta \) denotes the dimensionless theory-result, \( c \) is the distance between neighbor sites, and \( \mu_B \) is the Bohr magneton. Note that \( L_{EM} \) has a factor \( 1/T \) with respect to \( L_{EM} \); hence a third factor \( J_z \beta \) in (15). In-
spection of that formula shows the units of $L_{ME}$ to be J/(Tesla)$^{-2}$m/(Ks$^2$).

For the sake of completeness we state the analogous results

$$L_{MM} = \frac{J_x \mu_B \mu_B C}{\hbar} (J_x \beta) \tilde{L}_{MM}$$

for the magnetic Drude weight and

$$L_{EE} = \frac{k_B J_x J_x C}{\hbar} (J_x \beta)^2 \tilde{L}_{EE}$$

for the thermal Drude weight. The units can be read off as $[L_{MM}] = J/(\text{Tesla})^{-2}\text{m/s}^2$ and $[L_{EE}] = J\text{m}/(\text{Ks})^2$. Note that $[L_{ij}] = [L_{ij}]s$, see (3).

We take the well studied one-dimensional Heisenberg chain Sr$_2$CuO$_3$ as an example with the following parameters $c = 3.91 \text{Å}$, $J_x/k_B = 2.2 \cdot 10^3 \text{K}$, and $J_x/k_B = 2.2 \cdot 10^3 \text{K}$. There are two chains in an area of $12.68 \times 3.48 \text{Å}^2$. This leads to a magnon path $\lambda_s(T)$ extracted from a quasi-classical interpretation of thermal conductivity data which is strongly temperature dependent, i.e., it ranges from $\lambda_s(200\text{K}) \approx 100 \text{Å}$ to $\lambda_s(50\text{K}) \approx 800 \text{Å}$. This results via $\lambda_s = v_s \tau$ in a relaxation time $\tau(200\text{K}) \approx 0.8 \cdot 10^{-13}\text{s}$ and $\tau(50\text{K}) \approx 6.6 \cdot 10^{-13}\text{s}$, in order of magnitude.

### B. Thermopower

For the *thermopower*, we obtain

$$Q'_M = \frac{L'_{ME}}{L_{MM}} = \frac{k_B J_x (J_x \beta)^2}{\hbar J_x} \tilde{L}'_{ME} = \frac{k_B}{J_x} Q'_M .$$

Typically, $k_B/J_x \approx 10^{-3}\text{K}^{-1}$ (e.g., in Sr$_2$CuO$_3$) and at room temperature $Q'_M \approx 0.1$. This yields $Q'_M \approx 10^{-4}\text{K}^{-1}$.

### C. Seebeck-effect

The dimensionless $B$-derivative of the magnetothermal response is $(J_x \beta)^2 \tilde{L}'_{ME} \approx 0.1$, in order of magnitude, see Fig. 1. We therefore obtain from Eq. (21) at $T = 200\text{K}$ for the magnetic particle current density a value of

$$0.036 \times B \times \nabla T \quad \text{moments/s}$$

per Tesla per (Kelvin/m), i.e., in SI-units. For a sample of length $1\text{cm} = 10^{-2}\text{m}$ with a temperature difference of $10\text{K}$ and a field of $10\text{Tesla}$ we have a current of $360$ spin-1 moments (magnons) per second. A sample of $\text{Sr}_2\text{CuO}_3$ with a cross-section of $1\text{mm}^2$ contains $4.5 \cdot 10^{12}$ chains. It would induce a magnetic current of $1.6 \cdot 10^{15}$ moments per second.

### D. Closed system

Finally, we consider again the setting of a *closed system*. We are given a sample with open ends such that no current may flow. A temperature gradient should therefore lead to a gradient in the magnetization. Using the Einstein relation for the magnetization current and Eq. (26) we have

$$\nabla M = \frac{L_{ME}}{D_{MM}} \nabla T = -B \frac{\partial \chi}{\partial T} \nabla T .$$

$\chi B = M$ is the magnetization caused by the presence of a magnetic field. Hence, dividing by $M$

$$\nabla M/M = -B \frac{\partial \chi}{\partial T} \nabla T$$

or multiplying both sides with the system length

$$\Delta M/M = - \frac{k_B}{J_x} \frac{\partial \chi}{\partial T} \nabla T \Delta T .$$

Note, that $\Delta M/M$ is not directly a function of magnetothermal coefficients. The magnitude of the dimensionless quantity $\frac{\partial \chi}{\partial T}$ varies about 0.1. We therefore find with $J_x/k_B = 2200\text{K}$ that the relative change in magnetization – from one end of the sample to the other – should be a fraction of the order of $5 \cdot 10^{-5}\text{K}^{-1} \times \Delta T$.

### E. Peltier-effect

We want to review now briefly the adjoint (Peltier) effect, described by the coefficient $L_{EM}$. We now turn once again to our reference system Sr$_2$CuO$_3$. Here it is instructive to compare the energy currents driven by a temperature gradient and a gradient in the magnetic field.

We set all quantities as above, with the exception of the values $(J_x \beta)^2 \tilde{L}'_{EM} \approx 0.01$, and $(J_x \beta)^2 \tilde{L}_{EE} \approx 0.1$, which we find more appropriate. We also do not compute the energy current density for one chain but per volume in SI-units. The result for the thermal response is

$$j_E = 16 \times \nabla T \quad \text{J/(s m}^2)$$

and for the magnetic response

$$j_E = 3.3 \cdot 10^{-4} \times \nabla B \times B \quad \text{J/(s m}^2).$$

### XI. CONCLUSION

We have shown that non-trivial magnetothermal currents may be induced in one-dimensional quantum-spin chains in an external magnetic field. We have argued that these effects might be especially important for the 1D Heisenberg chain where the energy-current operator...
commutes with the Hamiltonian and the magnetothermal response diverges. We have presented estimates of the size for the current of magnetic moments induced by a thermal temperature difference for Sr$_2$CuO$_3$. We believe the size of the induced magnetic current to be sizeable and note that the observability of magnetic currents in magnetic insulators has been discussed recently.

The support of the German Science Foundation is acknowledged.

XII. APPENDIX

A. Proof of Eq. (29)

1. Proof, first step

We present the proof of Eq. (29) in two steps. First we extend the Hamiltonian to comprise the static response to a thermal current:

\[ H(\lambda, B) = H(B) + \lambda J_E. \]

We indicate the expectation value at nonzero \( \lambda \) and \( B \) by indices. Moreover, we mean that these variables are zero, if we omit them in an index or an argument. ‘\( \Delta \)’ means subtraction of the expectation value.

We now show that

\[ \langle J_M \Delta H \rangle_{\lambda,B} = \langle J_E \Delta M \rangle_{\lambda,B}. \]  

(32)

We explicitly assume PBC – no polarization operators– and invoke the equation of continuity to obtain a local version of the above formula

\[ \langle (J_M^n - J_M^{n-1}) \Delta h_m \rangle_{\lambda,B} = -\langle [H, \Delta S^n_m] \Delta h_m \rangle_{\lambda,B} \]

\[ = (\Delta S^n_m [H, \Delta h_m])_{\lambda,B} = -\langle \Delta S^n_m (J_E - J_E^{m-1}) \rangle_{\lambda,B}. \]

On the right-hand side of the above equation we perform a reflexion in space

\[ \langle (J_M^n - J_M^{n-1}) \Delta h_m \rangle_{\lambda,B} = \langle \Delta S^n_m (J_E^{m-n} - J_E^{m+1}) \rangle_{-\lambda,B}. \]

Translational invariance leads for

\[ a_{n,m} := \langle J_M^n \Delta h_m \rangle_{\lambda,B} \quad b_{n,m} := -\langle J_E^n \Delta S_m^z \rangle_{-\lambda,B} \]

to \( a_{n,m} \equiv a_{n,-m} \) and to

\[ a_k - a_{k-1} = b_{k+1} - b_k \quad \iff \quad a_k - b_{k+1} = a_{k-1} - b_k, \]

where \( k = n - m \). This last equation implies that

\[ c := a_k - b_{k+1} \]

does not depend on the index \( k \). Our strategy is to show that \( c \) – a function on \( \lambda \) and \( B \) – may be neglected with impunity in the thermodynamic limit. To this end we look at the following estimate:

\[ |c(B,\lambda)| = |b_{k+1} - a_k| \leq \min_k \{ |b_{k+1}| + |a_k| \}. \]

The fact that all correlation function of the form \( \langle \Delta G_1 \Delta G_2 \rangle \) (as, e.g., \( a_k \) and \( b_k \)) decay to zero when the spatial extension (i.e., the index \( k \)) goes to infinity leads to \( \lim_{\text{Vol} \to \infty} c = 0 \). Hence we find that in the thermodynamic limit \( a_k = b_{k+1} \Rightarrow \sum a_k = \sum b_k \). And therefore:

\[ \langle J_M H \rangle_{\lambda,B}/\text{Vol} = -\langle J_E M \rangle_{-\lambda,B}/\text{Vol}. \]

The initial claim (32) follows – once again – by a reflexion in space on the second term.

2. Proof, second step

Having attained our first goal the further proceeding is standard. We apply consecutively derivatives with respect to \( \lambda \) and \( B \) on our result and obtain:

\[ \langle J_M J_E \Delta H \Delta M \rangle = -T \frac{d}{dB} \langle J_E J_E \Delta M \rangle_B. \]

We note that the \( \Delta H \) (resp., \( \Delta M \)) might come from a derivative with respect to \( -d/d\beta = T^2 d/dT \) (resp., \( -Td/dB \)) and use \( \langle T_E M (-\beta \Delta M) \rangle = -\beta \langle J_E E \rangle \) and \( -\langle T_E E \rangle = \beta^2 \langle J_E J_E \rangle \). Our formula may then be rewritten as:

\[ \frac{d}{dT} \langle T^2 E M (-\beta M) \rangle = T^2 \frac{d^2}{dB^2} \langle T E E \rangle_B, \]

Q.E.D.

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FIG. 1: Illustration of a quasi-one-dimensional magnetic insulator in the presence of an external magnetic field $B$, and a longitudinal temperature differential $\Delta T$. A magnetic current $j_M$, with the moments aligned along $B$ is induced.

FIG. 2: Monte-Carlo-data (48 & 96 sites, PBC) for the dimensionless $\langle (-\beta M)T_{EM}\rangle$ and various interaction strengths $J_z/J_{xx}$. The statistical MC-error-bars are given.

FIG. 3: Monte-Carlo-data (48 & 96 sites) at small $T$ for PBC in comparison (lines) with the estimates for $\langle (-\beta M)T_{EM}\rangle$ by Eq. (28) and data from Ref. [21] for the Drude weight. The cases $J_z = \cos(\pi/4)$ and $J_z = 1$ are offset for clarity.
FIG. 4: The linear part (in $B$) of $L_{EM}$ as a function of temperature, see Eq. (18), obtained by exact diagonalization for both $\langle (-\beta M)T_{EM} \rangle$ and the Drude weight. We plotted data for three system sizes (14, 16, 18 sites) with different line styles (long-dashed, dashed, solid, respectively).

FIG. 5: The part of the thermopower (19) linear in $B$ as a function of temperature, see Eq. (18) with exact-diagonalization-data for $\langle (-\beta M)T_{EM} \rangle$ and the Drude weight. We plotted data for three system sizes (14, 16, 18 sites) with different line styles (long-dashed, dashed, solid, respectively).