Non-dissipative Thermal Transport and Magnetothermal Effect for the Spin-1/2 Heisenberg Chain

Kazumitsu Sakai$^1$ and Andreas Klümp$^2$ *

$^1$Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan
$^2$Bergische Universität Wuppertal, Fachbereich Physik, D-42097 Wuppertal, Germany

Anomalous magnetothermal effects are discussed in the spin-1/2 Heisenberg chain. The energy current is related to one of the non-trivial conserved quantities underlying integrability and therefore both the diagonal and off diagonal dynamical correlations of spin and energy current diverge. The energy-energy and spin-energy current correlations at finite temperatures are exactly calculated by a lattice path integral formulation. The low-temperature behavior of the thermomagnetic (magnetic Seebeck) coefficient is also discussed. Due to effects of strong correlations, we observe the magnetic Seebeck coefficient changes sign at certain interaction strengths and magnetic fields.

KEYWORDS: transport properties, thermal conductivity, magnetothermal effect, Seebeck coefficient, Heisenberg chain

In the last two decades, 1D strongly correlated systems have attracted immense theoretical and experimental interest. One of the reasons stems from their unusual static and dynamical properties peculiar to 1D systems. The spin-1/2 Heisenberg chain is one of the most fundamental solvable models for 1D magnetic insulators and has served as a testing ground for many approaches. Recently, transport properties of low-dimensional strongly correlated quantum systems have been extensively studied from both theoretical and experimental sides. Among them anomalously enhanced thermal conductivity and unconventional large spin diffusion constants have been reported in experiments on one- or quasi 1D materials with weak interchain interactions. These observations indicate the existence of non-dissipative transport properties in 1D quantum systems. Theoretically, the existence of such anomalous properties has also been pointed out especially in quantum integrable systems. One of the criteria for anomalous transport is the existence of a non-zero Drude weight. In particular for the spin-1/2 XXZ chain, the Drude weight for the spin transport has been obtained by Zotos for finite temperature at zero magnetic field. In the massless regime, the Drude weight is non-zero and hence the spin transport is non-dissipative. In the massive regime without magnetic field a similar treatment yields zero Drude weight at any temperature implying dissipative spin transport. This feature, however, contradicts with numerical or field theoretical approaches and is still debated.

On the other hand, the thermal Drude weight $D_{th}(T)$ for zero magnetic field has been recently obtained by the Bethe ansatz showing that the thermal transport is non-dissipative in both massless and massive regimes. At low-temperature $D_{th}(T)$ behaves as $D_{th}(T) \sim \pi \nu v T/3$ where $\nu v$ is the velocity of excitations. This universal behavior was also found in general systems in which the low-energy excitations are described by a $c = 1$ conformal field theory. In the massive regime, we find that $D_{th}(T) \sim \exp(-\delta/T)/\sqrt{T}$ where $\delta$ is the one-spinon (respectively one-magnon) excitation gap for the antiferromagnetic (respectively ferromagnetic) regime.

In this article we will mainly discuss the thermal transport and magnetothermal effect in presence of finite magnetic fields. Because the spin-reversal symmetry vanishes for finite fields, the magnetothermal effect does appear. Consequently the thermomagnetic (magnetic Seebeck) coefficient is finite. Moreover we observe the magnetic Seebeck coefficient changes sign for certain interaction strengths and magnetic fields, which can be interpreted as effects of strong correlations.

Let us consider the spin-1/2 Heisenberg XXZ chain with magnetic fields $h$:

$$\mathcal{H} = \sum_{k=1}^{L} \hat{h}_{kk+1} = \sum_{k=1}^{L} \sigma_{k}^{z} \hat{h}_{kk+1},$$

$$\hat{h}_{kk+1} = J \left\{ \sigma_{k}^{+} \sigma_{k+1}^{-} + \sigma_{k}^{-} \sigma_{k+1}^{+} + \frac{\Delta}{2} (\sigma_{k}^{z} \sigma_{k+1}^{z} - 1) \right\}.$$

Here we restrict ourselves to the critical antiferromagnetic regime $0 \leq \Delta \leq 1$ and $J > 0$. In this case, the anisotropy parameter $\Delta$ is conveniently parametrized by $\Delta = \cos \gamma$ ($0 \leq \gamma \leq \pi$).

The spin and energy current operator of the present system are written as

$$\mathcal{J}_{s} = J \sum_{k=1}^{L} [(\sigma_{k}^{+} \sigma_{k+1}^{-} + h.c.)], \quad \mathcal{J}_{E} = iJ \sum_{k=1}^{L} [\hat{h}_{k-1k}, \hat{h}_{kk+1}],$$

respectively. The transport coefficients are determined by the Kubo formula in terms of the correlation functions of the above defined current operators. For instance, the thermal conductivity is determined by

$$\text{Re} \kappa(\omega) = \frac{1}{T} \text{Re} \left\{ \frac{L_{QQ}^{2} - L_{Qs}^{2}}{L_{ss}} \right\} = \pi D_{th}(T) \delta(\omega) + \kappa_{\text{reg}},$$

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$^*$E-mail address: sakai@stat.phys.titech.ac.jp

$^+$E-mail address: kluemper@physik.uni-wuppertal.de
Here the thermal current \( J_Q \) should be \( J_Q = \mathcal{J}_E - h \mathcal{J}_s \).

As already mentioned by Zotos in ref. 6, the energy current \( \mathcal{J}_E \) is a constant of motion \( [H, \mathcal{J}_E] = 0 \) and therefore the thermal Drude weight is finite \( D_{th}(T) > 0 \) at all finite temperatures. Hence the thermal transport is non-dissipative.

For zero magnetic field \( h = 0 \), the magnetothermal effect is always zero because the system exhibits the spin-reversal symmetry. In contrast, for finite magnetic fields \( h > 0 \) we see \( \langle \mathcal{J}_E, \mathcal{J}_s \rangle > 0 \), which leads to the diverging off diagonal dynamical correlations:

\[
\text{Re} \, L_{Qs} = \pi (\beta \langle \mathcal{J}_E, \mathcal{J}_s \rangle - h D_s(T)) \delta(\omega), \quad L_{sQ} = L_{Qs}.
\]

In this case the thermal Drude weight

\[
D_{th}(T) = \beta^2 \langle \mathcal{J}_E \rangle^2 - \beta^3 \frac{\langle \mathcal{J}_E, \mathcal{J}_s \rangle^2}{D_s(T)}, \quad (1)
\]

and the magnetic Seebeck coefficient

\[
S(T) = \text{Re} \left\{ \frac{1}{T} \frac{L_{Qs}}{\pi D_s(T)} \right\} = \frac{1}{T} \left\{ \frac{(\langle \mathcal{J}_E, \mathcal{J}_s \rangle)}{D_s(T)} - h \right\}, \quad (2)
\]

are both finite at finite temperatures.

To obtain them, we have to evaluate the correlations of \( \mathcal{J}_E \) and \( \mathcal{J}_s \). Let us consider the autocorrelation \( \langle \mathcal{J}_E \rangle \) first. To evaluate this quantity, we introduce the following extended Hamiltonian including \( \mathcal{J}_E \) as a perturbation: \( \mathcal{H} := \lambda_0 \mathcal{H}_0 - h \mathcal{M} + \lambda_1 \mathcal{J}_E \), where \( \mathcal{H}_0 \) is the Hamiltonian without the Zeeman term \( h \mathcal{M} \). The parameters \( \lambda_0 \) and \( \lambda_1 \) are introduced for later convenience and should be taken to be \( \lambda_0 = 1 \) and \( \lambda_1 = 0 \) after taking all necessary derivatives. Introducing the partition function \( Z = \text{Tr} e^{-\beta \mathcal{H}} \), we easily see that \( \langle \mathcal{J}_E \rangle \) is evaluated by taking the second logarithmic derivative with respect to \( \lambda_1 \): \( \langle \mathcal{J}_E \rangle = \frac{\partial^2 \ln Z[\lambda_1 = 0]}{\partial \lambda_1^2} / (L \beta^2) \). Note that from symmetric arguments we can prove \( \langle \mathcal{J}_E \rangle = 0 \). Applying a lattice path integral formulation, we introduce the quantum transfer matrix (QTM) in the imaginary time direction. In this formalism \( Z \) in the thermodynamic limit \( L \to \infty \) can be expressed as the largest eigenvalue of the QTM \( \Lambda(\lambda_0, \lambda_1) \), namely \( \lim_{L \to \infty} (\ln Z) / L = \ln \Lambda(\lambda_0, \lambda_1) \):

\[
\ln \Lambda(\lambda_0, \lambda_1) = \frac{\beta h}{2} + \oint_C a_1(x+i) \ln(1+\eta^{-1}(x+i)) dx, \quad (3)
\]

where the contour \( C \) encloses the real axis (for instance we take \( \text{Im} x = 1 \) (\( \text{Im} x = -i \)) for the upper (lower) contour) and \( a_n(x) = \gamma \sin n \gamma / (2\pi(\cosh \gamma x - \cos n \gamma)) \). The unknown function \( \eta(x) \) is determined by the following non-linear integral equation (NLIE):

\[
\text{In} \eta(x) = \beta(\lambda_0 + \lambda_1 A \partial_x) e(x) + \beta h + \oint_C a_2(x-y-i) \ln(1+\eta^{-1}(y+i)) dy, \quad (4)
\]

where \( e(x) = -2\pi A a_1(x) \) and \( A = 2J \sin \gamma / \gamma \). Consequently we obtain

\[
\langle \mathcal{J}_E \rangle = \frac{1}{\beta^2} \partial^2 \ln \Lambda(1, 1) \big|_{\lambda_1 = 0}, \quad (5)
\]

In Fig. 1, the temperature dependence of the correlation \( \langle \mathcal{J}_E \rangle \) for the isotropic point \( \Delta = 1 \) is depicted for various magnetic fields. For \( 0 < h < h_c \) (\( h_c = 4 \) is the critical magnetic field for \( \Delta = 1 \)), we find that \( \langle \mathcal{J}_E \rangle \) is linear in \( T \) at low-temperature \( T \ll 1 \). On the other hand, \( \langle \mathcal{J}_E \rangle \) exponentially decays for \( h > h_c \) due to the mass gap. At high temperature, \( \langle \mathcal{J}_E \rangle \) converges to a constant \( J_s^2(1+2\Delta)/2 \) not depending on the magnetic field \( h \).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{Illustration of \( \langle \mathcal{J}_E \rangle \) for the isotropic case \( \Delta = 1 \) as a function of temperature for various magnetic fields \( h \).}
\end{figure}

Next we consider the correlation \( \langle \mathcal{J}_E, \mathcal{J}_s \rangle \). Since the spin current \( \mathcal{J}_s \) is not a constant of motion (except for the XY model \( \Delta = 0 \)), the quantity \( \mathcal{J}_E \mathcal{J}_s \) is no longer conserved, namely \( [\mathcal{H}, \mathcal{J}_E \mathcal{J}_s] \neq 0 \). Hence the above procedure, which is useful to calculate the conserved quantities, is not applicable directly. Alternatively we use the following non-trivial identity relating \( \langle \mathcal{J}_E, \mathcal{J}_s \rangle \) to \( \langle \mathcal{J}_E \rangle \), which is valid for the thermodynamic limit \( L \to \infty \):

\[
\langle \mathcal{J}_E \mathcal{J}_s \Delta \mathcal{H}_0 \rangle = \langle \mathcal{J}_E^2 \Delta \mathcal{M} \rangle,
\]

where \( \Delta \mathcal{H}_0 = \mathcal{H}_0 - \langle \mathcal{H}_0 \rangle \) and \( \Delta \mathcal{M} = \mathcal{M} - \langle \mathcal{M} \rangle \). Using this identity, we express \( \langle \mathcal{J}_E \mathcal{J}_s \rangle \) in terms of the largest eigenvalue of the QTM \( \Lambda(\lambda_0, \lambda_1) \):

\[
\langle \mathcal{J}_E \mathcal{J}_s \rangle = -\frac{1}{\beta^2} \partial^2 \ln \Lambda(1, 1) \big|_{\lambda_0=1, \lambda_1=0}.
\]

To simplify the above equation further, we take the derivative with respect to \( h \) and \( \lambda_0 \) of both sides of eq. (4) after shifting the variable \( x \to x+i \). Comparing the re-
The other hand, \( \langle J \rangle \) has an isotropic case \( \Delta = 1 \) for various magnetic fields. As mentioned above, this correlation is strictly zero at \( \lambda_0 = 0 \). At finite magnetic fields, we find that \( \langle J \rangle \) is obtained from the condition \( \ln(1 + \eta^{-1}(x)) = 0 \) at \( \lambda_0 = 0 \) and \( \lambda_1 \) is obtained from the condition \( \ln(\Lambda_R) = \ln(\Lambda_L) = 0 \). To consider the \( O(T) \) correction to \( \ln \eta(x) \), we take into account the behavior near the Fermi point: \( \ln \eta(x) = \beta \varepsilon(x) + O(T) \), where \( \varepsilon(x) = \lambda_0 + \lambda_1 A x \) and eq. (3). Finally substituting the above equation into eq. (6), we arrive at
\[
\langle J_E J_s \rangle = \frac{1}{2 \pi A^2} \int_C \partial \lambda \ln(1 + \eta^{-1}(x)) dx.
\]

In Fig. 2, we show the temperature dependence of the current correlation \( \langle J_E J_s \rangle \) for the isotropic point \( \Delta = 1 \). As mentioned above, this correlation is strictly zero at \( h = 0 \). At finite magnetic fields, we find that \( \langle J_E J_s \rangle \) has a finite temperature maximum which increases with increasing magnetic field for \( 0 < h < h_c = 4 \). For \( h > h_c \), the maximum decreases and the corresponding temperature \( T_0 \) shifts to higher values with increasing magnetic field. At \( h \to \infty \) in which all spins point up, the temperature \( T_0 \) moves to infinity for fixed \( J \). Consequently \( \langle J_E J_s \rangle = 0 \) at \( h = \infty \). For \( h \) weaker than the critical field \( h_c \), \( \langle J_E J_s \rangle \) is linear in \( T \) at low-temperature. On the other hand, \( \langle J_E J_s \rangle \) exponentially decays for \( h > h_c \) because of the existence of the mass gap.

**Low-temperature asymptotics \( (T \ll h) \).** Next we would like to discuss the leading contributions at low temperature \( T \ll 1 \) and \( T \ll h \) (i.e. \( \beta h \gg 1 \)) in which the “logarithmic correction” terms especially for the isotropic case are next-leading contributions. In this case the auxiliary function \( \eta^{-1}(x) \) is exponentially small on the upper contour, i.e. \( \eta^{-1}(x) \sim \exp(-\beta h \delta) \). Moreover the function on the lower contour \( \ln x = 0 \) behaves as \( \ln(1 + \eta^{-1}(x)) \gg 1 \) for the region \( x \in [\Lambda_L, \Lambda_R] \) and \( \ln(1 + \eta^{-1}(x)) \ll 1 \) for \( x < \Lambda_L \) and \( x > \Lambda_R \). Therefore the NLIE (4) reduces to \( \ln \eta(x) = \beta \varepsilon(x) + O(T) \), where \( \varepsilon(x) = \lambda_0 + \lambda_1 A x \) and eq. (3). Finally substituting the above equation into eq. (6), we arrive at
\[
\langle J_E J_s \rangle = \frac{1}{2 \pi A^2} \int_C \partial \lambda \ln(1 + \eta^{-1}(x)) dx.
\]

The right (left) “Fermi point” \( \Lambda_R (\Lambda_L) \) depending on \( \lambda_0 \) and \( \lambda_1 \) is obtained from the condition \( \ln(\Lambda_R) = \ln(\Lambda_L) = 0 \). To consider the \( O(T) \) correction to \( \ln \eta(x) \), we take into account the behavior near the Fermi point: \( \ln \eta(x) = \beta \varepsilon(\Lambda_R/L)(x - \Lambda_R/L) \) for \( x \sim \Lambda_R/L \). Using this, we evaluate the \( O(T) \) contribution
\[
\frac{\pi^2}{6 \beta} \left\{ \frac{a_2(x - \Lambda_R)}{\varepsilon'(\Lambda_R)} - \frac{a_2(x - \Lambda_L)}{\varepsilon'(\Lambda_L)} \right\}.
\]

Thus we obtain the auxiliary function \( \ln \eta(x) \) up to \( O(T) \):
\[
\ln \eta(x) = \beta \varepsilon(x) + \frac{\pi^2}{6 \beta} \left\{ \frac{a_2(x - \Lambda_R)}{\varepsilon'(\Lambda_R)} - \frac{a_2(x - \Lambda_L)}{\varepsilon'(\Lambda_L)} \right\},
\]

Applying the same procedure and using the above obtained relations, we have the low-temperature behavior of the eigenvalue (3) up to \( O(T) \):
\[
\ln \Lambda = \frac{\beta h}{2} - \beta \int_{\Lambda_L}^{\Lambda_R} a_1(x) \varepsilon(x) dx + \frac{\pi^2}{6 \beta} \left\{ \frac{\rho(\Lambda_R)}{\varepsilon'(\Lambda_R)} - \frac{\rho(\Lambda_L)}{\varepsilon'(\Lambda_L)} \right\} + O(T^2),
\]

where \( \rho(x) \) is the density function given by
\[
\rho(x) = a_1(x) - \int_{\Lambda_L}^{\Lambda_R} a_2(x - y)\rho(y) dy.
\]

Combining (9) with (5) and (6), we obtain \( \langle J_E \rangle \) and \( \langle J_E J_s \rangle \) for \( \beta h \gg 1 \):
\[
\langle J_E \rangle^2 = h^2 D_0(0) T + \frac{(\pi A)^2 T^3}{3} \left\{ \frac{\alpha'(\Lambda) \rho(\Lambda)}{\varepsilon'^2(\Lambda)} + \frac{\alpha(\Lambda) \rho'(\Lambda)}{\varepsilon^2(\Lambda)} - \frac{2 \alpha(\Lambda) \varepsilon''(\Lambda) \rho(\Lambda)}{\varepsilon'^3(\Lambda)} - \frac{\alpha(\Lambda)}{2 \pi A \varepsilon'(\Lambda)} + \frac{\alpha^2(\Lambda) \rho(\Lambda)}{\varepsilon'^2(\Lambda)} \right\},
\]
\[
\langle J_E J_s \rangle = h D_0(0) T + \frac{\pi A T^3}{6} \left\{ \frac{\alpha'(\Lambda) \xi(\Lambda)}{\varepsilon'^2(\Lambda)} + \frac{\alpha'(\Lambda) \xi(\Lambda)}{\varepsilon'^2(\Lambda)} \right\},
\]
where \( \Lambda \) is the Fermi point determined by \( \varepsilon(\pm \Lambda) = 0 \) (note that we set \((\lambda_0, \lambda_1) = (1,0) \) in (7) and (10)); \( D_\theta(0) \) is the zero temperature spin stiffness \( D_\theta(0) = v_F^2 \tau \xi(\Lambda)/\pi; \) \( v_F \) is the Fermi velocity defined by \( v_F = \varepsilon'(\Lambda)/(2\pi \rho(\Lambda)) \); the function \( \alpha(x) \) and the dressed charge \( \xi(x) \) are given by

\[
\alpha(x) = \varepsilon'(v) - \int_{-\Lambda}^{\Lambda} a_2(x-y)\alpha(y)dy,
\]

\[
\xi(x) = 1 - \int_{-\Lambda}^{\Lambda} a_2(x-y)\xi(y)dy.
\]

**Drude weights and Seebeck Coefficient.**—Finally we discuss the thermal Drude weight \( D_{th}(T) \) and the magnetic Seebeck coefficient \( S \) at low-temperature \((\beta h \gg 1)\). To evaluate them, we have to explicitly determine the spin Drude weight \( D_\theta(T) \) as well as the above obtained current correlations \( \langle J_\theta^2 \rangle \) and \( \langle J_\theta J_s \rangle \). Though the Drude weight for the spin transport at finite temperatures and zero magnetic field has been evaluated by Zotos already \( \gamma \) a while ago, \(^7\) the validity of the results is still debated. Here, we determine the low-temperature behavior alternatively without directly calculating \( D_\theta(T) \). Utilizing the phenomenological relation between the thermal conductivity \( \kappa \) and the specific heat \( C \), i.e. \( \kappa = C(T)v_F^2 \tau \) (\( \tau \): relaxation time), we assume the low-temperature asymptotics of the thermal Drude weight as

\[
D_{th}(T) = \frac{\pi v_F}{3} T + O(T^2). \tag{12}
\]

Here we have used \( \kappa = D_{th}(T)\tau \) and \( C = \pi T/(3v_F). \) \(^20\) Note that \( \tau = \infty \) for the present case. The validity of eq.(12) is verified at \( h = 0 \) \(^1\) and for the XY model \((\Delta = 0) \) for \( 0 \leq h \leq h_c \) \((h_c = 2)\). Combining (12) with (1) and using the result (11), we determine the low-temperature behavior of \( D_\theta(T) \). From the resultant equation and (11), we obtain the ratio of \( \langle J_\theta J_s \rangle \) and \( D_\theta(T) \):

\[
\frac{\langle J_\theta J_s \rangle}{D_\theta(T)} = hT - \frac{\pi T^3}{6A\rho(\Lambda)\xi(\Lambda)} \left\{ 1 + \frac{A\alpha(\Lambda)}{2\pi \rho(\Lambda)v_F^2} \right\}.
\]

Finally substituting this into (2), we arrive at the leading low-temperature behavior of the magnetic Seebeck coefficient for \( T \ll h \):

\[
S(T) = -\frac{\pi T}{6A\rho(\Lambda)\xi(\Lambda)} \left\{ 1 + \frac{A\alpha(\Lambda)}{2\pi \rho(\Lambda)v_F^2} \right\} + O(T^2).
\]

In Fig. 3, the coefficient of the leading correction is depicted as a function of the magnetic field for various anisotropy parameters. For weak interaction strengths \( \Delta < \Delta_0 \sim 0.5 \), the leading behavior is negative. On the contrary, for \( \Delta > \Delta_0 \), due to effects of strong correlations, the Seebeck coefficient changes sign at certain magnetic field \( h_0 \) (or equivalently certain magnetization \( M_0 \)). The value \( h_0 \) shifts to higher values with increasing the interaction strengths. Recently similar behavior has also been observed in the electric Seebeck coefficient of the Hubbard model for finite \( U \) and \( T \) by the numerical diagonalization for small systems. \(^{21}\)

In summary, we have discussed the magnetothermal effects and the thermal transport at finite magnetic fields. The magnetic Seebeck coefficient changes sign above certain interaction strengths, because of effects of strong correlations.

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