A TBA approach to thermal transport in the XXZ Heisenberg model

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Abstract. We show that the thermal Drude weight and magnetothermal coefficient of the 1D easy-plane Heisenberg model can be evaluated by an extension of the Bethe ansatz thermodynamics formulation by Takahashi and Suzuki (1972 Prog. Theor. Phys. 48 2187). They have earlier been obtained by the quantum transfer matrix method (Klümper 1999 Z. Phys. B 91 507). Furthermore, this approach can be applied to the study of the far-out of equilibrium energy current generated at the interface between two semi-infinite chains held at different temperatures.

Keywords: integrable spin chains and vertex models, quantum integrability (Bethe Ansatz), quantum transport in one-dimension, thermodynamic Bethe Ansatz
1. Introduction

The one dimensional spin-1/2 Heisenberg chain is the prototype model integrable by the Bethe ansatz method [3–5]. Its thermodynamic properties have been studied, first by a method proposed by Takahashi and Suzuki (TS) [1] along the lines proposed by Yang and Yang [6] and later by a quantum transfer matrix method (QTM) proposed by Klümper [2].

Concerning the spin and thermal transport, the existence of conservation laws generically implies unconventional-ballistic-transport [7]. In particular, the energy current commutes with the Hamiltonian resulting in purely ballistic thermal transport characterized by the thermal Drude weight \( D_{\text{th}} \). This fact has further promoted the study of thermal conduction by magnetic excitations in novel, high quality, quasi-one dimensional magnetic compounds [8]. The temperature and magnetic field dependence of \( D_{\text{th}} \) as well as of the magnetothermal coefficient have been evaluated as well by an extension of the QTM method [9, 10].

On the spin transport, the situation is more involved as the spin current is not a conserved quantity. Although ballistic transport can be established at finite magnetization using the Mazur inequality [7], at zero magnetization a finite spin Drude weight was found at all temperatures in the easy-plane regime using a TBA approach [11]. These results were recently corroborated by the finding of a family of quasi-local conservation laws that provided a bound on the spin Drude weight [12, 13] and a generalized hydrodynamics approach (GHD) [14–16]. In this note, we point out that the thermal Drude weight \( D_{\text{th}} \) and magnetothermal coefficient can similarly be obtained by an extension of the TS formulation.

On the far-out of equilibrium thermal conductance, the idea that the steady state energy current between two semi-infinite ballistic systems held at different temperatures can be studied within a ‘Landauer’ approach has a long history [17]. It has recently been investigated in a series of pioneering numerical simulation studies [18–21] and the GHD approach. Here we show that recent numerical simulation and GHD results of the non-equilibrium steady current can be fairly accurately reproduced by the same extended TBA approach. The resulting fermionic quasi-particle

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description of the thermal Drude weight and far-out of equilibrium thermal current is rather appealing as it promotes a semi-phenomenological description of this system.

2. Thermal Drude weight

The XXZ anisotropic Heisenberg Hamiltonian for a chain of \( N \) sites with periodic boundary conditions \( \sigma_{N+1}^a = \sigma_1^a \) is given by,

\[
H = J \sum_{i=1}^{N} \left( \frac{1}{2} e^{i\phi} \sigma_i^+ \sigma_{i+1}^- + \text{h.c.} \right) + \frac{\Delta}{4} \sigma_i^z \sigma_{i+1}^z - \frac{\hbar}{2} \sigma_i^z ,
\]

where \( \sigma_i^a \) are Pauli spin operators and a spin current generating fictitious flux \( \phi \) is introduced \([11, 22]\). The region \( 0 \leq \Delta \leq 1 \) is commonly parametrized by \( \Delta = \cos \theta \), \( J \) taken as the unit of energy. In the following we will consider the case \( \theta = \pi/\nu \) (\( \nu \) integer) although it is straightforward to consider a more general anisotropy range. Following the TS formulation the pseudomomenta \( k_\alpha \) characterizing the Bethe ansatz wavefunctions are expressed in terms of the rapidities \( x_\alpha \),

\[
\cot \left( \frac{k_\alpha}{2} \right) = \cot \left( \frac{\theta}{2} \right) \tanh \left( \frac{\theta x_\alpha}{2} \right) .
\]

For \( M \) down spins and \( N-M \) up spins the energy \( E \) and momentum \( K \) are given by:

\[
E = J \sum_{\alpha=1}^{M} (\cos k_\alpha - \Delta), \quad K = \sum_{\alpha=1}^{M} k_\alpha .
\]

Imposing periodic boundary conditions on the Bethe ansatz wavefunctions the following relations on the allowed values of the rapidities are obtained,

\[
\left\{ \frac{\sinh \frac{1}{2} \theta (x_\alpha + i)}{\sinh \frac{1}{2} \theta (x_\alpha - i)} \right\}^N = e^{i\phi N} \prod_{\beta=1}^{M} \left\{ \frac{\sinh \frac{1}{2} \theta (x_\alpha - x_\beta + 2i)}{\sinh \frac{1}{2} \theta (x_\alpha - x_\beta - 2i)} \right\}, \quad \alpha = 1, 2, \ldots M .
\]

In the thermodynamic limit, the solutions of equations (4) are grouped into strings of order \( n_j, j = 1, \ldots, \nu \) and parity \( v_j = +1 \) or \(-1\). In the case \( \theta = \pi/\nu \) the allowed strings are of order \( n_j = j \), for \( j = 1, \ldots, \nu - 1 \) and parity \( v_j = +1 \) of the form,

\[
x_{\alpha,+}^{n,k} = x_\alpha^n + (n + 1 - 2k)i + O(e^{-\delta N}); \quad k = 1, 2, \ldots n ,
\]

and strings of order \( n_\nu = 1 \) and parity \( v_\nu = -1 \),

\[
x_{\alpha,-} = x_\alpha + i\nu + O(e^{-\delta N}), \quad \delta > 0 .
\]

Multiplying the terms in equation (4) corresponding to different members of a string and taking the logarithm we obtain the relations,

\[
Nt_j(x_\alpha^j) = 2\pi i J^j + \sum_{k=1}^{\infty} \sum_{\beta=1}^{M_k} \Theta_{jk}(x_\alpha^j - x_\beta^k) + n_j\phi N, \quad \alpha = 1, 2, \ldots M_j ,
\]

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where $I_{a}^{j}$ are integers (or half-integers) and $M_{k}$ is the number of strings of type $k$, 

\[ t_{j}(x) = f(x; n_{j}, v_{j}), \]

\[ \Theta_{jk}(x) = f(x; |n_{j} - n_{k}|, v_{j}v_{k}) + f(x; n_{j} + n_{k}, v_{j}v_{k}) + 2 \sum_{i=1}^{\min(n_{j}, n_{k})-1} f(x; |n_{j} - n_{k}| + 2i, v_{j}v_{k}), \]

\[ f(x; n, v) = 2v \tan^{-1}[(\cot(n\pi/2\nu))^\nu \tanh(\pi x/2\nu)]. \]

Concerning the finite temperature spin Drude weight $D_{s}$, it was evaluated in [11] using the Kohn relation [22, 23]:

\[ D_{s} = \frac{1}{N} \sum_{n} p_{n} \frac{1}{2} \frac{\partial^{2} E_{n}(\phi)}{\partial \phi^{2}} \bigg|_{\phi \to 0}, \tag{8} \]

where $E_{n}$ are the eigenvalues of the Hamiltonian and $p_{n}$ the corresponding Boltzmann weights. Following Fujimoto and Kawakami [24] the finite size corrections to the energy eigenvalues for a system of size $N$ are expressed by introducing the functions $g_{1j}$,

\[ x_{N}^{j} = x_{\infty}^{j} + \frac{g_{1j}}{N} + \ldots. \tag{9} \]

where $x_{N}^{j}$ are the rapidities for a system of size $N$, $x_{\infty}^{j}$ of size $\infty$. Expanding (7) to order $1/N$ and in the thermodynamic limit the densities of excitations $\rho_{j}$ and hole densities $\rho_{j}^{h}$ are introduced. The sums over the pseudomomenta are replaced by integrals over excitation densities plus boundary terms using the Euler-Maclaurin formula. To $O(1)$ we recover the integral equations for the excitation densities in the thermodynamic limit [1],

\[ a_{j} = \lambda_{j}(\rho_{j} + \rho_{j}^{h}) + \sum_{k} T_{jk} * \rho_{k}, \tag{10} \]

where $*$ denotes the convolution $a * b(x) = \int_{-\infty}^{+\infty} a(x-y)b(y)dy$, $T_{jk}(x) = (1/2\pi) d\Theta_{jk}(x)/dx$ and

\[ a_{j}(x) = \frac{1}{2\pi} dt_{j}(x)/dx = \frac{v_{j}}{2\nu} \frac{\sin(\frac{\pi x}{\nu})}{\cosh(\frac{\pi x}{\nu}) - v_{j} \cos(\frac{\pi x}{\nu})}. \tag{11} \]

The sum over $k$ is constrained to the allowed strings, given in our case by the equations (5), (6) and $\lambda_{j} = v_{j}$. Furthermore to $O(1/N)$:

\[ \lambda_{j} g_{1j}(\rho_{j} + \rho_{j}^{h}) = \frac{n_{j}\phi}{2\pi} - \sum_{k} T_{jk} * (g_{1k}\rho_{k}). \tag{12} \]

Minimizing the free energy we obtain the standard Bethe ansatz equations for the effective dispersions $\epsilon_{j} = (1/\beta) \ln(\rho_{j}^{h}/\rho_{j})$ at temperature $T(\beta = 1/\kappa_{B} T)$,

\[ \epsilon_{j} = \epsilon^{(0)}_{j} - \ln n_{j} + T \sum_{k} \lambda_{k} T_{jk} * \ln(1 + e^{-\beta \epsilon_{k}}), \tag{13} \]

where $\epsilon^{(0)}_{j} = -Aa_{j}$ ($A = 2\pi J \sin(\theta)/\theta$) are the zero excitation energies. The spin Drude weight is finally given by [11],
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\[
D_s = \frac{\beta}{2} \sum_j \int_{-\infty}^{+\infty} dx (\rho_j^\dagger + \rho_j^\dagger)(n_j)(1 - \langle n_j \rangle)(\frac{\partial \epsilon_j}{\partial x} \frac{\partial g_{1j}}{\partial \phi})^2
\]  

(14)

with \( \langle n_j \rangle = 1/(1 + e^{\beta \epsilon_j}) \). We should note that this expression can be recast in the form,

\[
D_s = \frac{\beta}{2} \sum_j \int_{-\infty}^{+\infty} dx (\rho_j^\dagger + \rho_j^\dagger)(n_j)(1 - \langle n_j \rangle)(j_j^s)^2
\]  

(15)

by introducing an effective velocity \( v_j \), dressed charge \( Q_j \) and current \( j_j^s \) of the excitations [24],

\[
j_j^s = v_j Q_j, \quad Q_j = 2\pi \lambda_j (\rho_j^\dagger + \rho_j^\dagger) \frac{\partial g_{1j}}{\partial \phi}, \quad v_j = \frac{1}{2\pi \lambda_j (\rho_j^\dagger + \rho_j^\dagger)} \frac{\partial \epsilon_j}{\partial x}.
\]  

(16)

It resembles that of independent fermion-like excitations with dispersion \( \epsilon_{\mu} \),

\[
D \approx \frac{\beta}{2N} \sum_{\mu} \langle n_{\mu} \rangle (1 - \langle n_{\mu} \rangle)(\frac{\partial \epsilon_{\mu}}{\partial \phi})^2|_{\phi \to 0}.
\]  

(17)

To study thermal transport, we cannot use a similar phase approach but we note that the derivatives of the monodromy matrix with respect to the spectral parameter generate the conservation laws of the system [5]. In particular, in the Heisenberg model the first derivative generates the Hamiltonian \( H \), while the second the energy current \( J_E \). The energy of a BA state is then given by,

\[
E/N = \sum_j \int_{-\infty}^{+\infty} dx \left( \epsilon_j^{(0)} - h n_j + \xi_j j_j^{(0)} \right) \rho_j
\]  

(18)

where \( j_j^{(0)} = (-A/2\pi) \frac{\partial \epsilon_j^{(0)}}{\partial x} \) are the corresponding eigenvalues of the energy current operator. Introducing the fictitious fields \( \xi_j(x) \) coupled to the eigenvalues of the conserved energy current operator \( J_E \) and minimizing the free energy, extended Bethe ansatz equations for the temperature dependent effective dispersions are obtained,

\[
\epsilon_j = \epsilon_j^{(0)} - h n_j + \xi_j j_j^{(0)} + T \sum_k \lambda_k T_{jk} \ln(1 + e^{-\beta \epsilon_k}).
\]  

(19)

We derive an analogous expression for the thermal Drude weight by first writing the free energy density \( f \) in the convenient form [1],

\[
f = -T \sum_j \int_{-\infty}^{+\infty} dx \lambda_j a_j \ln(1 + e^{-\beta \epsilon_j}).
\]  

(20)

The thermal Drude weight is given by the 2nd derivative with respect to \( \xi \) \((\xi_j(x) = \xi)\),

\[
D_{th} = \frac{\beta^2}{2N} \langle J_E^2 \rangle = \left. -\frac{\beta}{2} \frac{\partial^2 f}{\partial \xi^2} \right|_{\xi = 0}.
\]  

(21)
It is evaluated as,
\[
\frac{\partial^2 f}{\partial \xi^2} = \sum_i \int dx \lambda_i a_i \left( -\beta \langle n_i \rangle (1 - \langle n_i \rangle) \left( \frac{\partial \epsilon_i}{\partial \xi} \right)^2 + \langle n_i \rangle \left( \frac{\partial^2 \epsilon_i}{\partial \xi^2} \right) \right)
\]
and by using (10), (13),
\[
\frac{\partial^2 f}{\partial \xi^2} = -\beta \sum_j \int dx (\rho_j + \rho_j^h)(n_j)(1 - \langle n_j \rangle) \left( \frac{\partial \epsilon_j}{\partial \xi} \right)^2
+ \sum_j \int dx (\rho_j + \rho_j^h)(n_j) \cdot \left( \frac{\partial^2 \epsilon_j}{\partial \xi^2} + \sum_k \lambda_k T_{jk} \ast \left( -\beta \langle n_k \rangle (1 - \langle n_k \rangle) \left( \frac{\partial \epsilon_k}{\partial \xi} \right)^2 + \langle n_k \rangle \left( \frac{\partial^2 \epsilon_k}{\partial \xi^2} \right) \right) \right),
\]
\[
\frac{\partial^2 f}{\partial \xi^2} = -\beta \sum_j \int dx (\rho_j + \rho_j^h)(n_j)(1 - \langle n_j \rangle) \left( \frac{\partial \epsilon_j}{\partial \xi} \right)^2.
\]
Finally using the key observation that \(\partial \epsilon_j/\partial \xi = (-A/2\pi) \partial \epsilon_j/\partial x = j^e_j\) we obtain the thermal Drude weight,
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\[ D_{\text{th}} = \frac{\beta^2}{2} \sum_j \int_{-\infty}^{+\infty} dx (\rho_j + \rho_j^h)(n_j)(1 - \langle n_j \rangle)(j^s_j j^s_j), \]

(23)

with \( j^s_j \) the effective energy current of the string excitations. This formulation reproduces the QTM data [9] as a function of temperature and magnetic field.

Along the same line the magnetothermal correlation [10, 25] can also be expressed as,

\[ \langle J_S J_E \rangle / N = -T \frac{\partial^2 f}{\partial \phi \partial \xi} \bigg|_{\phi, \xi = 0} \]

\[ = \sum_j \int_{-\infty}^{+\infty} dx (\rho_j + \rho_j^h)(n_j)(1 - \langle n_j \rangle)(j^s_j j^s_j). \]

(24)

While the QTM is an elegant and powerful method as it provides directly data at all values of the anisotropy parameter \( \Delta \), the TBA approach offers an appealing fermionic quasi-particle picture. We should note that a similar extension of TBA was proposed in [26, 27] in the context of the Lieb-Liniger model. It is clear that ‘Drude weights’ of conserved quantities in integrable models can be obtained along the same line as derivatives of the corresponding free energy density.

3. Thermal quench—an ansatz

In recent theoretical studies of far-out of equilibrium thermal transport, two semi-infinite chains (L—left, R—right) initially held at different temperatures \( T_L, T_R \) are brought into contact and the long time energy current at the junction is observed. A physically motivated ansatz to evaluate the expectation value of the current \( \langle J_E \rangle \) at the junction is to assume that the far from the junction thermal baths impose left (right) currents \( \langle J_L(R) \rangle \) so that \( \langle J_E \rangle = \langle J_L \rangle + \langle J_R \rangle \). \( \langle J_L(R) \rangle \) is the energy current carried by positive (negative) velocity excitations. Of course this ansatz relies on the integrability of

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the XXZ chain implying that each eigenstate is also an eigenstate of the energy current operator. Using the relation

$$\langle J_L \rangle = \left. \frac{\partial f}{\partial \xi_L} \right|_{\xi_L=0},$$

(25)

with the condition $\xi_j(x) = \xi_L$ for $x > 0$ and $\xi_j(x) = 0$ for $x < 0$ at $\beta_L = 1/T_L$, $\langle J_L \rangle$ is given by,

$$\langle J_L \rangle = \sum_j \int_0^{+\infty} dx \lambda_j a_j \langle n_j \rangle \epsilon_j.$$  

(26)

where $j_j = \partial \epsilon_j / \partial \xi$ is obtained from (19) under the above condition by,

$$\left. \frac{\partial \epsilon_j}{\partial \xi} \right|_{x>0} = j_j^{(0)} - \sum_k \lambda_k T_{jk} \ast (\langle n_k \rangle \frac{\epsilon_k}{\partial \xi})$$

$$\left. \frac{\partial \epsilon_j}{\partial \xi} \right|_{x<0} = - \sum_k \lambda_k T_{jk} \ast (\langle n_k \rangle \frac{\epsilon_k}{\partial \xi}).$$

(27)

Symmetrically, $\langle J_R \rangle$ (of opposite sign) is evaluated at inverse temperature $\beta_R = 1/T_R$ by integrating over $-\infty < x < 0$.

As shown in figures 1 and 2 data produced by this ansatz are in fair agreement with recent DMRG numerical simulation studies [19, 20]. Also the zero temperature limit $\langle J_L \rangle$ is numerically close to the $(\pi/12) T_L^2$ CFT value.

Finally, the dependence of the current at different magnetic fields is presented in figure 3, where the critical field from the gapless antiferromagnetic to the gapped ferromagnetic state occurs at $h = J(1 + \Delta) = 1.5$. The non-monotonic behavior observed approaching the critical field is puzzling but reminiscent of a similar behavior of other magnetothermal quantities [25]. Of course in a finite magnetic field the thermal current has also a component from the spin current, that although ballistic, is not conserved.

It remains an open question, why the physically motivated and straightforward ‘Landauer’ approach introduced in the framework of independent particle systems, when applied to quantum many-body systems far-out of equilibrium, reproduces with minimal computational effort and high accuracy (of the order of percent discrepancy) DMRG numerical simulation and GHD results [14, 15] over an extended temperature and parameter range.

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