On the finite temperature Drude weight of the anisotropic
Heisenberg chain

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Abstract

We present a study of the Drude weight \( D(T) \) of the spin-1/2 XXZ chain in the gapless regime. The thermodynamic Bethe ansatz (TBA) is applied in two different ways. In the first application we employ the particle basis of magnons and their bound states. In this case we rederive and considerably extend earlier work in the literature. However, in the course of our investigation we find arguments that cast doubt on the applicability of the TBA in this case. In a second application by use of the spinon and anti-spinon particle basis we obtain completely different results. Only for anisotropy parameter \( \Delta \) close to 0 we find that \( D(T) \) is a monotonously decaying function of temperature. For \( \Delta \) close to 1 the behaviour is entirely different showing a finite temperature maximum. Also for the isotropic antiferromagnetic chain (\( \Delta = 1 \)) the results for \( D(T) \) are finite for \( T = 0 \) as well as for \( T > 0 \) with an infinite positive slope at \( T = 0 \).

1 Introduction

In this work we are studying transport properties of the spin-1/2 Heisenberg chain with longitudinal anisotropy (XXZ chain). Depending on the representation of the system the quantity of interest is the spin conductivity of a quantum spin system with anisotropic spin exchange or the electrical conductivity of a system of spinless fermions with density-density interaction. Both representations are related by a Jordan-Wigner transformation. The recent interest in these quantities has several reasons. We want to mention only two of these. First, in low-dimensional systems the question has been raised whether spin diffusion exists or not and the role of integrability for anomalous transport properties was discussed. (For a review see [1].) Second, the Drude peak at zero frequency in the dynamical conductivity is in principle accessible to analytical studies.

Let us consider a Hamiltonian of the form

\[
\hat{H} = \hat{H}_0 + \hat{V} = -t \sum_j \left( e^{i e A_x(j,t)} c_{j+1}^\dagger c_j + e^{-i e A_x(j,t)} c_j^\dagger c_{j+1} \right) + \mathcal{H}_{\text{int}}
\]  

(1)

representing a one-dimensional system of length \( L \) with periodic boundary conditions subject to a vector potential \( A \). In our case \( \mathcal{H}_{\text{int}} \) describes density-density interactions and hence does not depend on the vector potential.

Within Kubo theory [2], i.e. linear response for \( \mathcal{H}_{\text{int}} \) in \( A \), the dynamical conductivity is obtained in terms of current-current correlation functions. The Drude weight \( D \) is the zero
frequency distribution of the dynamical conductivity \( \sigma = D \delta(\omega) + \sigma_{\text{reg}} \) and has a spectral representation in terms of eigenstates and eigenvalues of the system with vector potential \( A = 0 \)

\[
D = \frac{1}{2L} \left\{ \langle -\hat{T} \rangle - 2 \sum_{m \neq n} p_n \frac{|\langle n|\hat{j}|m \rangle|^2}{\epsilon_m - \epsilon_n} \right\},
\]

(2)

where \( \hat{j} \) is the current operator, \( \langle \hat{T} \rangle \) is the thermal expectation value of the kinetic energy, and \( p_n = e^{-\epsilon_n/T}/Z \) is the Boltzmann weight for the eigenstate \( |n\rangle \) of the Hamiltonian with energy \( \epsilon_n \).

On the other hand, a static magnetic flux leads to a site and time independent vector potential \( A_x(j, t) = \phi/e \) with characteristic dependence of the eigenvalues on \( \phi \). Denoting the Hamiltonian (1) by \( \hat{H}(\phi) \) we find in second order perturbation theory in \( \phi \)

\[
\epsilon_n(\phi) = \langle n|\hat{H}(0)|n \rangle - \phi \langle n|\hat{j}|n \rangle - \phi^2 \sum_{m \neq n} \frac{|\langle n|\hat{j}|m \rangle|^2}{\epsilon_m - \epsilon_n} - \frac{1}{2} \phi^2 \langle n|\hat{T}|n \rangle.
\]

(3)

Comparing second order terms we see that

\[
D = \frac{1}{L} \sum_n p_n \frac{1}{2} \frac{\partial^2 \epsilon_n(\phi)}{\partial \phi^2} \bigg|_{\phi \to 0}.
\]

(4)

This is the generalization of Kohn’s result [3], see also [4, 5] to finite temperature [6]. In this way the Drude weight \( D \) is connected to the twist \( \phi \) in the boundary conditions caused by the applied external field.

The expression (4) is very interesting as it allows for the calculation of the Drude weight just from the eigenvalues of the Hamiltonian without the knowledge of matrix elements. This is essential for analytic calculations of integrable systems rendering the task feasible although the remaining work is still formidable. In [7] an extension of the traditional Thermodynamic Bethe Ansatz (TBA) to cover the mean curvature of energy levels was presented. This method was applied to the spin-1/2 XXZ chain in [8]. The numerical evaluation of the Drude weight showed a curious behaviour especially for the isotropic chain suggesting that \( D(T > 0) = 0 \).

Our own interest in the finite temperature Drude weight was triggered by the peculiar findings of [8]. The treatment of the (strictly) isotropic Heisenberg chain within the TBA approach is rather challenging as it involves infinitely many functions to be solved from infinitely many non-linear integral equations. Hence, we suspected that the findings in [8] might be based on inappropriate numerical treatments of these integral equations. This however, is not the case as will become clear in section 3.

In Sec.2 we present some necessary elements of TBA and the generalization for calculating the Drude weight along reference [7]. In Sec.3 we describe the application of the TBA approach to the Heisenberg chain on the particle basis of magnons and their bound states (strings) somewhat following the treatment of [8]. Our main technical achievement in this section is that we manage to reduce the many integral equations to just two. Among other things, this allows for much simplified numerical calculations in comparison to [8], however confirming the obtained data and the steep drop of the Drude weight as discussed above.
In section 4, we apply the extended TBA method on the basis of spinons and anti-spinons. The resulting equations are studied analytically and numerically yielding results that are completely different from those of section 3 and ref. [8]. Most of the discussion of our results is presented in section 5. Some more technical material related to the derivation presented in section 4 can be found in the appendix.

2 TBA formalism for free energy and Drude weight

We consider a system of particles with bare energy \( \epsilon_\alpha(x) \) and momentum \( p_\alpha(x) \) parametrized by the spectral parameter \( x \). The index \( \alpha \) labels the species of particles. As we do not use in this work the notion of the dressed energy function we take the liberty of dropping the commonly used upper index 0 (\( \epsilon_\alpha(x) \) instead of \( \epsilon_\alpha^{(0)}(x) \)). Furthermore we have diagonal scattering of two particles of species \( \alpha \) and \( \beta \) with scattering phase \( \Theta_{\alpha\beta}(x_\alpha - x_\beta) \). The quantization condition for an eigenstate characterized by a set of particles with rapidities \( x_\alpha^{(k)} \) for twisted boundary condition with angle \( \phi_\alpha \) reads

\[
L p_\alpha(x_\alpha^{(k)}) + \sum_{\beta l} \Theta_{\alpha\beta}(x_\alpha^{(k)} - x_{\beta l}) = 2\pi I_{\alpha k} + \phi_\alpha,
\]

where \( \phi_\alpha \) is a multiple of the applied twist angle \( \phi_\alpha = \phi \cdot n_\alpha \) with some (integer) number \( n_\alpha \). (Note that Bethe ansatz equations usually take such a form.) We introduce the counting function

\[
Z_\alpha(x) := \frac{1}{2\pi} p_\alpha(x) + \frac{1}{2\pi L} \sum_\beta \sum_l \Theta_{\alpha\beta}(x - x_{\beta l}) - \frac{\phi_\alpha}{2\pi L}.
\]

The set of solutions to (5) for \( x_\alpha^{(k)} \) in an interval of width \( \Delta x_\alpha \) comprises actual rapidities as well as holes with density functions \( \rho_\alpha \) and \( \rho_h^\alpha \) the sum of which is related to the counting function \( Z_\alpha \)

\[
\#\text{particles} + \#\text{holes} = (\rho_\alpha + \rho_h^\alpha) \Delta x = Z_\alpha(x + \Delta x) - Z_\alpha(x),
\]

or explicitly

\[
\rho_\alpha(x) + \rho_h^\alpha(x) = \frac{1}{2\pi} p_\alpha'(x) + \frac{1}{2\pi L} \sum_\beta \sum_l \Theta_{\alpha\beta}'(x - x_{\beta l}).
\]

The summation over rapidities on the r.h.s. can be written in the thermodynamic limit in terms of integrals over \( \rho_\beta \)

\[
(1 + \eta_\alpha) \rho_\alpha(x) = \frac{1}{2\pi} p_\alpha'(x) + \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} \ast \rho_\beta, \quad \kappa_{\alpha\beta} := \Theta_{\alpha\beta}', \quad \eta_\alpha := \frac{\rho_h^\alpha}{\rho_\alpha}.
\]

This set of integral equations is equivalent to the Bethe ansatz equations (5). The state representing the macrostate for finite temperature \( T \) is obtained from the minimization of the free energy functional

\[
f = e - Ts = \sum_\alpha \left( \int_{-\infty}^{\infty} \epsilon_\alpha \rho_\alpha dx - T \int_{-\infty}^{\infty} \left( [\rho_\alpha + \rho_h^\alpha] \ln(\rho_\alpha + \rho_h^\alpha) - \rho_\alpha \ln \rho_\alpha - \rho_h^\alpha \ln \rho_h^\alpha \right) dx \right).
\]
This results into the non-linear integral equations (thermodynamic Bethe ansatz equations)

\[
\ln \eta_{\alpha}(x) = \beta \epsilon_{\alpha}(x) - \frac{1}{2\pi} \sum_{\beta} \kappa_{\alpha\beta} \ast \ln \left(1 + \eta_{\beta}^{-1}\right),
\]

where we have used the symmetry property \( \kappa_{\alpha\beta}(x) := \kappa_{\beta\alpha}(-x) \). By use of this set of equations we can simplify the expression for the free energy \( \beta f \) yielding

\[
-\beta f = \frac{1}{2\pi} \sum_{\alpha} \int_{-\infty}^{\infty} p'_{\alpha}(x) \ln(1 + \eta_{\alpha}^{-1}(x)) \, dx.
\]

The equations \( (10-12) \) are valid for finite magnetic field \( h \) if the term \( \epsilon_{\alpha} \) is replaced by \( \epsilon_{\alpha} - hn_{\alpha} \) where \( n_{\alpha} \) is the same number that occurred below \( (5) \). We do not give the details of these calculations. The interested reader is referred to the book [9]. Here we are more concerned with the finite size analysis of the rapidities for which we closely follow the treatment of [7]. For \( x_{\alpha j} \) we make the ansatz

\[
x_{\alpha j} = x_{\alpha j}^{\infty} + \frac{g_{\alpha j}^{(1)}}{L} + \frac{g_{\alpha j}^{(2)}}{L^2} = x_{\alpha j}^{\infty} + \frac{g_{\alpha}^{(1)}(x_{\alpha j}^{\infty})}{L} + \frac{g_{\alpha}^{(2)}(x_{\alpha j}^{\infty})}{L^2},
\]

with finite size coefficients \( g_{\alpha j}^{(1,2)} \) taking the form of smooth functions \( g_{\alpha}^{(1,2)}(x) \) in the thermodynamic limit. Inserting this into the counting function leads to an expansion

\[
Z_{\alpha}(x) = \frac{1}{2\pi} p_{\alpha}(x) + \frac{1}{2\pi L} \sum_{\beta} \sum_{l} \Theta_{\alpha\beta}(x - x_{\beta l}^{\infty})
\]

\[
- \frac{1}{2\pi L} \sum_{\beta} \sum_{l} \Theta'_{\alpha\beta}(x - x_{\beta l}^{\infty}) \frac{g_{\beta l}^{(1)}}{L} - \frac{\phi_{\alpha}}{2\pi L}
\]

\[
+ \frac{1}{2\pi L} \sum_{\beta} \sum_{l} \Theta''_{\alpha\beta}(x - x_{\beta l}^{\infty}) \left(\frac{g_{\beta l}^{(1)}}{2L}\right)^2
\]

\[
- \frac{1}{2\pi L} \sum_{\beta} \sum_{l} \Theta'_{\alpha\beta}(x - x_{\beta l}^{\infty}) \frac{g_{\beta l}^{(2)}}{L^2}.
\]

We identify the \( O(1), O(1/L), O(1/L^2) \) contributions to the counting function

\[
Z_{\alpha}(x) = Z_{\alpha}^{\infty}(x) + \frac{Z_{\alpha}^{(1)}}{L}(x) + \frac{Z_{\alpha}^{(2)}}{L^2}(x)
\]

\[
Z_{\alpha}^{(\infty)}(x) = \frac{1}{2\pi} p_{\alpha}(x) + \frac{1}{2\pi} \sum_{\beta} \Theta_{\alpha\beta} \ast \rho_{\beta}(x)
\]

\[
Z_{\alpha}^{(1)}(x) = -\frac{1}{2\pi} \sum_{\beta} \Theta'_{\alpha\beta} \ast (g_{\beta}^{(1)} \rho_{\beta}) - \frac{\phi_{\alpha}}{2\pi}
\]

\[
Z_{\alpha}^{(2)}(x) = \frac{1}{2\pi} \sum_{\beta} \left( \frac{1}{2} \Theta''_{\alpha\beta} \left(g_{\beta}^{(1)^2} \rho_{\beta}\right) - \Theta'_{\alpha\beta} \ast (g_{\beta}^{(2)} \rho_{\beta}) \right),
\]

where we have replaced the summations over \( x_{\beta l}^{\infty} \) by integrals involving the density functions. For studying the quantization condition \( (5) \) we have to expand terms of \( Z \) like

\[
Z_{\alpha}(x_{\alpha j}) = Z_{\alpha} \left(x_{\alpha j}^{\infty} + \frac{g_{\alpha j}^{(1)}}{L} + \frac{g_{\alpha j}^{(2)}}{L^2}\right).
\]
leading to
\[
Z_\alpha(x_{\alpha j}) = Z_\alpha(x_{\alpha j}^\infty) + \frac{1}{L} Z'_\alpha(x_{\alpha j}^\infty) g_{\alpha j}^{(1)} \\
+ \frac{1}{L^2} \left[ \frac{1}{2} Z''_\alpha(x_{\alpha j}^\infty) g_{\alpha j}^{(1)^2} + Z'_\alpha(x_{\alpha j}^\infty) g_{\alpha j}^{(2)} \right] \\
= Z_\alpha^\infty(x_{\alpha j}) + \frac{1}{L} \left[ Z_\alpha^{(1)}(x_{\alpha j}^\infty) + Z_\alpha^{\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)} \right] \\
+ \frac{1}{L^2} \left[ Z_\alpha^{(2)}(x_{\alpha j}^\infty) + Z_\alpha^{(1)'}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)} + \frac{1}{2} Z_\alpha^{\prime\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)^2} \right] \\
+ Z_\alpha^{\prime\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(2)}
\]
(20)

This equation imposes for the corrections
\[
Z_\alpha^{(1)}(x_{\alpha j}^\infty) + Z_\alpha^{\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)} = 0 \\
Z_\alpha^{(2)}(x_{\alpha j}^\infty) + Z_\alpha^{(1)'}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)} + \frac{1}{2} Z_\alpha^{\prime\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(1)^2} + Z_\alpha^{\prime\prime\prime}(x_{\alpha j}^\infty) g_{\alpha j}^{(2)} = 0,
\]
(21)

reading in the thermodynamic limit
\[
(1 + \eta_\alpha) \cdot (g_{\alpha}^{(1)} \rho_\alpha) = \frac{\phi_\alpha}{2\pi} + \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} * (g_{\beta}^{(1)} \rho_\beta) \\
(1 + \eta_\alpha) \cdot (g_{\alpha}^{(2)} \rho_\alpha) = l'_\alpha + \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} * (g_{\beta}^{(2)} \rho_\beta) \\
l_\alpha = \frac{1}{2} (\rho_\alpha + \rho_h^\alpha) g_{\alpha}^{(1)^2} - \frac{1}{4\pi} \sum_\beta \kappa_{\alpha\beta} * (g_{\beta}^{(1)^2} \rho_\beta)
\]
(22)

Focusing again on the Drude weight we are rather interested in the derivatives with respect to \(\phi\) which we denote by dots
\[
(1 + \eta_\alpha) \cdot (\dot{g}_{\alpha}^{(1)} \rho_\alpha) = \frac{\eta_\alpha}{2\pi} + \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} * (\dot{g}_{\beta}^{(1)} \rho_\beta), \\
(1 + \eta_\alpha) \cdot (\ddot{g}_{\alpha}^{(2)} \rho_\alpha) = \ddot{l}_\alpha + \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} * (\ddot{g}_{\beta}^{(2)} \rho_\beta),
\]
(23)
\[
\ddot{l}_\alpha = (\rho_\alpha + \rho_h^\alpha) \dot{g}_{\alpha}^{(1)^2} - \frac{1}{2\pi} \sum_\beta \kappa_{\alpha\beta} * (\dot{g}_{\beta}^{(1)^2} \rho_\beta).
\]

Next we note the second order term in \(\phi\) of the energy function
\[
E_2 = \sum_\alpha \int_{-\infty}^{\infty} \left( \frac{1}{2} \epsilon_\alpha'' g_{\alpha}^{(1)^2} \rho_\alpha + \epsilon_\alpha' g_{\alpha}^{(2)} \rho_\alpha \right) dx,
\]
(24)

the second derivative of this is
\[
2D = \ddot{E}_2 = \sum_\alpha \int_{-\infty}^{\infty} \left( \epsilon_\alpha'' g_{\alpha}^{(1)^2} \rho_\alpha + \epsilon_\alpha' g_{\alpha}^{(2)} \rho_\alpha \right) dx.
\]
(25)
At this point we want to comment on some potentially fatal problem residing in the last expressions. By inspection of explicit examples we see that separate integrals of the individual summands occurring in the integrands of (24) and (25) diverge! Ignoring this problem we may reformulate the last expression

\[
D = \frac{1}{2} \sum_{\alpha} \left( \int_{-\infty}^{\infty} \epsilon_{\alpha}'' (y_{\alpha}^{(1)})^2 \rho_{\alpha} dx + \int_{-\infty}^{\infty} \epsilon_{\alpha}' y_{\alpha}^{(2)} \rho_{\alpha} dx \right)
\]

\[
= \frac{1}{2\beta} \sum_{\alpha} \int_{-\infty}^{\infty} \frac{y_{\alpha}^{(1)} \rho_{\alpha} [\partial_{\beta} \ln \eta_{\alpha}]^2}{(1 + \eta_{\alpha}^{-1})} dx,
\]

where in the last line we have used among other things an identity following from the “dressed function” formalism applied to (11) (after taking the derivative with respect to the spectral parameter) and (24).

Expression (26) was derived in [7] for the study of the Hubbard model. Here we like to simplify this expression by showing that all functions appearing in the integrand of (26) are simply related to \( \eta_{\alpha} \). For this we note the relation

\[
\epsilon_{\alpha} = J \frac{\sin \gamma}{\gamma} P_{\alpha},
\]

and the validity of (11) for finite field \( h \) provided \( \epsilon_{\alpha} \) is replaced by \( \epsilon_{\alpha} - hn_{\alpha} \). This yields

\[
J \frac{\sin \gamma}{\gamma} \rho_{\alpha} = -\frac{1}{2\pi} \frac{\partial}{\partial \beta} \ln (1 + \eta_{\alpha}^{-1}),
\]

\[
y_{\alpha}^{(1)} \rho_{\alpha} = \pm \frac{1}{2\pi} \frac{\partial}{\partial \beta h} \ln (1 + \eta_{\alpha}^{-1}),
\]

just because both sides of each equation satisfy the same integral equation. Putting together (28) and (26) we find

\[
D = \frac{J \sin \gamma}{4\pi \beta \gamma} \sum_{\alpha} \int_{-\infty}^{\infty} \frac{[\partial_{\beta} \ln \eta_{\alpha}]^2 [\partial_{\beta} \ln \eta_{\alpha}]^2}{(1 + \eta_{\alpha})(1 + \eta_{\alpha}^{-1}) \partial_{\gamma} \ln \eta_{\alpha}} dx.
\]

This expression is amazingly symmetric as the identity

\[
\frac{[\partial_{\beta} \ln \eta]^2 [\partial_{\beta} \ln \eta]^2}{(1 + \eta)(1 + \eta^{-1}) \partial_{\gamma} \ln \eta} = -\frac{[\partial_{\beta} \ln \frac{1}{\eta}]^2 [\partial_{\beta} \ln \frac{1}{\eta}]^2}{(1 + \eta^{-1})(1 + \eta) \partial_{\gamma} \ln \frac{1}{\eta}}
\]

may be interpreted (up to the sign change) as invariance under a “particle hole transformation” \( (\eta = \rho^h/\rho \leftrightarrow 1/\eta = \rho/\rho^h) \). Formulas like (29) with the additional minus sign also appeared in [8].

3 TBA and Fusion Hierarchy for the Heisenberg chain

In general the number of particles entering the TBA formalism as sketched in the foregoing section is infinite. In the case of the spin-1/2 Heisenberg chain we have to deal with the single magnon and its many bound states (strings). For the special case of

\[
\mathcal{H} = J \sum_{i} [S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \cos(\gamma) S_{i}^{z} S_{i+1}^{z}] - h \sum_{i} S_{i}^{z}
\]

(31)
with anisotropy parameter \( \gamma = \pi/\nu \) with integer \( \nu \) the number of bound states is finite and the TBA equations close for a finite set of \( \eta \)-functions. This is the case studied in [8] with the main equation being (26) for which the functions \( \eta \) etc. are calculated from (11) etc.

We want to calculate the functions appearing in (29) in a different manner by employing an alternative approach to the thermodynamics of quantum systems making use of a lattice path integral formulation [10, 11]. The quantum system at finite temperature is mapped to a classical model. In the case of the Heisenberg chain we are led to the study of a staggered six-vertex model on the square lattice. The size of this lattice is \( L \times N \) where \( L \) is the length of the quantum chain and \( N \) is the Trotter number. The partition function of this model is calculated within a transfer matrix approach. For these calculations it turns out that the quantum transfer matrix (QTM), i.e. the column-to-column transfer matrix, is most appropriate as it shows a spectral gap between the largest and next-largest eigenvalues even in the limit \( L, N \to \infty \).

There are mainly two different ways of analysing the spectrum of the QTM: the Bethe ansatz analysis and the fusion hierarchy. Here we make use of both approaches. The fusion hierarchy was studied carefully in [12] which we are going to utilize extensively in the first part of this section. In [12] a hierarchy of functions \( Y_\alpha(x), \alpha = 1, 2, \ldots, \) is derived from the basic object of the QTM. These functions satisfy the functional equations

\[
Y_\alpha(x + 1)Y_\alpha(x - 1) = (1 + Y_{\alpha-1}(x))(1 + Y_{\alpha+1}(x)),
\]

relating each function \( Y_\alpha \) to two other functions, one with lower index, the other with higher index. For anisotropy \( \gamma = \pi/\nu \) with integer \( \nu \) the functional equations close at a finite level. (In [12] \( \nu \) is denoted by \( p_0 \); otherwise we follow their notation closely.) The closure happens as \( 1 + Y_{\nu-1} \) factorizes

\[
1 + Y_{\nu-1}(x) = \left(1 + e^{\beta h\nu/2}K(x)\right)\left(1 + e^{-\beta h\nu/2}K(x)\right)
\]

with a function \( K(x) \) satisfying

\[
K(x + 1)K(x - 1) = 1 + Y_{\nu-2}(x).
\]

These equations can be put into a more canonical form by the definition

\[
\eta_\alpha(x) := Y_\alpha(x), \quad \text{for } 1 \leq \alpha \leq \nu - 2
\]

\[
\eta_{\nu-1}(x) := e^{\beta h\nu/2}K(x),
\]

\[
\eta_{\nu}(x) := e^{+\beta h\nu/2}/K(x).
\]

These \( \nu \)-many functions satisfy the functional equations

\[
\eta_\alpha(x + 1)\eta_\alpha(x - 1) = (1 + \eta_{\alpha-1}(x))(1 + \eta_{\alpha+1}(x)), \quad \text{for } 1 \leq \alpha \leq \nu - 3
\]

\[
e^{-\beta h\nu}\eta_{\nu-2}(x + 1)\eta_{\nu-2}(x - 1) = (1 + \eta_{\nu-2}(x))(1 + \eta_{\nu-1}(x))(1 + \eta_{\nu-1}^{-1}(x))
\]

\[
e^{-\beta h\nu}\eta_{\nu-1}(x + 1)\eta_{\nu-1}(x - 1) = e^{+\beta h\nu}\eta_{\nu-1}^{-1}(x + 1)\eta_{\nu-1}^{-1}(x - 1) = 1 + \eta_{\nu-2}(x).
\]

These equations can be brought into the form of \( \nu \)-many non-linear integral equations identical to the TBA equations of [8] that are the starting point of [8].

We want to present a method of computation of the relevant functions avoiding an explicit solution of the TBA equations. To this end we observe two important properties of the functions \( \eta_\alpha \):
(i) All objects \( Y_\alpha \) and \( K \) are even functions of the magnetic field \( h \). Hence the first order derivatives of \( \eta_\alpha \) with respect to \( h \) evaluated at \( h = 0 \) yield zero for all \( \alpha \) except \( \alpha = \nu - 1, \nu \) where we have

\[
\partial_{\beta h} \log \eta_{\nu - 1} = \partial_{\beta h} \log \eta_\nu = \nu / 2. \tag{37}
\]

(ii) For vanishing magnetic field we have a remarkably simple identity

\[
1 + \eta_{\nu - 1}(x) = 1 + \eta_{\nu - 1}(x) \frac{Q(x + i(\nu - 1))Q(x - i(\nu - 1))}{Q(x + i(\nu + 1))Q(x - i(\nu + 1))} \] \( \times \) \( \sinh \left( \frac{\gamma}{2} (x + i(\nu + 1)) \right) \sinh \left( \frac{\gamma}{2} (x - i(\nu + 1)) \right) \] \( \right)^{\nu / 2} \tag{38}\]

involving the function \( Q \) that can be computed without solving the \( \nu \)-many TBA equations. The alternative computation is done on the basis of a set of non-linear integral equations for two functions \( a \) and \( \bar{a} \) \[11\]

\[
\log a(x) = -\beta \epsilon_+(x) + \int_{-\infty}^{\infty} \kappa(x - y) \log(1 + a(y)) dy
\]

\[
- \int_{-\infty}^{\infty} \kappa(x - y + 2i) \log(1 + \bar{a}(y)) dy
\]

\[
\log \bar{a}(x) = -\beta \epsilon_-(x) + \int_{-\infty}^{\infty} \kappa(x - y) \log(1 + \bar{a}(y)) dy
\]

\[
- \int_{-\infty}^{\infty} \kappa(x - y - 2i) \log(1 + a(y)) dy, \tag{39}\]

where the driving terms \( \epsilon_\pm \) and integration kernels \( \kappa \) are explicitly given by

\[
\epsilon_\pm(x) = J \frac{\pi}{2} \sin \frac{\gamma}{\gamma} e_\pm(x) = \frac{\pi}{2(\pi - \gamma)} h, \quad e_\pm(x) = \frac{1}{\cosh \frac{\pi}{2} x}, \quad \tag{40}\]

\[
\kappa(x) = \frac{1}{2 \pi} \int_{-\infty}^{\infty} \frac{\sinh(\frac{\pi}{\gamma} - 2)k}{2 \cosh k \sinh \left( \frac{\pi}{\gamma} - 1 \right) k} e^{ikx} dk. \tag{41}\]

In the course of the derivation of these two non-linear integral equations, explicit expressions for the function \( \log Q(x) \) occur. By use of these results we find for \[13\] straightforwardly

\[
1 + \eta_{\nu - 1}(x) = 1 + \eta_{\nu - 1}(x)
\]

\[
= \nu \cdot \exp \left( \int_{-\infty}^{\infty} \omega(x - y - 1) \log(1 + a(y)) - \omega(x - y + 1) \log(1 + \bar{a}(y)) \right) dy \tag{42}\]

where the function \( \omega(...) \) is given by

\[
\omega(x) = \frac{1}{2 \pi} \int_{-\infty}^{\infty} \frac{1}{2 \sinh \left( \frac{\pi}{\gamma} - 1 \right) k} e^{ikx} dk. \tag{43}\]

The \( k \)-integral may be regularized by either choosing a path along the real axis avoiding \( k = 0 \) in the upper or in the lower half plane: the term in brackets on the r.h.s. of \[17\] containing convolution terms of \( \omega \) with \( a \) and \( \bar{a} \) does not depend on the choice of regularization as the asymptotics of \( a \) and \( \bar{a} \) are identical.

The last equations are the main result of this section. The r.h.s. of \[19\] can be calculated as the terms with \( 1 \leq \alpha \leq \nu - 2 \) are zero and those with \( \alpha = \nu - 1, \nu \) are obtained from \[17\] and \[12\]. Most importantly, in this formulation the number \( \nu \), that used to be the level of
closure of the TBA equations, only enters via the anisotropy parameter \( \gamma \). Hence, we may regard the above formulation as an analytic continuation to all anisotropies \( 0 < \gamma < \pi \).

Finally, we like to mention that the largest eigenvalue may be calculated from

\[
-\beta f = \frac{1}{4} \int_{-\infty}^{\infty} e_0(x) \log [(1 + a(x))(1 + \bar{a}(x))] \, dx
\]

(44)

where an irrelevant constant, i.e. independent of \( T \) and \( h \) has been ignored.

3.1 Numerical results

Here we present the results of numerical treatments of the equations \( (39)-(42) \) derived above. For any anisotropy \( 0 \leq \Delta < 1 \) we obtain Drude weights \( D(T) \) that are monotonously decaying for increasing temperature \( T \), see Fig. In the zero temperature limit the analytically known values \( D_0 \) are reproduced (the formula is given in \( (64) \) below). At high temperatures the data \( D(T) \) follow the behaviour derived analytically in \( (48) \).

Most striking is the behaviour of \( D(T) \) for parameters \( \Delta \) close to 1. At \( T = 0 \) the slope of \( D(T) \) gets steeper the closer \( \Delta \) approaches 1. For \( \Delta = 1 \) the Drude weight shows singular behaviour with a finite value of \( D(T = 0) \) and a drop to \( D(T) = 0 \) for all \( T > 0 \). This is in perfect agreement with the results obtained in [8] by a completely different and much more elaborate treatment of the TBA equations comprising \( \nu \) many non-linear integral equations (with \( \nu \to \infty \) for \( \Delta \to 1 \)).

On the technical side we like to note that our treatment is not restricted to anisotropy parameters \( \Delta = \cos \pi \nu \) with integer \( \nu \). Also, we conclude from the agreement of the two different numerical treatments of the TBA equations (here and in [8]) that both results are either correct, or both are wrong in which case the failure must arise from assumptions underlying the analytical derivation of [20]. We will return to this discussion at the end of the next subsection.

3.2 High temperature asymptotics

The analytical solution to the non-linear integral equations (NLIE) \( (39) \) in first order in \( \beta = 1/T \) is obtained by writing the auxiliary functions

\[
\log a(x) := -\beta e(x) + O(\beta^2) \\
\log \bar{a}(x) := -\beta \bar{e}(x) + O(\beta^2).
\]

(45)

These expressions are inserted into the NLIE and \( \log(1 + a) \), \( \log(1 + \bar{a}) \) are expanded up to first order in \( \beta \) leading to the linear integral equations

\[
-\beta e(x) = -\beta e_+(x) \\
- \frac{\beta}{2} \int_{-\infty}^{\infty} \kappa (x - y) e(y) \, dy + \frac{\beta}{2} \int_{-\infty}^{\infty} \kappa (x - y + 2i) \bar{e}(y) \, dy,
\]

\[
-\beta \bar{e}(x) = -\beta e_-(x) \\
- \frac{\beta}{2} \int_{-\infty}^{\infty} \kappa (x - y) \bar{e}(y) \, dy + \frac{\beta}{2} \int_{-\infty}^{\infty} \kappa (x - y - 2i) e(y) \, dy.
\]

(46)
Figure 1: The Drude weight in the temperature range $T/J = 0, ..., 1$ for different anisotropy parameters $\Delta = 0, 0.1, ..., 0.9$ as obtained in the TBA approach. For $\Delta = 1$ the corresponding data consist of a finite value of the Drude weight for $T = 0$ and zero for all $T > 0$.

This system of linear integral equations is solved in Fourier space yielding explicit expressions for the Fourier transforms of $e$ and $\overline{e}$. Transforming back yields the result

$$
\log a(x) = -\sin \gamma \beta i \left( \frac{2}{1 - e^{-\gamma x - \gamma i}} - \frac{1}{1 - e^{-\gamma x + \gamma i}} - \frac{1}{1 - e^{-\gamma x - 3\gamma i}} \right) - \beta h.
$$

$$
\log \overline{a}(x) = -\sin \gamma \beta i \left( \frac{1}{1 - e^{-\gamma x - \gamma i}} + \frac{1}{1 - e^{-\gamma x + 3\gamma i}} - \frac{2}{1 - e^{-\gamma x + \gamma i}} \right) + \beta h
$$

(47)

This has to be inserted into the expressions \[12\] and \[20\] for the Drude weight $D$. The integral was solved by means of Mathematica yielding the analytical high temperature result

$$
D \simeq \frac{C(\Delta)}{T}, \quad C(\Delta) = J^2 \frac{\gamma - \frac{1}{2} \sin 2\gamma}{16 \gamma},
$$

(48)

for $\gamma = \frac{\pi}{\nu}, \ \nu = 2, 3, ...$. This was compared to the numerical data for $D(T)T$ obtained by numerical iteration of the NLIEs for several anisotropy parameters in the high temperature limit. We observed very good agreement in this regime with high accuracy. (Prior to publication of our work we communicated the analytical results with the authors of [1] who also found very good agreement with the numerical data of [8].)

A fundamental problem appears with \[15\] if we recall the unitary transformation $U$ acting on every second lattice site $j$ by a rotation in spin space by an angle $\pi$ around the $z$-axis and
thus transforming $S^x_j, S^y_j, S^z_j$ into $-S^x_j, -S^y_j, S^z_j$. Actually, in fermionic operator language this is equivalent to changing $c^\dagger_j, c_j$ to $-c^\dagger_j, -c_j$ on every second site without affecting the anti-commutation rules. Hence we have $U H(J, \Delta) U^{-1} = \hat{H}(-J, -\Delta)$ and from (4) we conclude

$$D(T, J, \Delta) = D(T, -J, -\Delta) = -D(-T, J, -\Delta),$$

where we also used the fact that $U$ does not change the dependence of the energy levels on the twist angle $\phi$.

Equation (49) relates the Drude weight at positive temperature $T$ and interaction parameters $J, \Delta$ to the Drude weight at negative temperature $-T$ and interaction parameters $J, -\Delta$. In general we do not learn much from this with respect to the properties of a system at “physical” temperatures, e.g. for $T \to 0^+$ equation (49) relates the Drude weight of the ground state of the system with $J, \Delta$ to the Drude weight of the highest energy state of the system with $J, -\Delta$. Quite differently, for high temperatures the asymptotical behaviour is valid for large positive and negative temperatures $T$! In fact, a high temperature series in $\beta (= 1/T)$ is meaningful and has to have some finite convergence radius such that sufficiently small, but otherwise arbitrary (complex) arguments $\beta$ are allowed. Hence we may apply (48) in the form $D \simeq C(J, \Delta)/T$ for positive and negative temperatures and from (49) we obtain $C(J, \Delta) = C(-J, -\Delta)$ or $C(\gamma) = C(\pi - \gamma)$ a relation certainly not satisfied by (48). There are several possible reasons for this failure. It may simply be that (48) is valid only for the discrete values of $\gamma = \pi \nu$ with $\nu = 2, 3, \ldots$. In other words, the analytical continuation is simply not allowed (at least not in the “most natural” way). We do not want to discuss this point any further.

Another reason may be due to assumptions usually taken for granted in TBA calculations, but failing in the derivation of (26). We already pointed out that there are convergence problems in the transformation of (25) to (26). Yet another problem is due to the fact that (26) has been applied to the Heisenberg chain by dealing with magnons and their bound states (“string”) as elementary, i.e. stable particles. This is –as we nowadays know– not strictly the case. The perfect string picture may be strongly violated, especially if the string is located at large spectral parameters. This explanation is actually corroborated by numerical studies [13].

### 4 TBA based on spinons and antispinons

The above set of NLIEs has been derived in the QTM setting which is mathematically quite different from the TBA. In this sense the QTM approach is an independent method based on algebraic and analytical reasoning rather than combinatorial arguments in the case of the TBA approach. However, the structure of the NLIEs is similar to that of TBA. In fact, it has been argued that can be viewed as the TBA equations of spinons and anti-spinons with bare energies and scattering data given in (41) (with $\eta_1 := 1/a$ and $\eta_2 := 1/\bar{a}$). Such a description of the thermodynamics of a system based on its exact low energy excitations would usually be expected to be possible, but restricted to the low temperature regime. Surprisingly, for the thermodynamical potential of the Heisenberg chain it is quantitatively correct for all temperatures and fields! Note also that is valid for all $\gamma$, not just for the discrete set for which the number of bound states of magnons is finite.

The idea of our work in this section is to utilize the spinon and anti-spinon particle basis for
describing the spectrum of the model. The advantage in comparison to the basis of magnons and their bound states is obvious: from the beginning there will be just two coupled NLIEs to be solved and only two terms in the sum of \(26\) in contrast to in general infinitely many for generic values of \(\Delta\). Also we no longer deal with disintegrating or deformating strings. Of course, this approach is phenomenological and for the computation of the Drude weight it can not be expected to be as successful as for the free energy. With respect to the justification of our approach and its limitation to low temperatures some arguments are given in the appendix.

The reader short of time may directly go to equation \((56)\) obtained from \((29)\) for just two particles: spinon and anti-spinon with \(\eta_1 := 1/a\) and \(\eta_2 := 1/\bar{a}\). In the following treatment we want to address certain subtle, but important issues like the response of spinons and anti-spinons to twist angles \(\phi\) and magnetic fields \(h\). In section 2, the two types of response were assumed for any particle species \(\alpha\) to be governed by just one number \(n_\alpha\) which is usually an integer. From \((41)\) we see that the Zeeman energy for spinons involves a number \(\pm \frac{\pi}{2} (\pi - \gamma)\) that in general is non-integer. From \([15]\) we may infer that also the response to the twist angle \(\phi\) is governed by the same number. Here however, we want to treat the problem in a different way by a mapping to a system where the numbers \(n_\alpha\) are just 1 as usual. This system will involve just one closed integration contour thereby also avoiding the divergence problem mentioned in the final paragraph of the preceding section.

To achieve the outlined goals we reformulate the equations \((39)\) from which we see that the functions \(a(x)\) and \(\bar{a}(x)\) can be analytically continued into the complex plane where they turn into each other due to the identity \(\bar{a}(x) = \frac{1}{a(x - 2i)}\).

Substituting \(\log(1 + a) = \log(1 + 1/a) + \log a\) in \((39)\) and resolving for \(\log a\) yields

\[
\log \eta_+(x) = \beta \epsilon(x) - \int_{-\infty}^{\infty} \kappa(x - y) \log(1 + \eta^+_1(y))dy \\
+ \int_{-\infty}^{\infty} \kappa(x - y + 2i) \log(1 + \eta^-_1(y))dy, \tag{50}
\]

where \(\eta_+(x) := a(x)\) and \(\eta_-(x) := 1/\bar{a}(x)\). The function \(\epsilon(x)\) happens to be the energy of a single magnon parametrized by the spectral parameter \(x\)

\[
\epsilon(x) = -J \frac{\sin \gamma}{\gamma} p'(x) - h, \\
p(x) = -i \log \frac{\sinh(\frac{\gamma}{2} (x - i))}{\sinh(\frac{\gamma}{2} (x + i))}, \tag{51}
\]

and \(p(x)\) is the momentum. Furthermore, \(\kappa(x)\) is given by

\[
\kappa(x) = \frac{1}{2\pi} \Theta'(x), \quad \Theta(x) := -i \log \frac{\sinh(\frac{\gamma}{2} (x - 2i))}{\sinh(\frac{\gamma}{2} (x + 2i))}, \tag{52}
\]

where \(\Theta(x - y)\) is the scattering phase of two magnons with spectral parameters \(x\) and \(y\).

Due to the relation \(\eta_-(x + 2i) = \eta_+(x)\) we can immediately write down a second equation from \((50)\) yielding a complete set of equations for \(\eta_\pm\).

These equations are quite different from the standard TBA equations for the spin-1/2 Heisenberg model since those are based on up to infinitely many bound states (strings). However, the above equations may be obtained within the TBA method if the following two modifications with respect to the standard approach are applied
• ignore bound states,

• consider the single magnon with energy $\epsilon(x)$ and momentum $p(x)$ parametrized by the spectral parameter $x$ on the real axis $\text{Im } x = 0$ (“$C_+$”) as well as on the axis $\text{Im } x = -2$ (“$C_-$”).

A posteriori we find that this prescription renders the single magnon a complete particle basis for the thermodynamics of the system. In other words, if we take the magnon with bare momentum $p$ and energy $\epsilon$ on the axes $C_{\pm}$ the TBA method of the previous section yields exactly (50). The free energy then reads

\[ -\beta f = \frac{1}{2\pi} \sum_{\alpha=\pm} \int_{-\infty}^{\infty} p_\alpha(x) \ln(1 + \eta_\alpha^{-1}(x)) \, dx. \]

where $p_+(x) = p(x)$, $p_-(x) = -p(x - 2i)$ (both functions are monotonously increasing with increasing $x$) and $\eta_\alpha$ are determined from (50) or

\[ \ln \eta_\alpha(x) = \beta \epsilon_\alpha(x) - \frac{1}{2\pi} \sum_{\beta} \chi_{\alpha\beta} \ln \left( 1 + \eta_\beta^{-1} \right), \]

with $\epsilon_+(x) = \epsilon(x)$, $\epsilon_-(x) = \epsilon(x - 2i)$ and $\chi_{++}(z) = \chi_{--}(z) = \chi(z)$, $\chi_{+-}(z) = -\chi(z + 2i)$, $\chi_{-+}(z) = -\chi(z - 2i)$.

Finally, we note for the Drude weight formula (29) with $\alpha$ ranging only over $\alpha = +, -$. As (27) has to be slightly modified by $\pm$ signs, because of $\epsilon_{\pm} = \pm J \frac{\sin \gamma}{\gamma} p_\alpha'$, we find (28) consequently modified to $J \frac{\sin \gamma}{\gamma} \rho_\alpha = \pm \frac{1}{2\pi} \frac{\partial}{\partial \beta} \ln(1 + \eta_\alpha^{-1})$. The Drude weight is

\[ D = \frac{J \sin \gamma}{4\pi \beta \gamma} \sum_{\alpha = \pm} \alpha \int_{-\infty}^{\infty} \frac{(\frac{\partial}{\partial \alpha} \ln \eta_\alpha)^2 (\frac{\partial}{\partial \alpha} \ln \eta_\alpha)}{(1 + \eta_\alpha)(1 + \eta_\alpha^{-1})} \, d\alpha. \]

Alternatively, in terms of $a (= \eta_+)$, $\bar{a} (= \eta_-^{-1})$ and due to the relation (30) we get

\[ D = \frac{J \sin \gamma}{4\pi \beta \gamma} \sum_{\alpha = 1, 2} \int_{-\infty}^{\infty} \frac{(\frac{\partial}{\partial a} \ln a_\alpha)^2 (\frac{\partial}{\partial a} \ln a_\alpha)}{(1 + a_\alpha)(1 + a_\alpha^{-1})} \, da. \]

with the notation $a_1 := a$, $a_2 := a$. This expression with functions $a$ and $\bar{a}$ calculated from (39) is our final analytic result for the finite temperature Drude weight within the spinon approach. In the next subsections we will numerically evaluate $D$ for arbitrary temperatures and study analytically the zero temperature limit and the high temperature asymptotics.

### 4.1 Numerical results

Our numerical results are obtained for arbitrary temperatures $T$ and various anisotropy parameters $\Delta = \cos \gamma$ in the repulsive regime $[0, 1]$, cf. Fig[2]. We find qualitatively different behaviour depending on the value of $\Delta$.

For $\Delta$ close to the free fermion point $\Delta = 0$ the Drude weight $D(T)$ is a monotonously decreasing function of temperature, see Fig[2]. However, for larger values of $\Delta$ close to $\Delta = 1$ corresponding to the isotropic antiferromagnetic Heisenberg point the dependence of $D(T)$ on temperature is non-monotonous! For sufficiently low $T$ the function $D(T)$ increases with
temperature. After taking a finite temperature maximum the function $D(T)$ decreases. In particular, the values of $D(T)$ at the isotropic point ($\Delta = 1$) are non-zero for any value of temperature $T$, see Fig.3. This is in striking contrast to the results of [8] and those of the preceding section. A discussion of this will be given in the final section of this paper.

Figure 2: The Drude weight in the temperature range $T/J = 0, ..., 1$ for different anisotropy parameters $\Delta = 0, 0.1, ..., 0.9, 1$ as obtained in the spinon approach.

4.2 Drude weight at $T = 0$

In the limit of $T \to 0$ and large argument $x$ we have the scaling behaviour of the driving term in the NLIE

$$\frac{\beta}{\cosh \frac{x}{\beta}} \to 2\beta e^{-\frac{x}{2}}.$$  \hspace{1cm} (57)

From this observation it was concluded [11] that the leading low $T$ asymptotics of the physical properties is determined by values of the spectral parameter $x \simeq \pm \frac{2}{\pi} \ln \beta$. Indeed we find that $\lim_{T \to 0} a_\alpha(x \pm \frac{2}{\pi} \ln \beta)$ yields a well defined function of $x$ still satisfying a non-linear integral equation. However the associated functions like $\frac{\partial}{\partial x} a_\alpha$ and $\frac{\partial}{\partial \beta} a_\alpha$ satisfy linear integral equations. Actually, both sets of integral equations are identical up to different driving terms.
Figure 3: The Drude weight at the isotropic point $\Delta = 1$ ($\gamma = 0$). A very steep slope close to $T = 0$ is observed. This slope is infinite at precisely $T = 0$.

Those, however, are strictly proportional to each other as they are given by

$$\frac{\partial}{\partial x} \left( \frac{\beta}{\cosh \frac{\beta}{2} x} \right) \to \mp \pi \beta e^{-\frac{\pi}{2} |x|},$$

$$\frac{\partial}{\partial \beta} \left( \frac{\beta}{\cosh \frac{\beta}{2} x} \right) \to 2e^{-\frac{\pi}{2} |x|},$$

(58) with proportionality factor $\pm \frac{\pi}{2} \beta$. Therefore, in the limit $T \to 0$ and for the relevant range of spectral parameters $x$ the derivatives of $\ln a_\alpha$ with respect to $x$ and $\beta$ satisfy

$$\frac{\partial}{\partial x} \ln a_\alpha \frac{\partial}{\partial \beta} \ln a_\alpha = \mp \frac{\pi}{2} \beta.$$ (59)

Hence in (58) we find the simplification

$$D_0 = \frac{J \sin \gamma}{4 \gamma} \sum_{\alpha=1,2} \int_0^\infty \frac{(\frac{\partial}{\partial \beta} \ln a_\alpha)^2 \frac{\partial}{\partial x} a_\alpha}{(1 + a_\alpha)(1 + a_\alpha^{-1})} dx.$$ (60)

By use of the “dressed function” formalism we obtain the identity

$$\sum_{\alpha=1,2} \int_0^\infty \frac{(\frac{\partial}{\partial \beta} a_\alpha)^2 \frac{\partial}{\partial x} a_\alpha}{a_\alpha^2 (1 + a_\alpha)^2} dx = -\beta \sum_{\alpha=1,2} \int_0^\infty \frac{\partial^2}{\partial (\beta h)^2} \ln(1 + a_\alpha) \frac{\partial}{\partial x} \epsilon_\alpha dx,$$ (61)
Hence the Drude weight is
\[
D_0 = \frac{\beta}{4} \left( \frac{\pi \sin \gamma}{2} J \right)^2 \frac{\partial^2}{\partial(\beta h)^2} \sum_{\alpha=1,2} \int_0^\infty [\ln(1 + a_\alpha)] \epsilon_0 dx,
\] (62)
where the term to the right of the partial derivative is identical to \(-2\beta f\). The second derivative with respect to \(\beta h\) leads to the magnetic susceptibility
\[
\chi_0 = \frac{\pi \sin \gamma}{2v(\pi - \gamma)} J.
\] (63)
Finally the zero temperature Drude weight is found to be
\[
D_0 = \frac{\pi \sin \gamma}{8\gamma(\pi - \gamma)} J.
\] (64)
This result agrees exactly with the Drude weight directly obtained from the groundstate energy of a finite system with twist [4, 5].

4.3 High temperature asymptotics

As an illustration of the high temperature behaviour we show a plot of \(TD(T)\) for some value of \(\Delta\) close to 1, see Fig. 4. The analytic evaluation using (48) in (56) yields
\[
D \simeq \frac{C(\Delta)}{T}, \quad C(\Delta) = J^2 \frac{\Delta^2 + 2}{32}
\] (65)
Again there is a problem with the analytically derived expression for \(C(\Delta)\). Here it contradicts certain rigorously known properties of the high temperature limit that we are going to derive from the spectral representation (2). First we symmetrize the summation
\[
D = \frac{1}{L} \left[ \frac{1}{2} \langle -\hat{T} \rangle \right]_{\geq 0} - \sum_{m \neq n} \frac{p_n |\langle n|J|m \rangle|^2}{\epsilon_m - \epsilon_n}
\] (66)
As \(D\) is the difference of two non-negative terms we see
\[
D \leq \frac{1}{2L} \langle -\hat{T} \rangle
\] (67)
where equality holds if the second term in (66) disappears; this happens for \(\Delta = 0\) where the matrix elements \(\langle n|J|m \rangle\) for different states \(n\) and \(m\) yield zero.
From direct calculations at high \(T\) we find \(\langle -\hat{T} \rangle \simeq \tilde{C}/T\) with a constant \(\tilde{C}\) independent of \(\Delta\). From (67) we see \(C(\Delta) \leq \tilde{C}/2L\). On the other hand we know that equality holds in the case \(\Delta = 0\), therefore
\[
C(\Delta) \leq C(0),
\] (68)
an inequality that has been obtained earlier on grounds of the optical sum rule, see e.g. [1]. This is clearly violated by our analytic result (65)!

The status of the high temperature results in the spinon approach and those in the TBA approach are equally problematic: in the spinon approach the inequality (68) is violated, in the TBA approach the symmetry with respect to \(\Delta\) is violated.
5 Discussion

In section 2 we reviewed the analytical method of computation of the finite temperature Drude weight as proposed in [7] and used in [8] for the study of the spin-1/2 Heisenberg chain. We then employed this method as the starting point of our own analysis of the Heisenberg chain. This was done in two different ways.

In section 3 we utilized the particle basis of magnons and their bound states. Within this approach we managed to reduce the resultant equations to only two non-linear integral equations. These results are totally equivalent to those of [8], however, they allowed for an analytic continuation to the treatment of all anisotropies $-1 < \Delta \leq 1$. Also, we derived an analytic formula for the high temperature asymptotics.

In section 4 we employed the spinon and anti-spinon particle basis. The results obtained in this approach strongly deviate from those of the preceding section and hence from [8]. We observed qualitatively different behaviour of $D(T)$ for $\Delta$ close to 0 and 1 showing monotonous and non-monotonous temperature dependence, respectively. Instead of a drop of $D(T)$ at $T = 0$ our results show an increase with apparently infinite slope at $T = 0$, see Fig.3. This is reminiscent of the behaviour of the magnetic susceptibility with infinite slope due to logarithmic corrections at $T = 0$.
Though disagreeing with [8] we find strong similarities of our results in the spinon approach with the numerical work [16] which is based on complete diagonalization of quantum chains up to length $L = 14$. Unfortunately, the non-monotonous dependence of the Drude weight data obtained in [16] may still be considered as plagued by finite size corrections. In a later numerical analysis in [17] the size dependence was carefully studied for system sizes up to $N = 18$. It was argued [17] that a non-monotonous behaviour found at $\Delta = 1$ was not an artefact of finite size effects and qualitatively agreed with our (then unpublished) data that we presented here in section 4. Also, by use of quantum Monte Carlo calculations at low temperatures, the authors of [18] found quantitative agreement of their results for anisotropy $\Delta = \cos \pi/6$ with our (then unpublished) findings in the spinon approach, which are in strong disagreement with [8].

Still, the numerical treatments have to be considered with care as the size dependence is indeed very strong. However, also the analytical treatments have to be considered with care. For the case of the TBA approach on the basis of bound states (strings) we have indicated certain problems and mechanisms of possible failure. In our understanding, signatures of this are even visible at high temperatures, cf. subsections 3.2 and 4.3. This will be studied in more detail in [13].

In the case of the spinon approach we are confident that the results are reliable at low temperature, whereas they are not trustworthy at high temperatures. The reason for this is simply that the concept of the spinon and anti-spinon particles is field theoretic and restricted to low energies and low temperatures. (Strangely, for the static properties encoded in the free energy, the spinon-concept gives correct results for all temperatures and fields! Some further aspects along this line are discussed in the appendix.)

Finally, we like to mention that our results in the spinon approach have been confirmed by conformal field theoretical arguments developed in [19] for certain anisotropy values $\Delta$, however for some other values (notably those close to 1) there is still strong disagreement. A comparison of all data in collaboration with the authors of [19] is on the way.

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Appendix

Here we address the question whether the relations (50) and (53) are more than accidental. We want to argue that the functions $\rho_\alpha (\alpha = \pm)$ obtained from equations (28) in the spinon approach (and satisfying (9,11)) are true density functions. A (necessary) criterion to be satisfied is the requirement that $\rho_\alpha$ determine all thermal expectation values of the higher
conserved quantities $F_n$ where

$$F_n = \frac{\partial^n}{\partial x^n} \log T(x) \bigg|_{x=0},$$

(A.1)

and $T(x)$ is the six-vertex model row-to-row transfer matrix in dependence on the spectral parameter $x$ with decoupling point $x = 0$. For $n = 0, 1$ we have $F_0 \sim P$ (momentum operator) and $F_1 \sim H$ (Hamiltonian). We are interested in the cases $n \geq 1$ and define the differential operator $D_n = \partial^n / \partial x^n$.

The contribution of a magnon with spectral parameter $x$ to the eigenvalue of any $F_n$ is

$$\langle F_n \rangle = \sum_{\alpha = \pm} \int_{-\infty}^{\infty} (D_n p_{\alpha})(x) \rho_{\alpha}(x) \, dx.$$  

(A.2)

We want to verify this expectation and calculate

$$\langle F_n \rangle = \langle D_n \log T(x) \rangle = \frac{\partial}{\partial z} \log \text{Tr} \left[ \exp(1 + z D_n \log T) e^{-\beta H} \right],$$

(A.3)

where the derivative is to be taken at $z = 0$. The reason for introducing the rather involved expression on the r.h.s. is that exactly this quantity can be calculated in the QTM approach resulting into almost literally (54) except the replacement

$$\beta \epsilon_{\alpha}(x) \to (\beta - z D_{n-1}) \epsilon_{\alpha}(x),$$

(A.4)

which can be derived by simple but lengthy calculations. Note the subscript $n - 1$! The free energy (or more precisely the quantity $\log \text{Tr} [...]$ in (A.3)) is still given by the r.h.s. of (53). Hence the thermal average of $F_n$ is

$$\langle F_n \rangle = \sum_{\alpha = \pm} \int_{-\infty}^{\infty} p'_{\alpha}(x) \frac{\partial}{\partial z} \ln(1 + \eta^{-1}_{\alpha}(x)) \, dx.$$  

(A.5)

The expressions (A.2) and (A.5) look quite different. Still they are equivalent as can be seen in the “dressed functions” formalism. To this end we note (54) with the replacement (A.4), and take the derivative with respect to $z$ at $z = 0$

$$(1 + \eta_{\alpha}) \frac{\partial}{\partial z} \ln(1 + \eta^{-1}_{\beta}) = -D_{n-1} e_{\alpha} + \frac{1}{2\pi} \sum_{\beta} \chi_{\alpha \beta} * \frac{\partial}{\partial z} \ln(1 + \eta^{-1}_{\beta}).$$

(A.6)

This equation can be regarded as an integral equation for $\frac{\partial}{\partial z} \ln(1 + \eta^{-1}_{\beta})$ and is very similar to that one for $\rho_{\alpha}$ (9), just the inhomogeneity (driving term) is different

$$(1 + \eta_{\alpha}) \rho_{\alpha}(x) = \frac{1}{2\pi} p'_{\alpha}(x) + \frac{1}{2\pi} \sum_{\beta} \chi_{\alpha \beta} * \rho_{\beta}.$$  

(A.7)

It is now a standard exercise in mathematical analysis to show the identity of (A.2) and (A.5).

Unfortunately, the criterion that the functions $\rho_{\alpha}$ yield the correct expectation values is necessary, but not sufficient. True density functions are usually real and non-negative. In our case, however, complex valued functions are in principle allowed as we may have distributions along curved lines in the complex plane. Along these lines just the ratio of particle and hole densities (i.e. the function $\eta_{\alpha}$) must take positive values. In the spinon approach this is satisfied for low temperatures, but not for high temperatures.
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