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The thermal conductivity of the spin-$\frac{1}{2}$ XXZ chain at arbitrary temperature

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Abstract

Motivated by recent investigations of transport properties of strongly correlated 1D models and thermal conductivity measurements of quasi 1D magnetic systems, we present results for the integrable spin-$\frac{1}{2}$ XXZ chain. The thermal conductivity $\kappa(\omega)$ of this model has $\mathrm{Re}\,\kappa(\omega) = \tilde{\kappa}\delta(\omega)$, i.e. it is infinite for zero frequency ω. The weight $\tilde{\kappa}$ of the delta peak is calculated exactly by a lattice path integral formulation. Numerical results for wide ranges of temperature and anisotropy are presented. The low- and high-temperature limits are studied analytically.

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1. Introduction

Transport properties of strongly correlated quantum systems have recently attracted immense theoretical and experimental interest. For the XXZ chain as a quantum spin model (or alternatively as a lattice gas model), the spin transport (electrical transport) was investigated analytically [1] by using a method suggested in [2] and numerically [3, 4] with inconclusive results so far about the finite-temperature Drude weight. In [5–7] the thermal conductivities of spin-$\frac{1}{2}$ Heisenberg chain compounds were measured and in [8–10] the thermal conductivity of the quasi one-dimensional magnetic (ladder) system $(\mathrm{Sr,Ca})_{14}\mathrm{Cu}_{24}\mathrm{O}_{41}$ was investigated showing anomalous transport properties along the chain directions. In [10] it was argued that the large thermal conductivity cannot be explained in terms of phonons.

Here we want to use an approach as microscopic as possible and apply Kubo's theory to the strongly correlated spin-$\frac{1}{2}$ XXZ chain. This approach closely follows [11]. We explicitly avoid the notion of particles and Boltzmann equations that take account of scattering as is commonly done in the Fermi liquid theory. In strongly correlated low-dimensional quantum systems, there is no particle picture with finite quasi-particle weight nor do we restrict ourselves to low temperatures in comparison to some reference ('Fermi') energy. Rather on the contrary, we are interested in temperatures comparable to the exchange energy of neighbouring spins.

The Kubo formulae [12, 13] are obtained within linear response theory and yield the (thermal) conductivity κ relating the (thermal) current $\mathcal{J}_{\rm E}$ to the (temperature) gradient ∇T,

$$\mathcal{J}_{\rm E} = \kappa \nabla T \tag{1.1}$$

where

$$\kappa(\omega) = \beta \int_0^\infty {\rm d}t\, {\rm e}^{-{\rm i}\omega t} \int_0^\beta {\rm d}\tau \, \langle \mathcal{J}_{\rm E}(-t - {\rm i}\tau) \mathcal{J}_{\rm E} \rangle \tag{1.2}$$

and β is the reciprocal temperature $1/(k_{\rm B}T)$.[1] The current–current correlation function is to be evaluated in thermal equilibrium and poses the main problem of our study. However, as already pointed out in [11, 14–18], the total thermal current operator $\mathcal{J}_{\rm E}$ commutes with the Hamiltonian $\mathcal{H}$ of the XXZ chain. Hence we find

$$\kappa(\omega) = \frac{1}{{\rm i}(\omega - {\rm i}\epsilon)} \beta^2 \left\langle \mathcal{J}_{\rm E}^2 \right\rangle \qquad (\epsilon \to 0+) \tag{1.3}$$

with $\mathrm{Re}\, \kappa(\omega) = \tilde{\kappa} \delta(\omega)$, where

$$\tilde{\kappa} = \pi \beta^2 \left\langle \mathcal{J}_{\rm E}^2 \right\rangle . \tag{1.4}$$

As a consequence, the thermal conductivity at zero frequency is infinite! The property of a non-decaying thermal current is a feature of 1D systems, in particular of integrable systems with many integrals of motion (for a discussion see [26]). We expect that additional interactions, especially residual interchain couplings in quasi one-dimensional materials, will lead to a broadening of the delta peak, however with the same weight. Instead of speculations about the possible scenarios of such a broadening, we want to present results for the weight $\tilde{\kappa}$ as a function of temperature and anisotropy.

The paper is organized as follows. In section 2 we discuss the integrability of the XXZ chain and identify the thermal current as one of the integrals of motion. In section 3 we present our method of calculation of thermodynamical quantities and discuss the results. In section 4 we treat analytically the low- and high-temperature limits and give a summary in section 5.

2. Thermal current and conserved quantities

Here we begin the microscopic approach to the heat conductivity of the spin-$\frac{1}{2}$ quantum chain with a construction of the conserved currents. The Hamiltonian of the XXZ model on a periodic lattice of size L is

$$\mathcal{H} = \sum_{k=1}^{L} h_{kk+1} \qquad h_{kk+1} = J \left(\sigma_k^+ \sigma_{k+1}^- + \sigma_{k+1}^+ \sigma_k^- + \frac{\Delta}{2} \sigma_k^z \sigma_{k+1}^z \right) \tag{2.1}$$

where $\sigma_k^{\pm} = \left(\sigma_k^x \pm {\rm i}\sigma_k^y\right)/2$ and σ_k^x, σ_k^y, σ_k^z denote the usual Pauli matrices acting on the kth space.

In this paper we restrict ourselves to the critical regime $-1 < \Delta \leqslant 1$, where the system displays algebraically decaying correlation functions at zero temperature. The anisotropy parameter Δ is conveniently parametrized by

$$\Delta = \cos\gamma \qquad 0 \leqslant \gamma < \pi. \tag{2.2}$$

We will give our analytical results for the entire regime $0 \leqslant \gamma < \pi$ $(-1 < \Delta \leqslant 1)$; numerical results will be given for the repulsive range $0 \leqslant \gamma \leqslant \pi/2$ $(0 \leqslant \Delta \leqslant 1)$.

Our first goal is the determination of the thermal current operator $j^{\rm E}$. To this end we impose the continuity equation relating the time derivative of the local Hamiltonian (interaction) and

[1] In this paper we set $k_{\rm B} = 1$.

the divergence of the current: $\dot{h} = -\mathrm{div}\, j^{\mathrm{E}}$. The time evolution of the local Hamiltonian in (2.1) is obtained from the commutator with the total Hamiltonian and the divergence of the local current on the lattice given by a difference expression

$$\frac{\partial h_{kk+1}(t)}{\partial t} = \mathrm{i}[\mathcal{H}, h_{kk+1}(t)] = -\left\{ j^{\mathrm{E}}_{k+1}(t) - j^{\mathrm{E}}_{k}(t)\right\}. \tag{2.3}$$

Apparently, the last equation is satisfied with a local thermal current operator j^{E}_k defined by

$$j^{\mathrm{E}}_k = \mathrm{i}[h_{k-1k}, h_{kk+1}]. \tag{2.4}$$

In fact the total thermal current $\mathcal{J}_{\mathrm{E}} = \sum_{k=1}^{L} j^{\mathrm{E}}_k$,

$$\mathcal{J}_{\mathrm{E}} = -\mathrm{i}J^2 \sum_{k=1}^{L} \left\{ \sigma^z_k(\sigma^+_{k-1}\sigma^-_{k+1} - \sigma^+_{k+1}\sigma^-_{k-1}) - \Delta\left(\sigma^z_{k-1} + \sigma^z_{k+2}\right)(\sigma^+_k\sigma^-_{k+1} - \sigma^+_{k+1}\sigma^-_k)\right\} \tag{2.5}$$

commutes with the Hamiltonian, $[\mathcal{H}, \mathcal{J}_{\mathrm{E}}] = 0$, as it is closely connected with a non-trivial conserved quantity derived from the underlying integrability of the model. To see this, we introduce the transfer matrix constructed from the R-matrix $R \in \mathrm{End}(V \otimes V)$, where V denotes a two-dimensional irreducible module over the quantum algebra $U_q(\hat{s}l(2))$. The six non-zero elements of the R-matrix with the spectral parameter v are given by

$$R^{11}_{11}(v) = R^{22}_{22}(v) = \frac{[v+2]}{[2]} \qquad R^{12}_{12}(v) = R^{21}_{21}(v) = \frac{[v]}{[2]} \qquad R^{21}_{12}(v) = R^{12}_{21}(v) = 1 \tag{2.6}$$

where $[v] = \sin(\gamma v/2)/\sin(\gamma/2)$ and the indices of the above relations can be interpreted as

$$|1\rangle = |\uparrow\rangle \qquad |2\rangle = |\downarrow\rangle \qquad R(v)|\alpha\rangle \otimes |\beta\rangle = \sum_{\gamma,\delta} |\gamma\rangle \otimes |\delta\rangle R^{\gamma\delta}_{\alpha\beta}(v). \tag{2.7}$$

The R-matrix satisfies the Yang–Baxter equation (YBE)

$$R_{12}(u-v)R_{13}(u)R_{23}(v) = R_{23}(v)R_{13}(u)R_{12}(u-v). \tag{2.8}$$

Due to the YBE the transfer matrix $T(v) = \overset{\curvearrowleft}{\prod}_k R_{kk+1}(v)$ is commutative with respect to different spectral parameters v and v', i.e

$$[T(v), T(v')] = 0. \tag{2.9}$$

As is well known, $\ln T(v)$ is the generating function for the conserved quantities

$$\mathcal{J}^{(n)} = \left(\frac{\partial}{\partial v}\right)^n \ln T(v)\Big|_{v=0}. \tag{2.10}$$

In particular, the Hamiltonian (2.1) and the thermal current (2.5) are expressed in terms of $\mathcal{J}^{(1)}$ and $\mathcal{J}^{(2)}$, respectively. Explicitly, they read

$$\mathcal{H} = \frac{2J\sin\gamma}{\gamma}\mathcal{J}^{(1)} - \frac{JL}{2}\Delta \qquad \mathcal{J}_{\mathrm{E}} = \mathrm{i}\left(\frac{2J\sin\gamma}{\gamma}\right)^2 \mathcal{J}^{(2)} + \mathrm{i}J^2L. \tag{2.11}$$

Due to the commutativity of (2.9), every operator $\mathcal{J}^{(n)}$ commutes with the Hamiltonian $\mathcal{H}$.

3. Thermal conductivity

Our goal is to calculate the second moment of the thermal current. Generally, the expectation values of conserved quantities may be calculated by using a suitable generating function. As such we want to define a modified partition function

$$Z = \mathrm{Tr}\exp(-\beta\mathcal{H} + \lambda\mathcal{J}_{\mathrm{E}}) \tag{3.1}$$

from which we find the expectation values by differentiating with respect to λ at $\lambda = 0$,

$$\frac{\partial}{\partial\lambda}\ln Z\bigg|_{\lambda=0} = \langle\mathcal{J}_{\mathrm{E}}\rangle = 0 \qquad \left(\frac{\partial}{\partial\lambda}\right)^2 \ln Z\bigg|_{\lambda=0} = \left\langle\mathcal{J}_{\mathrm{E}}^2\right\rangle - \langle\mathcal{J}_{\mathrm{E}}\rangle^2 = \left\langle\mathcal{J}_{\mathrm{E}}^2\right\rangle \tag{3.2}$$

where we have used the fact that the expectation value of the thermal current in thermodynamical equilibrium is zero.

Instead of Z we find it slightly more convenient to work with a partition function

$$\bar{Z} = \mathrm{Tr}\exp\bigl(-\lambda_1\mathcal{J}^{(1)} - \lambda_n\mathcal{J}^{(n)}\bigr). \tag{3.3}$$

Keeping in view (2.11), we choose

$$\lambda_1 = \beta\frac{2J\sin\gamma}{\gamma} \qquad \lambda_2 = -\mathrm{i}\lambda\left(\frac{2J\sin\gamma}{\gamma}\right)^2 \tag{3.4}$$

and obtain the desired expectation values from $\bar{Z}$

$$\left\langle\mathcal{J}_{\mathrm{E}}^2\right\rangle = \left(\frac{\partial}{\partial\lambda}\right)^2 \ln\bar{Z}\Big|_{\lambda=0}. \tag{3.5}$$

We can deal with $\bar{Z}$ rather easily. Consider the trace of the product of N row-to-row transfer matrices $T(u_j)$ and some spectral parameters u_j close to zero, but still to be specified, and the Nth power of the inverse of $T(0)$

$$\begin{aligned} Z_N &= \mathrm{Tr}\left[T(u_1)\cdots T(u_N)T(0)^{-N}\right] \\ &= \mathrm{Tr}\,\exp\left(\sum_j[\ln T(u_j) - \ln T(0)]\right). \end{aligned} \tag{3.6}$$

Now, it is a standard exercise in mathematics to devise a sequence of N numbers $u_1,\ldots,u_N$ (actually $u_j = u_j^{(N)}$) such that

$$\lim_{N\to\infty}\sum_j[f(u_j) - f(0)] = -\lambda_1\frac{\partial}{\partial v}f(v)\bigg|_{v=0} - \lambda_n\left(\frac{\partial}{\partial v}\right)^n f(v)\bigg|_{v=0}. \tag{3.7}$$

We only need the existence of such a sequence of numbers, the precise values are of no importance. In the limit $N\to\infty$, we note

$$\lim_{N\to\infty} Z_N = \bar{Z}. \tag{3.8}$$

We can proceed along the established path of the quantum transfer matrix (QTM) formalism [19–25] and derive the partition function Z_N in the thermodynamic limit $L\to\infty$,

$$\lim_{L\to\infty} Z_N^{1/L} = \Lambda \tag{3.9}$$

where Λ is the largest eigenvalue of the QTM. The integral expression for Λ reads

$$\ln\Lambda = \sum_j[e(u_j) - e(0)] + \int_{-\infty}^{\infty} K(v)\ln[\mathfrak{U}(v)\bar{\mathfrak{U}}(v)]\,\mathrm{d}v \qquad K(v) = \frac{1}{4\cosh\frac{\pi}{2}v} \tag{3.10}$$

with some function $e(v)$ given in [24]. In the limit $N\to\infty$, the first term on the r.h.s of equation (3.10) turns into

$$\lim_{N\to\infty}\sum_j[e(u_j) - e(0)] = -\lambda_1\frac{\partial}{\partial v}e(v)\bigg|_{v=0} - \lambda_n\left(\frac{\partial}{\partial v}\right)^n e(v)\bigg|_{v=0} \tag{3.11}$$

a rather irrelevant term as it is linear in λ_1 and λ_n, and therefore the second derivatives with respect to λ_1 and λ_n vanish. The functions $\mathfrak{A}(v)$ and $\bar{\mathfrak{A}}(v)$ are determined from the following set of non-linear integral equations (NLIEs):

$$\begin{aligned} \ln \mathfrak{a}(v) &= \sum_j [\varepsilon_0(v - \mathrm{i}u_j) - \varepsilon_0(0)] + \kappa * \ln \mathfrak{A}(v) - \kappa * \ln \bar{\mathfrak{A}}(v + 2\mathrm{i}) \\ \ln \bar{\mathfrak{a}}(v) &= \sum_j [\varepsilon_0(v - \mathrm{i}u_j) - \varepsilon_0(0)] + \kappa * \ln \bar{\mathfrak{A}}(v) - \kappa * \ln \mathfrak{A}(v - 2\mathrm{i}) \\ \mathfrak{A}(v) &= 1 + \mathfrak{a}(v) \qquad \bar{\mathfrak{A}}(v) = 1 + \bar{\mathfrak{a}}(v). \end{aligned} \tag{3.12}$$

with a function $\varepsilon_0(v)$ given in terms of hyperbolic functions [24]. The symbol $*$ denotes the convolution $f * g(v) = \int_{-\infty}^{\infty} f(v - v')g(v')\,\mathrm{d}v'$ and the function $\kappa(v)$ is defined by

$$\kappa(v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh\left(\frac{\pi}{\gamma} - 2\right)k}{2\cosh k \sinh\left(\frac{\pi}{\gamma} - 1\right)k}\, \mathrm{e}^{\mathrm{i}kv}\, \mathrm{d}k. \tag{3.13}$$

Again, the summations in (3.12) can be simplified in the limit $N \to \infty$,

$$\lim_{N\to\infty} \sum_j [\varepsilon_0(v - \mathrm{i}u_j) - \varepsilon_0(v)] = -\lambda_1 \underbrace{\left(-\mathrm{i}\frac{\partial}{\partial v}\right) \varepsilon_0(v)}_{=:\varepsilon_1(v)} - \lambda_n \underbrace{\left(-\mathrm{i}\frac{\partial}{\partial v}\right)^n \varepsilon_0(v)}_{=:\varepsilon_n(v)} \tag{3.14}$$

where the first function can be found in [24] and is simply

$$\varepsilon_1(v) = 2\pi K(v) = \frac{\pi}{2\cosh \frac{\pi}{2} v} \tag{3.15}$$

and hence the second function is

$$\varepsilon_n(v) = \left(-\mathrm{i}\frac{\partial}{\partial v}\right)^{n-1} \varepsilon_1(v). \tag{3.16}$$

We would like to note that the structure of the driving term (3.14) appearing in the NLIE (3.12) reflects the structure of the generalized Hamiltonian in the exponent on the rhs of (3.3). We could have given an alternative derivation of the NLIE along the lines of the thermodynamic Bethe ansatz. In such an approach the driving term is typically the one-particle energy corresponding to the generalized Hamiltonian. Hence it has contributions due to the first as well as the nth logarithmic derivative of the row-to-row transfer matrix, i.e. due to the terms ε_1 and ε_n.

In figure 1 we show $\tilde{\kappa}(T)$ for various anisotropy parameters γ. Note that $\tilde{\kappa}(T)$ has a linear T dependence at low temperatures. In the free-fermion case ($\gamma = \pi/2$), we observe that the ratio of the thermal conductivity κ to the electrical conductivity σ obeys the Wiedemann–Franz law (see the next section). There is a finite temperature maximum at roughly half the temperature of the maximum in the specific heat $c(T)$ data, cf inset to figure 2. At high temperatures $\tilde{\kappa}(T)$ behaves as $1/T^2$. This and the low-temperature asymptotics will be studied analytically in the next section.

In general the data of $\tilde{\kappa}(T)$ show a much stronger variation with the anisotropy γ than the specific heat $c(T)$ data. In figure 2 we show the ratio $\tilde{\kappa}(T)/c(T)$ which has finite low- and high-temperature limits and strongly depends on the anisotropy parameter.

4. Low- and high-temperature limits

In certain limits we can analytically evaluate the NLIEs. For high temperatures the NLIEs linearize and hence can be solved. At low temperatures the NLIEs remain non-linear, but the

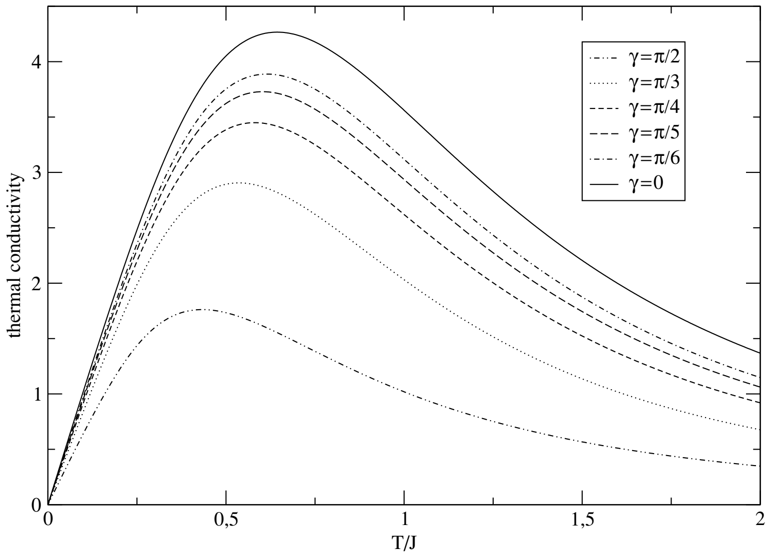

Figure 1. Illustration of numerical results for the thermal conductivity $\tilde{\kappa}$ (in units of J^2) as a function of temperature T for various anisotropy parameters $\gamma = 0, \pi/6, \pi/5, \pi/4, \pi/3, \pi/2$.

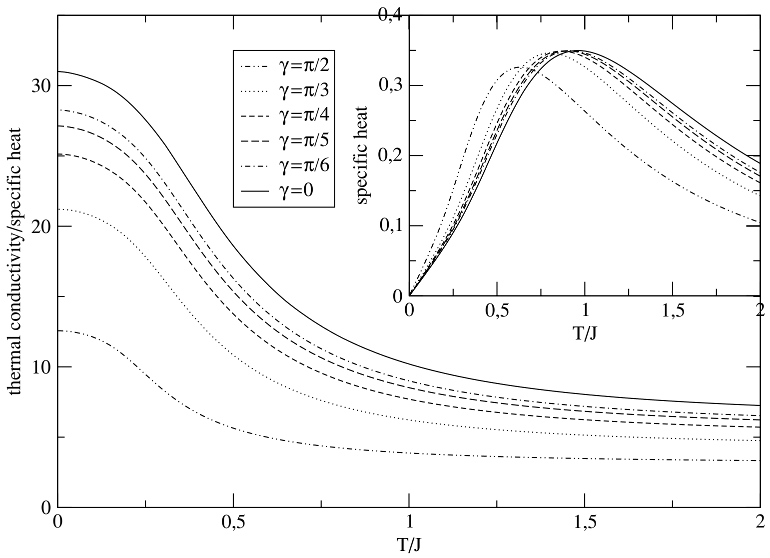

Figure 2. Depiction of the ratio of thermal conductivity and specific heat $\tilde{\kappa}/c$ (in units of J^2) as a function of temperature T for various anisotropy parameters $\gamma = 0, \pi/6, \pi/5, \pi/4, \pi/3, \pi/2$. The zero-temperature limits of the data completely agree with the analytical result (4.12). In the inset, numerical data for the specific heat c are illustrated.

driving terms simplify. Then the symmetry of the integration kernel allows for an evaluation of the physically interesting quantities by avoiding the explicit solution of the NLIEs.

4.1. Low-temperature limit

We consider the low-temperature behaviour of the current–current correlation function of the thermal current $\mathcal{J}_{\mathrm{E}}$ by making use of the dilogarithm trick. The functions $\mathfrak{a}(v)$ and $\bar{\mathfrak{a}}(v)$ in the NLIEs (3.12) exhibit a cross-over behaviour

$$\begin{array}{llll} \mathfrak{a}(v) \ll 1 & \bar{\mathfrak{a}}(v) \ll 1 & \text{for} & -\mathcal{K}_- < v < \mathcal{K}_+ \\ \mathfrak{a}(v) \simeq 1 & \bar{\mathfrak{a}}(v) \simeq 1 & \text{for} & v < -\mathcal{K}_-, \mathcal{K}_+ < v \end{array} \tag{4.1}$$

where

$$\mathcal{K}_\pm = \frac{2}{\pi} \ln \left\{ \frac{2\pi J \sin\gamma}{\gamma} \left(\beta \pm \frac{\lambda\pi J \sin\gamma}{\gamma} \right) \right\}. \tag{4.2}$$

We introduce the scaling functions

$$a_\pm(v) = \mathfrak{a}\left(\pm\frac{2}{\pi} v \pm \mathcal{K}_\pm \right) \qquad \bar{a}_\pm(v) = \bar{\mathfrak{a}}\left(\pm\frac{2}{\pi} v \pm \mathcal{K}_\pm \right) \tag{4.3}$$

and similarly the functions $A_\pm$ ($\bar{A}_\pm$) for $\mathfrak{U}$ ($\bar{\mathfrak{U}}$). From the NLIEs (3.12), one sees that the scaling functions satisfy the following 'scaled' equations in the limit $\beta \to \infty$:

$$\begin{aligned} &\ln a_\pm(v) = -\mathrm{e}^{-v} + \kappa_1 * \ln A_\pm(v) - \kappa_{2\pm} * \ln \bar{A}_\pm(v) \\ &\ln \bar{a}_\pm(v) = -\mathrm{e}^{-v} + \kappa_1 * \ln \bar{A}_\pm(v) - \kappa_{2\mp} * \ln A_\pm(v) \\ &\kappa_1(v) = \frac{2}{\pi}\kappa\left(\frac{2v}{\pi}\right) \qquad \kappa_{2\pm}(v) = \frac{2}{\pi}\kappa\left(\frac{2v}{\pi} \pm 2\mathrm{i}\right). \end{aligned} \tag{4.4}$$

In this limit, the integrals of the functions $\mathfrak{U}$, $\bar{\mathfrak{U}}$ in equation (3.10) can be written as

$$\begin{aligned} \ln\Lambda &= \int_{-\infty}^{\infty} K(v) \ln[\mathfrak{U}(v)\bar{\mathfrak{U}}(v)]\,\mathrm{d}v \\ &= \frac{\gamma^2}{2\pi^2 J \sin\gamma(\beta\gamma + \lambda\pi J \sin\gamma)} \int_{-\infty}^{\infty} \mathrm{e}^{-v}(\ln A_+(v) + \ln \bar{A}_+(v))\,\mathrm{d}v \\ &\quad + \frac{\gamma^2}{2\pi^2 J \sin\gamma(\beta\gamma - \lambda\pi J \sin\gamma)} \int_{-\infty}^{\infty} \mathrm{e}^{-v}(\ln A_-(v) + \ln \bar{A}_-(v))\,\mathrm{d}v. \end{aligned} \tag{4.5}$$

The right-hand side of the above equation is evaluated as follows. (A) After taking the derivatives of the first and second equations in (4.4), we multiply them by $\ln A_\pm(v)$ and $\ln \bar{A}_\pm(v)$, respectively and take the summation of them with respect to each side. (B) Next we multiply the first and second equations in (4.4) by $[\ln A_\pm(v)]'$ and $[\ln \bar{A}_\pm(v)]'$, respectively and take the summation. Then we subtract the resultant equation of (B) from that of (A). After integrating over v, we obtain

$$D_\pm = 2\int_{-\infty}^{\infty} \mathrm{e}^{-v}[\ln A_\pm(v) + \ln \bar{A}_\pm(v)]\,\mathrm{d}v \tag{4.6}$$

where

$$\begin{aligned} D_\pm &= \int_{-\infty}^{\infty} \left(\ln A_\pm(v) \frac{\mathrm{d}}{\mathrm{d}v} \ln a_\pm(v) + \ln \bar{A}_\pm(v) \frac{\mathrm{d}}{\mathrm{d}x} \ln \bar{a}_\pm(v) \right. \\ &\qquad \left. - \ln a_\pm(v) \frac{\mathrm{d}}{\mathrm{d}v} \ln A_\pm(v) - \ln \bar{a}_\pm(v) \frac{\mathrm{d}}{\mathrm{d}x} \ln \bar{A}_\pm(v) \right) \mathrm{d}v \\ &= \int_{a_\pm(-\infty)}^{a_\pm(\infty)} \left(\frac{\ln(1+a)}{a} - \frac{\ln a}{1+a} \right) \mathrm{d}a + \int_{\bar{a}_\pm(-\infty)}^{\bar{a}_\pm(\infty)} \left(\frac{\ln(1+\bar{a})}{\bar{a}} - \frac{\ln \bar{a}}{1+\bar{a}} \right) \mathrm{d}\bar{a}. \end{aligned} \tag{4.7}$$

The quantities $D_\pm$ can be expressed in terms of Roger's dilogarithm $\mathcal{L}(v)$,

$$D_\pm = 2\mathcal{L}\left(\frac{a_\pm(\infty)}{1+a_\pm(\infty)}\right) + 2\mathcal{L}\left(\frac{\bar{a}_\pm(\infty)}{1+\bar{a}_\pm(\infty)}\right) - 2\mathcal{L}\left(\frac{a_\pm(-\infty)}{1+a_\pm(-\infty)}\right) - 2\mathcal{L}\left(\frac{\bar{a}_\pm(-\infty)}{1+\bar{a}_\pm(-\infty)}\right)$$

$$\mathcal{L}(v) = -\frac{1}{2}\int_0^v \left(\frac{\ln(1-x)}{x} + \frac{\ln x}{1-x}\right) \mathrm{d}x. \tag{4.8}$$

Using the asymptotic value of the scaling functions $a_\pm(\pm\infty) = \bar{a}_\pm(\pm\infty) = 1$ and substituting equation (4.6) for equation (4.5), we arrive at

$$\ln \Lambda = \frac{\gamma^2}{12\beta J \sin\gamma}\left(\frac{1}{\beta\gamma + \lambda\pi J \sin\gamma} + \frac{1}{\beta\gamma - \lambda\pi J \sin\gamma}\right). \tag{4.9}$$

Here we have used the identity $\mathcal{L}(v) + \mathcal{L}(1-v) = \pi^2/6$. Hence the low-temperature asymptotics of the current–current correlation function are evaluated to

$$\left\langle \mathcal{J}_{\mathrm{E}}^2 \right\rangle \simeq \frac{J\pi^2 \sin\gamma}{3\beta^3\gamma} + O\left(\frac{1}{\beta^4}\right). \tag{4.10}$$

From this result we see that $\tilde{\kappa}(T)$ is linear in T at low T,

$$\tilde{\kappa}(T) \simeq \frac{\pi^2}{3} v T \tag{4.11}$$

with $v = J\pi \sin\gamma/\gamma$ being the velocity of the elementary excitations. From the low-temperature behaviour of the specific heat $c(T) = (\pi/3v)T$, we find

$$\frac{\tilde{\kappa}(T)}{c(T)} \to \pi v^2. \tag{4.12}$$

Finally, we want to compare the thermal conductivity κ and the electrical conductivity σ which, in the low-temperature limit, can be described by the Drude weight D_{c} [27],

$$\mathrm{Re}\, \sigma(\omega) = 2\pi D_{\mathrm{c}} \delta(\omega) \qquad D_{\mathrm{c}} = \frac{v}{4(\pi - \gamma)}. \tag{4.13}$$

This yields

$$\frac{\kappa}{\sigma} \simeq \frac{2}{3}\pi(\pi - \gamma) T \qquad (T \to 0) \tag{4.14}$$

which in the free-fermion case ($\gamma = \pi/2$) gives the Wiedemann–Franz law.

4.2. High-temperature limit

In the high-temperature limit ($\beta \to 0$), the auxiliary functions satisfy the following integral equations linear in $(\partial/\partial\lambda)^2 \ln \mathfrak{U}$:

$$\left(\frac{\partial}{\partial\lambda}\right)^2 \ln \mathfrak{U}(v) = \left(\frac{\partial}{\partial\lambda}\ln \mathfrak{U}(v)\right)^2 + \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2 \ln \mathfrak{U}(v) - \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2 \ln \bar{\mathfrak{U}}(v + 2\mathrm{i})$$

$$\left(\frac{\partial}{\partial\lambda}\right)^2 \ln \bar{\mathfrak{U}}(v) = \left(\frac{\partial}{\partial\lambda}\ln \bar{\mathfrak{U}}(v)\right)^2 + \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2 \ln \bar{\mathfrak{U}}(v) - \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2 \ln \mathfrak{U}(v - 2\mathrm{i}). \tag{4.15}$$

Here we have used the high-temperature asymptotics $\mathfrak{a}(v), \bar{\mathfrak{a}}(v) \simeq 1$. By using the dressed function formalism, we obtain the identity

$$\left(\frac{\partial}{\partial\lambda}\right)^2 \ln \Lambda \bigg|_{\lambda=0} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \varepsilon_1(v) \left(\frac{\partial}{\partial\lambda}\right)^2 \ln \mathfrak{U}(v)\bar{\mathfrak{U}}(v)\bigg|_{\lambda=0} \mathrm{d}v$$

$$= -\frac{\gamma}{8\pi J \sin\gamma}\int_{-\infty}^{\infty} \frac{\partial \mathfrak{a}(v)}{\partial\beta}\left(\frac{\partial \mathfrak{a}(v)}{\partial\lambda}\right)^2\bigg|_{\lambda=0} \mathrm{d}v. \tag{4.16}$$

The integrand in the above equation is found analytically,

$$\left.\frac{\partial \mathfrak{a}(v)}{\partial \beta}\right|_{\lambda=0} = \frac{J \sin^2 \gamma}{2 \sinh \frac{\gamma}{2}(v+\mathrm{i})} \left(\frac{1}{\sinh \frac{\gamma}{2}(v+3\mathrm{i})} - \frac{1}{\sinh \frac{\gamma}{2}(v-\mathrm{i})} \right)$$
$$\left.\frac{\partial \mathfrak{a}(v)}{\partial \lambda}\right|_{\lambda=0} = -\frac{\partial}{\partial v} \left.\left(\frac{\partial \mathfrak{a}(v)}{\partial \beta} \right)\right|_{\lambda=0}. \tag{4.17}$$

By using these explicit expressions, we obtain the high-temperature limit of $\tilde{\kappa}(T)$,

$$\tilde{\kappa}(T) \simeq \frac{J^4}{4} \left(3 + \frac{\sin 3\gamma}{\sin \gamma} \right) \beta^2 + O(\beta^3). \tag{4.18}$$

This result generalizes the known results for the special cases $\gamma = \pi/2$ (free-fermion model) in [28] and $\gamma = 0$ (isotropic Heisenberg chain) in [29].

5. Summary and discussion

In this paper we have presented a method for the calculation of the thermal conductivity $\kappa(\omega)$ of the integrable spin-$\frac{1}{2}$ XXZ chain. The investigation of this system is drastically simplified in comparison to other systems as here the thermal current is a conserved quantity. This led to $\mathrm{Re}\, \kappa(\omega) = \tilde{\kappa}\delta(\omega)$, where the weight $\tilde{\kappa}$ was calculated for arbitrary temperature and various anisotropy parameters in the repulsive, critical regime of the XXZ model.

We would like to comment on possible generalizations of our investigation. First of all, the computation of $\kappa(q, \omega)$, i.e. the thermal conductivity for a thermal current operator $\mathcal{J}_{\mathrm{E}}(q)$ with non-zero momentum q, is desirable. Unfortunately, it is only the case $q = 0$ that allows for an analytical approach. On the other hand, for small values of q a behaviour of $\kappa(q, \omega)$ similar to the $q = 0$ case is expected with the $\delta(\omega)$ factor replaced by $\delta(\omega - vq)$, where v is the velocity of the elementary excitations. Finally, the investigation of the thermal conductivity of the general XXZ chain with arbitrary anisotropies in the easy plane (gapless) and easy axis (gapped) regimes should be possible. This will be reported elsewhere.

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