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Non-dissipative thermal transport in the massive regimes of the XXZ chain

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Abstract
We present exact results on the thermal conductivity of the one-dimensional spin-1/2 *XXZ* model in the massive antiferromagnetic and ferromagnetic regimes. The thermal Drude weight is calculated by a lattice path integral formulation. Numerical results for wide ranges of temperature and anisotropy as well as analytical results in the low- and high-temperature limits are presented. At finite temperature, the thermal Drude weight is finite and hence there is non-dissipative thermal transport even in the massive regime. At low temperature, the thermal Drude weight behaves as $D_{\mathrm{th}}(T) \sim \exp(-\delta/T)/\sqrt{T}$ where δ is the one-spinon (respectively one-magnon) excitation energy for the antiferromagnetic (respectively ferromagnetic) regime.

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1. Introduction

Recently, transport properties of low-dimensional strongly correlated quantum systems have been extensively studied from both theoretical and experimental sides (see, for example, [1] and references therein). Among them anomalously enhanced thermal conductivity [2–7] and ballistic spin transport [8, 9] have been reported in experiments on one- or quasi one-dimensional materials with weak interchain interactions. Theoretically, the existence of such anomalous properties has also been pointed out especially in quantum integrable systems. One of the criteria for anomalous transport is the existence of a non-zero Drude weight.

In particular for the spin-1/2 *XXZ* chain, the spin transport was investigated analytically [10] using a method developed in [11]. In the massless regime, the Drude weight is non-zero at arbitrary temperatures resulting into non-dissipative (ballistic) spin transport. In contrast, in the massive regime without magnetic field, results on the basis of [10] and [11] indicate a zero Drude weight for any temperature implying that the spin transport is dissipative. The validity, however, of these results is still controversial due to the complexity of the analysis at finite temperatures and debated in [12–14] (see also [15–19] for Haldane gap systems). For the heat conduction, the *thermal* Drude weight $D_{\text{th}}(T)$ (the delta peak of the thermal conductivity at zero-frequency) in the critical regime was more recently calculated by the Bethe ansatz technique in [20] which shows that the thermal transport is non-dissipative at any finite temperature. In the low-temperature limit ($T \ll 1$), we found that $D_{\text{th}}(T)$ behaves as

$$D_{\text{th}}(T) = \pi v T/3 \tag{1.1}$$

where v is the velocity of excitations[3]. This universal behaviour was also found in general systems in which the low-energy excitations are described by $c = 1$ conformal field theory [21, 22]. The study was extended by field theoretical and numerical approaches to more general models including non-integrable systems, and the existence of a non-zero Drude weight was actively discussed [21–28].

In this paper we discuss the thermal conductivity in the massive regime of the *XXZ* model using the approach developed in our previous work [20]. In the case that the response of a physical system to a perturbation is proportional to the force, the quantitative relation is obtained from linear response theory. Transport coefficients are universally given by the Kubo formulae [29, 30] in terms of correlation functions in thermal equilibrium without perturbation. In this way the thermal conductivity $\kappa(\omega)$ relating the thermal current $\mathcal{J}_{\text{th}}$ to the temperature gradient, $\mathcal{J}_{\text{th}} = \kappa \nabla T$, is given by the correlation function of the thermal current operator $\mathcal{J}_{\text{th}}$:

$$\kappa(\omega) = \frac{1}{T}\int_0^{\infty} \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\omega t}\phi(t) \qquad \phi(t) = \int_0^{\beta} \mathrm{d}\tau \, \langle \mathcal{J}_{\text{th}}(-t - \mathrm{i}\tau)\mathcal{J}_{\text{th}}\rangle \tag{1.2}$$

where β is the reciprocal temperature; $\beta = 1/T$ and $\langle \cdots \rangle$ denotes the thermal expectation value per site. Note that here we do not take into account thermomagnetic effects (cf section 5). The real part of equation (1.2) reduces to

$$\operatorname{Re} \kappa(\omega) = \pi D_{\text{th}}(T)\delta(\omega) + \kappa_{\text{reg}}(\omega) \tag{1.3}$$

where $D_{\text{th}}(T)$ is the thermal Drude weight given by

$$D_{\text{th}}(T) = \frac{1}{TL}\left\{\phi(0) - 2\sum_{E_n \neq E_m} p_n \frac{|\langle n|\mathcal{J}_{\text{th}}|m\rangle|^2}{E_m - E_n}\right\} \qquad p_n = \frac{\mathrm{e}^{-\beta E_n}}{\sum_k \mathrm{e}^{-\beta E_k}}. \tag{1.4}$$

In general, the evaluation of the above correlation function is very difficult. Fortunately, as already pointed out by Zotos *et al* [31], the thermal current operator of certain integrable systems commutes with the Hamiltonian. Indeed, the thermal current can be identified as one of the infinitely many conserved quantities underlying the integrability. In this fortuitous situation the thermal current correlations are not time dependent, they reduce to ordinary static correlations. Hence we find

$$D_{\text{th}}(T) = \beta^2 \langle \mathcal{J}_{\text{th}}^2 \rangle. \tag{1.5}$$

Consequently, this quantity is exactly calculable within a lattice path integral formulation as described in [20]. At any finite temperature, the thermal Drude weight is finite implying non-dissipative thermal transport even in the massive regimes. At low temperature, due to the energy gap of the elementary excitations, the thermal Drude weight decays exponentially with decrease of temperature (cf equation (1.1) for the massless regime).

This paper is organized as follows. In section 2 we briefly review the relation between the thermal current operator and conserved quantities. In section 3 we consider the thermal Drude weight at finite temperatures and discuss the results. In section 4 analytical results in the low- and high-temperature limits are presented. Section 5 is devoted to a summary of the present work and an outlook on the case of finite magnetic field.

[3] In the previous work [20] the thermal Drude weight (written by $\tilde{\kappa}$) is defined as $\tilde{\kappa} = \pi D_{\text{th}}(T)$.

2. Ideal thermal current

Let us consider the *XXZ* model on a periodic chain with L sites:

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

where $\sigma_k^{\pm} = \left(\sigma_k^x \pm \mathrm{i}\sigma_k^y\right)/2$ and $\sigma_k^x, \sigma_k^y, \sigma_k^z$ denote the Pauli matrices acting on the kth space. The transfer integral J together with the anisotropy parameter Δ determine the physical nature of the system. In this paper we focus our attention on the massive regime $\Delta > 1$, where correlation functions decay exponentially at zero temperature. Here $J > 0$ (respectively $J < 0$) corresponds to the antiferromagnetic (respectively ferromagnetic) model. In this regime it is convenient to introduce the parameter γ instead of Δ:

$$\Delta = \cosh\gamma \qquad \gamma \in \mathbb{R}_{\geqslant 0}. \tag{2.2}$$

Our first aim is to determine the local energy current operator j_k^{E}. To achieve this we relate the time derivative of the local Hamiltonian to the (discrete) divergence of the thermal current via the continuity equation $\dot{h} = -\mathrm{div}\, j^{\mathrm{E}}$. Since $\dot{h}$ is written as the commutator with the Hamiltonian, we obtain

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

Obviously the local energy current j_k^{E} defined by

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

satisfies the last relation in (2.3). For zero magnetic field the energy current operator $\mathcal{J}_{\mathrm{E}} = \sum_{k=1}^{L} j_k^{\mathrm{E}}$ is equivalent to the thermal current operator $\mathcal{J}_{\mathrm{E}} = \mathcal{J}_{\mathrm{th}}$ (cf section 5 for non-zero magnetic field). Explicitly it reads

$$\mathcal{J}_{\mathrm{th}} = -\mathrm{i}J^2\sum_{k=1}^{L}\left\{\sigma_k^z\left(\sigma_{k-1}^+\sigma_{k+1}^- - \sigma_{k+1}^+\sigma_{k-1}^-\right) - \Delta\left(\sigma_{k-1}^z + \sigma_{k+2}^z\right)\left(\sigma_k^+\sigma_{k+1}^- - \sigma_{k+1}^+\sigma_k^-\right)\right\}. \tag{2.5}$$

As already shown by Zotos *et al* in [31], this thermal current operator is a conserved quantity.

To show this from the underlying integrability, we consider the six vertex model which is the classical counterpart of the *XXZ* chain. There are six spin configurations carrying non-zero Boltzmann weights. This corresponds to six non-zero elements of the R-matrix:

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

where $[v]$ is an abbreviation for $[v] = \sinh(\gamma v/2)$ and the meaning of the indices is exactly as in [20]. The original quantum spin chain is connected with the classical model by a relation of the Hamiltonian $\mathcal{H}$ and the row-to-row transfer matrix $T(v) = \mathrm{Tr}_a \prod_{k=1}^{L} R_{ak}(v)$

$$\mathcal{H} = A\frac{\mathrm{d}}{\mathrm{d}v}\ln T(v)\Big|_{v=0} \qquad A = \frac{2J\sinh\gamma}{\gamma} \tag{2.7}$$

where $T(v)$ is a commuting family with respect to different parameters: $[T(v), T(v')] = 0$. Due to the commutativity, the transfer matrix is a generator of conserved currents $\mathcal{J}^{(n)}$:

$$\mathcal{J}^{(n)} = \mathrm{i}^{n-1}(AD)^n \ln T(v)\big|_{v=0} \qquad D = \frac{\mathrm{d}}{\mathrm{d}v}. \tag{2.8}$$

Note that $\mathcal{J}^{(1)}$ corresponds to the Hamiltonian (2.1). For $n = 2$, we directly find

$$\mathcal{J}^{(2)} = \mathrm{i}A^2\sum_{k=1}^{L}\left\{\check{R}''_{kk+1}(0) - \check{R}'^2_{kk+1}(0) + [\check{R}'_{k-1k}(0), \check{R}'_{kk+1}(0)]\right\} \qquad \check{R}(v) := PR(v) \tag{2.9}$$

where P denotes the permutation operator. Thanks to the unitarity $\check{R}(v)\check{R}(-v) = 1$, the first two terms in the above equation cancel! Using the identity $A\check{R}'_{kk+1}(0) = h_{kk+1}$ and equation (2.4), we see that $\mathcal{J}^{(2)}$ coincides with the thermal current $\mathcal{J}_{\mathrm{th}}$. Due to this and the fact that the thermomagnetic power is always zero for zero magnetic field (being equivalent to half-filling), the thermal Drude weight $D_{\mathrm{th}}(T)$ is given by (1.5) (cf (5.2) in section 5).

Here we only used the difference property and the unitarity of the R-matrix to show the conservation law of the thermal current operator. These properties hold not only for the *XXZ* chain but also for any integrable system whose Hamiltonian is defined as in (2.7), hence the thermal current operator for such an integrable system also satisfies the conservation law[4].

3. Thermal conductivity

In order to obtain the thermal Drude weight (1.5), we have to evaluate the expectation value of the square of the thermal current operator. In fact, we are able to derive explicit results for the generating function of the expectation values of any power of any conserved current. Let us introduce the following extended Hamiltonian $\widetilde{\mathcal{H}}$ including the conserved currents (2.8) as a perturbation; $\widetilde{\mathcal{H}} := \mathcal{H} - T\lambda_n\mathcal{J}^{(n)}$ (throughout this paper we set $\lambda_n \ll 1$). Introducing the partition function $Z(\lambda_n) = \mathrm{Tr}\,\mathrm{e}^{-\beta\widetilde{\mathcal{H}}}$, we easily see that the autocorrelations of the conserved quantities can be calculated by taking the second logarithmic derivative with respect to the variable λ_n:

$$\langle\mathcal{J}^{(n)2}\rangle - \langle\mathcal{J}^{(n)}\rangle^2 = \frac{1}{L}\frac{\partial^2 \ln Z(\lambda_n)}{\partial\lambda_n^2}\bigg|_{\lambda_n=0}. \tag{3.1}$$

To evaluate $Z(\lambda_n)$ explicitly, we follow a procedure developed in the previous work [20]. Taking into account relation (2.8), we express the partition function $Z(\lambda_n)$ in terms of the row-to-row transfer matrices $T(v)$.

$$Z(\lambda_n) = \lim_{N\to\infty}\mathrm{Tr}\exp\left[T(0)^{-N}\prod_{j=1}^{N}T(u_j)\right] = \mathrm{Tr}\exp\left[\lim_{N\to\infty}\sum_{j=1}^{N}\{\ln T(u_j) - \ln T(0)\}\right] \tag{3.2}$$

where a sequence of N numbers $u_1, \ldots, u_N$ should be chosen such that

$$\lim_{N\to\infty}\sum_{j=1}^{N}\{\ln T(u_j) - \ln T(0)\} = AD\{-\beta + \lambda_n\,\mathrm{i}^{n-1}(AD)^{n-1}\}\ln T(v)|_{v=0}. \tag{3.3}$$

Applying a lattice path integral formulation, we introduce the quantum transfer matrix (QTM) in the imaginary time direction [32–36]. In this formalism the partition function $Z(\lambda_n)$ and the quantity (3.1) in the thermodynamic limit $L \to \infty$ can be expressed as the largest eigenvalue of the QTM Λ:

$$\lim_{L\to\infty}\frac{1}{L}\ln Z(\lambda_n) = \ln\Lambda \qquad \langle\mathcal{J}^{(n)2}\rangle - \langle\mathcal{J}^{(n)}\rangle^2 = \left(\frac{\partial}{\partial\lambda_n}\right)^2\ln\Lambda. \tag{3.4}$$

The integral expression for Λ is given by[5]

$$\ln\Lambda = \{-\beta + \lambda_n(AD)^{n-1}\}\mathcal{E}(v)|_{v=0} + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} K(v)\ln[\mathfrak{A}(v)\overline{\mathfrak{A}}(v)]\,\mathrm{d}v$$

$$K(v) = \frac{\gamma}{2\pi}\sum_{k=-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}k\gamma v}}{2\cosh k\gamma} \tag{3.5}$$

[4] One of the exceptions is the Hubbard model for which the R-matrix does not have the difference property.

[5] For convenience, we change here the spectral parameter $v \to \mathrm{i}v$.

where $\mathcal{E}(0)$ is the ground state energy of the antiferromagnetic system. Explicitly $\mathcal{E}(v)$ reads

$$\mathcal{E}(v) = \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} K(v-x)\epsilon(x)\,\mathrm{d}x \qquad \epsilon(v) = \frac{2J\sinh^2\gamma}{\cos\gamma v - \cosh\gamma}. \tag{3.6}$$

The functions $\mathfrak{A}(v) := 1 + \mathfrak{a}(v)$ and $\overline{\mathfrak{A}}(v) := 1 + \overline{\mathfrak{a}}(v)$ are determined from the following set of non-linear integral equations (NLIEs):

$$\begin{aligned} \ln\mathfrak{a}(v) &= \{-\beta + \lambda_n (AD)^{n-1}\}\varepsilon(v) + \kappa * \ln\mathfrak{A}(v) - \kappa * \ln\overline{\mathfrak{A}}(v + 2\mathrm{i} - \mathrm{i}\epsilon) \\ \ln\overline{\mathfrak{a}}(v) &= \{-\beta + \lambda_n (AD)^{n-1}\}\varepsilon(v) + \kappa * \ln\overline{\mathfrak{A}}(v) - \kappa * \ln\mathfrak{A}(v - 2\mathrm{i} + \mathrm{i}\epsilon). \end{aligned} \tag{3.7}$$

Here ϵ is an infinitesimally small number and the symbol $*$ denotes the convolution $f * g(v) = \int_{-\pi/\gamma}^{\pi/\gamma} f(v-x)g(x)\,\mathrm{d}x$. The kernel $\kappa(v)$ and the function $\varepsilon(v)$ are given by

$$\kappa(v) = \frac{\gamma}{2\pi}\sum_{k=-\infty}^{\infty}\frac{\mathrm{e}^{-|k|\gamma}}{2\cosh k\gamma}\,\mathrm{e}^{-\mathrm{i}k\gamma v} \qquad \varepsilon(v) = 2\pi A K(v) = 2J\sum_{k=-\infty}^{\infty}\frac{\sinh\gamma}{2\cosh k\gamma}\,\mathrm{e}^{-\mathrm{i}k\gamma v}. \tag{3.8}$$

From the above NLIEs (3.5) and (3.7), or just symmetry arguments, we find that expectation values of the conserved quantities $\langle\mathcal{J}^{(2m)}\rangle_{m\geqslant 1}$ are always zero: $\langle\mathcal{J}^{(2m)}\rangle_{m\geqslant 1} = 0$. Therefore, due to relations (1.5) and (3.4) (note that $\mathcal{J}^{(2)} = \mathcal{J}_{\mathrm{th}}$), the thermal Drude weight $D_{\mathrm{th}}(T)$ is given by

$$D_{\mathrm{th}}(T) = \beta^2\langle\mathcal{J}^{(2)2}\rangle = \beta^2\left(\frac{\partial}{\partial\lambda_2}\right)^2 \ln\Lambda. \tag{3.9}$$

We would like to remark on the structure of the NLIEs. Our NLIEs (3.7) are consistent with those for $\lambda_n = 0$ in [35], and may be obtained from those by the replacement of the driving term

$$-\beta\varepsilon(v) \to \{-\beta + \lambda_n(AD)^{n-1}\}\varepsilon(v) \tag{3.10}$$

reflecting the structure of the general Hamiltonian $\widetilde{\mathcal{H}}$ and the generating function (2.8) (or (3.3)). Note that for the isotropic limit ($\gamma \to 0$), the NLIEs (3.7) coincide with those in the critical regime [20]. Employing the same analogy, we can derive an alternative expression based on the thermodynamic Bethe ansatz (TBA) [37–39]. The resultant TBA equation consists of infinitely many NLIEs. In contrast to the TBA method, in our approach the thermal quantities are determined from only two NLIEs, which allows us to evaluate physical quantities numerically with quite high accuracy.

In figure 1, the temperature dependence of the thermal Drude weight $D_{\mathrm{th}}(T)$ is depicted for various anisotropy parameters. We find that at low temperatures and $\Delta > 1$, the weight $D_{\mathrm{th}}(T)$ decays exponentially with decreasing temperature:

$$D_{\mathrm{th}}(T) \sim \frac{1}{\sqrt{T}}\exp\left(-\frac{\delta}{T}\right) \qquad \text{for} \quad T \ll 1 \tag{3.11}$$

where δ is the energy gap of the one-spinon[6] (respectively one-magnon) excitation in the antiferromagnetic (respectively ferromagnetic) regime (see the next section for details). On the other hand at high temperatures, $D_{\mathrm{th}}(T)$ behaves as

$$D_{\mathrm{th}}(T) \sim \frac{1}{T^2} \qquad \text{for} \quad T \gg 1. \tag{3.12}$$

One finds that $D_{\mathrm{th}}(T)$ has a finite temperature maximum and the corresponding temperature T_0 shifts to higher values with increasing interaction strength. In the Ising limit $\Delta \to \infty$, the

[6] Note that the excitation gap (spectral gap) actually appearing in the energy spectrum is the two-spinon gap 2δ.

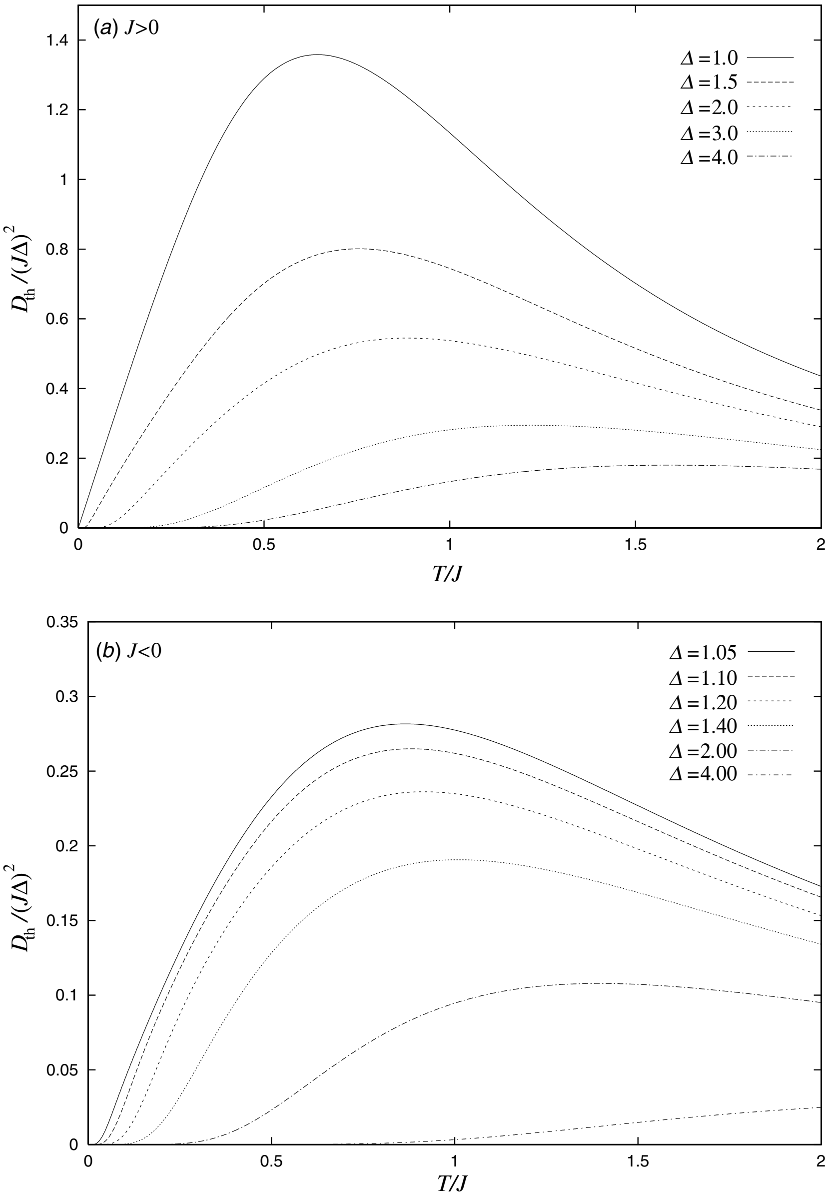

Figure 1. Illustration of numerical results for the thermal Drude weight $D_{\rm th}(T)$ (in units of $(J\Delta)^2$) in the antiferromagnetic $J > 0$ (*a*) and ferromagnetic $J < 0$ (*b*) regimes as a function of temperature T (in units of J) for various anisotropies.

temperature T_0 moves to infinity for fixed J or the height of the peak goes to zero for fixed $J\Delta$ and then the thermal Drude weight $D_{\rm th}(T)$ is always zero at arbitrary temperatures.

In figure 2, we show the ratio of the thermal Drude weight and the specific heat $D_{\rm th}(T)/C(T)$ as a function of the temperature T for various anisotropy parameters. Due to the mass-gap, this ratio goes to zero in the low-temperature limit (cf equation (4.12) in [20] for the massless regime). In the next section the aforementioned high- and low-temperature asymptotics are calculated analytically.

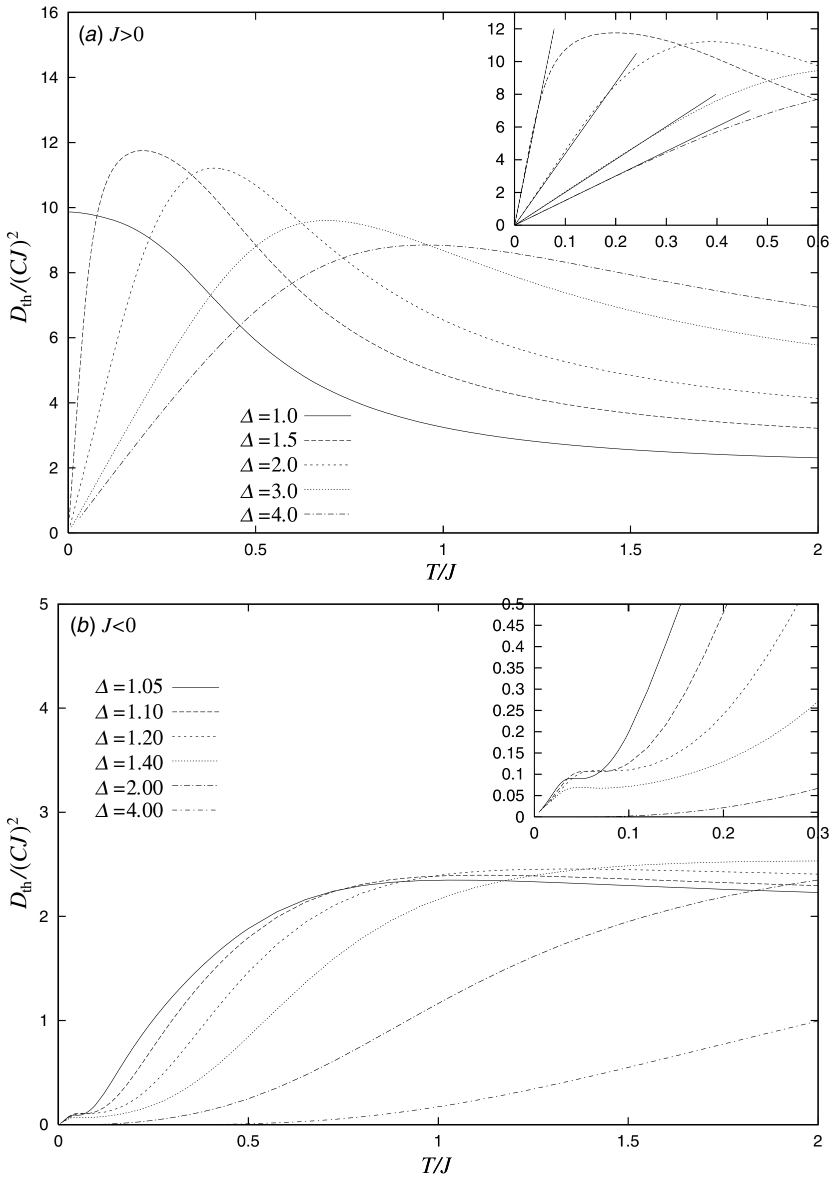

Figure 2. Illustration of the ratio of the thermal Drude weight and the specific heat $D_{\mathrm{th}}(T)/C(T)$ (in units of J^2) in the antiferromagnetic $J > 0$ (*a*) and ferromagnetic $J < 0$ (*b*) regimes as a function of temperature T (in units of J) for various anisotropies. In the inset numerical data at low temperatures are shown. The linear lines in the inset of figure 2(*a*) are the analytical results for the low-temperature asymptotics.

4. Low- and high-temperature limit

In this section we consider the low- and high-temperature behaviour of the thermal Drude weight for both ferromagnetic ($J < 0$) and antiferromagnetic ($J > 0$) regimes. In general, neither the NLIEs (3.7) nor the TBA equations can be solved analytically. However, in the low- and high-temperature limits, the equations simplify especially for the gapped regimes. Hence, we can exactly evaluate the asymptotic behaviour.

4.1. Low-temperature limit

4.1.1. Antiferromagnetic regime ($J > 0$). Let us consider the low-temperature asymptotics in the antiferromagnetic regime ($J > 0$). From the NLIEs (3.7) at low temperatures $\beta \gg 1$, the auxiliary functions $\mathfrak{a}(v)$ and $\overline{\mathfrak{a}}(v)$ reduce to

$$\mathfrak{a}(v) = \overline{\mathfrak{a}}(v) = \exp[\{-\beta + \lambda_n (AD)^{n-1}\}\varepsilon(v)] \qquad \text{for} \quad \beta \gg 1. \tag{4.1}$$

The sub-leading terms are exponentially smaller in T than the above expression. Substituting (4.1) into relation (3.5) and using (3.4), we have

$$\langle \mathcal{J}^{(n)2}\rangle - \langle \mathcal{J}^{(n)}\rangle^2 = 2\int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} K(v)\{(AD)^{n-1}\varepsilon(v)\}^2 \exp[-\beta\varepsilon(v)]\,\mathrm{d}v. \tag{4.2}$$

Applying the steepest descent method, we arrive at

$$\begin{aligned}\langle \mathcal{J}^{(n)2}\rangle - \langle \mathcal{J}^{(n)}\rangle^2 &= \frac{2(-1)^{n-1}(2J\sinh\gamma)^{\frac{4n-1}{2}}}{\sqrt{-2\pi\alpha_2}}\,\mathrm{e}^{\frac{-2J\alpha_0\sinh\gamma}{T}} \\ &\quad\times\left\{\alpha_0\alpha_{n-1}^2 T^{\frac{1}{2}} + \frac{\alpha_2\alpha_{n-1}^2 + 2\alpha_0\left(\alpha_n^2 + \alpha_{n-1}\alpha_{n+1}\right)}{4J\alpha_2\sinh\gamma}T^{\frac{3}{2}} + O\left(T^{\frac{5}{2}}\right)\right\}\end{aligned} \tag{4.3}$$

where

$$\alpha_n = \sum_{k=-\infty}^{\infty} \frac{(-1)^k k^n}{2\cosh k\gamma}. \tag{4.4}$$

Thus by setting $n = 2$ and using (3.9), we obtain the low-temperature asymptotics of the Drude weight $D_{\mathrm{th}}(T)$

$$D_{\mathrm{th}}(T) = \frac{-2(2J\sinh\gamma)^{\frac{5}{2}}\alpha_0\alpha_2}{\sqrt{-2\pi\alpha_2}}\,\mathrm{e}^{\frac{-2J\alpha_0\sinh\gamma}{T}}\left\{T^{-\frac{1}{2}} + O\left(T^{\frac{1}{2}}\right)\right\}. \tag{4.5}$$

Here we have used the fact $\alpha_{2m-1} = 0$ when $m \geqslant 1$. Note that the exponent $-2J\alpha_0\sinh\gamma$ in (4.5) is nothing but the one-spinon excitation energy of the model. This result indicates that the spinon excitation mainly contributes to the low-temperature heat conduction in the antiferromagnetic regime. Comparing the low-temperature limit for the specific heat $C(T) = \beta^2(\langle\mathcal{J}^{(1)2}\rangle - \langle\mathcal{J}^{(1)}\rangle^2)$

$$C(T) = \frac{2(2J\sinh\gamma)^{\frac{3}{2}}\alpha_0^3}{\sqrt{-2\pi\alpha_2}}\,\mathrm{e}^{\frac{-2J\alpha_0\sinh\gamma}{T}}\left\{T^{-\frac{3}{2}} + \frac{3}{4J\alpha_0\sinh\gamma}T^{-\frac{1}{2}} + O\left(T^{\frac{1}{2}}\right)\right\} \tag{4.6}$$

we have

$$\frac{D_{\mathrm{th}}(T)}{C(T)} = \frac{-2J\alpha_2\sinh\gamma}{\alpha_0^2}T + O(T^2). \tag{4.7}$$

In the inset of figure 2(*a*), we show these results for various anisotropy parameters.

4.1.2. Ferromagnetic regime ($J < 0$). Next we analyse the low-temperature asymptotics in the ferromagnetic regime ($J < 0$). In this regime the auxiliary functions $\mathfrak{a}(v)$ and $\overline{\mathfrak{a}}(v)$ are no longer small at low temperature, hence the analysis of the NLIEs becomes difficult. To deal with this situation, we introduce the alternative equations by taking the reciprocals [35]:

$$\begin{aligned} \mathfrak{b}(v) &= \frac{1}{\mathfrak{a}(v)} \qquad & \overline{\mathfrak{b}}(v) &= \frac{1}{\overline{\mathfrak{a}}(v)} \\ \mathfrak{B}(v) &= 1 + \mathfrak{b}(v) \qquad & \overline{\mathfrak{B}}(v) &= 1 + \overline{\mathfrak{b}}(v). \end{aligned} \tag{4.8}$$

Applying the Fourier transform, we derive the NLIEs in terms of these functions:

$$\begin{aligned} \ln \mathfrak{b}(v) &= \{\beta - \lambda_n (AD)^{n-1}\}\widetilde{\varepsilon}(v) + \widetilde{\kappa} * \ln \mathfrak{B}(v) - \widetilde{\kappa} * \ln \overline{\mathfrak{B}}(v + 2\mathrm{i} - \mathrm{i}\epsilon) \\ \ln \overline{\mathfrak{b}}(v) &= \{\beta - \lambda_n (AD)^{n-1}\}\widetilde{\varepsilon}^*(v) + \widetilde{\kappa} * \ln \overline{\mathfrak{B}}(v) - \widetilde{\kappa} * \ln \mathfrak{B}(v - 2\mathrm{i} + \mathrm{i}\epsilon) \end{aligned} \tag{4.9}$$

where the driving terms $\varepsilon(v)$ and $\varepsilon^*(v)$ are given by

$$\widetilde{\varepsilon}(v) = A\gamma \frac{\cosh \frac{\gamma}{2}(1 - \mathrm{i}v)}{2\sinh \frac{\gamma}{2}(1 - \mathrm{i}v)} \qquad \widetilde{\varepsilon}^*(v) = A\gamma \frac{\cosh \frac{\gamma}{2}(1 + \mathrm{i}v)}{2\sinh \frac{\gamma}{2}(1 + \mathrm{i}v)} \tag{4.10}$$

and the kernel $\widetilde{\kappa}(v)$ is defined as

$$\widetilde{\kappa}(v) = -\frac{\gamma}{2\pi} \sum_{k=1}^{\infty} \frac{\mathrm{e}^{-k\gamma} \cosh(\mathrm{i}k\gamma v)}{\sinh k\gamma}. \tag{4.11}$$

Accordingly, the largest eigenvalue Λ is written as

$$\begin{aligned} &\ln \Lambda = \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{K}(v) \ln \mathfrak{B}(v)\,\mathrm{d}v + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{K}^*(v) \ln \overline{\mathfrak{B}}(v)\,\mathrm{d}v \\ &\widetilde{K}(v) = \frac{\widetilde{\varepsilon}(v)}{2\pi A} \qquad \widetilde{K}^*(v) = \frac{\widetilde{\varepsilon}^*(v)}{2\pi A}. \end{aligned} \tag{4.12}$$

Applying an iteration procedure to (4.9), we obtain the low-temperature behaviour of the auxiliary functions:

$$\begin{aligned} \ln \mathfrak{b}(v) &= g(v) + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{\kappa}(v - x)\,\mathrm{e}^{g(x)}\,\mathrm{d}x - \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{\kappa}(v + 2\mathrm{i} - \mathrm{i}\epsilon)\,\mathrm{e}^{g^*(x)}\,\mathrm{d}x \\ \ln \overline{\mathfrak{b}}(v) &= g^*(v) + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{\kappa}(v - x)\,\mathrm{e}^{g^*(x)}\,\mathrm{d}x - \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{\kappa}(v - 2\mathrm{i} + \mathrm{i}\epsilon)\,\mathrm{e}^{g(x)}\,\mathrm{d}x \end{aligned} \tag{4.13}$$

where

$$g(v) = \{\beta - \lambda_n (AD)^{n-1}\}\widetilde{\varepsilon}(v) \qquad g^*(v) = \{\beta - \lambda_n (AD)^{n-1}\}\widetilde{\varepsilon}^*(v). \tag{4.14}$$

Identifying the poles of $\widetilde{\kappa}(v)$ at $v = \pm 2\mathrm{i}$ and applying Cauchy's theorem, the dominant contributions of the integrals for $T \ll 1$ are evaluated

$$\begin{aligned} &\int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{\kappa}(v - x + 2\mathrm{i} - \mathrm{i}\epsilon) \ln(1 + \mathrm{e}^{g^*(x)})\,\mathrm{d}x \\ &\qquad \sim -\frac{\gamma}{2\pi} \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \frac{\mathrm{e}^{-\frac{\mathrm{i}}{2}\gamma(v - x + \mathrm{i}\epsilon)}}{2\sinh \frac{\mathrm{i}}{2}\gamma(v - x + \mathrm{i}\epsilon)}\,\mathrm{e}^{g^*(x)}\,\mathrm{d}x = -\mathrm{e}^{g^*(v)}. \end{aligned} \tag{4.15}$$

Using this and neglecting the subdominant terms, we obtain

$$\ln \mathfrak{B}(v) \sim \mathfrak{b}(v) \sim \mathrm{e}^{g(v)}(1 + \mathrm{e}^{g^*(v)}) = \mathrm{e}^{g(v)} + \mathrm{e}^{g(v) + g^*(v)}. \tag{4.16}$$

For $\ln \overline{\mathfrak{B}}(v)$ a similar equation is valid. Substituting the results into (4.12), we have

$$\ln \Lambda = \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{K}(v)\,\mathrm{e}^{g(v)}\,\mathrm{d}v + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} \widetilde{K}^*(v)\,\mathrm{e}^{g^*(v)}\,\mathrm{d}v + \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} [\widetilde{K}(v) + \widetilde{K}^*(v)]\,\mathrm{e}^{g(v) + g^*(v)}\,\mathrm{d}v. \tag{4.17}$$

We can calculate the first (respectively second) term in (4.17) by shifting the contour to $-\mathrm{i}\infty$ (respectively $\mathrm{i}\infty$). The third integral is evaluated by a saddle point integration.

Using relation (3.4), we obtain the low-temperature asymptotics of the conserved quantities:

$$\langle \mathcal{J}^{(n)2}\rangle - \langle \mathcal{J}^{(n)}\rangle^2 = (J\sinh\gamma)^2\,\mathrm{e}^{\beta J\sinh\gamma}\delta_{n1} + \frac{(-1)^{n-1}(-2J\sinh\gamma)^{\frac{4n-1}{2}}}{\sqrt{-2\pi\beta_2}}\,\mathrm{e}^{\frac{2J\beta_0\sinh\gamma}{T}} \times \left\{\beta_0\beta_{n-1}^2 T^{\frac{1}{2}} + \frac{\beta_2\beta_{n-1}^2 + 2\beta_0\left(\beta_n^2+\beta_{n-1}\beta_{n+1}\right)}{-4J\beta_2\sinh\gamma}T^{\frac{3}{2}} + O\left(T^{\frac{5}{2}}\right)\right\} \tag{4.18}$$

where

$$\beta_n = \sum_{k=-\infty}^{\infty}(-1)^k k^n\,\mathrm{e}^{-|k|\gamma} \qquad \beta_0 = \frac{\sinh\gamma}{1+\Delta} \qquad \beta_1 = 0 \qquad \beta_2 = -\frac{\sinh\gamma}{(1+\Delta)^2}. \tag{4.19}$$

Setting $n = 2$, we derive the low-temperature asymptotics of the thermal Drude weight $D_{\mathrm{th}}(T)$:

$$D_{\mathrm{th}}(T) = \frac{(-2J)^{\frac{5}{2}}(\Delta-1)^2\,\mathrm{e}^{\frac{2J(\Delta-1)}{T}}}{\sqrt{2\pi}}\left\{T^{-\frac{1}{2}} + O\left(T^{\frac{1}{2}}\right)\right\}. \tag{4.20}$$

The exponent $2|J|(\Delta-1)$ in (4.20) agrees with the one-magnon gap. This result coincides with that from numerical diagonalization of the Hamiltonian for size $L = 18$ [21]. For the specific heat $C(T) = \beta^2(\langle\mathcal{J}^{(1)2}\rangle - \langle\mathcal{J}^{(1)}\rangle^2)$ we obtain

$$C(T) = \frac{(J\sinh\gamma)^2\,\mathrm{e}^{\frac{J\sinh\gamma}{T}}}{T^2} + \frac{(-2J)^{\frac{3}{2}}(\Delta-1)^2\,\mathrm{e}^{\frac{2J(\Delta-1)}{T}}}{\sqrt{2\pi}}\left\{T^{-\frac{3}{2}} + \frac{3}{-4J(\Delta-1)}T^{-\frac{1}{2}} + O\left(T^{\frac{1}{2}}\right)\right\}. \tag{4.21}$$

Here the exponent $|J|\sinh\gamma$ in the specific heat (4.21) is the one-spinon excitation gap in the ferromagnetic regime. We observe a crossover behaviour from dominant one-magnon excitation ($\Delta > 5/3$) and dominant one-spinon excitation ($\Delta \leqslant 5/3$) [39, 40]. In contrast to this, a crossover does not take place in the low-temperature thermal Drude weight, which implies that only the magnon excitation contributes to the low-temperature heat conduction. This result yields a different behaviour of the ratio of the thermal Drude weight and the specific heat (4.22) for small and large values of Δ, respectively

$$\frac{D_{\mathrm{th}}(T)}{C(T)} = \begin{cases} -2JT + O(T^2), & \text{for} \quad \Delta \leqslant \dfrac{5}{3} \\ \dfrac{(-2J)^{\frac{5}{2}}(\Delta-1)\,\mathrm{e}^{\frac{J\{2(\Delta-1)-\sinh\gamma\}}{T}}}{\sqrt{2\pi}\,J^2(\Delta+1)}\left\{T^{\frac{3}{2}} + O\left(T^{\frac{5}{2}}\right)\right\} & \text{for} \quad \Delta > \dfrac{5}{3}. \end{cases} \tag{4.22}$$

The ratio of $D_{\mathrm{th}}(T)$ and $C(T)$ depends linearly on the temperature and is independent of the anisotropy for $\Delta \leqslant 5/3$. On the other hand, for $\Delta > 5/3$ the ratio decays exponentially with temperature and explicitly depends on Δ. This behaviour is clearly observed in figure 2(*b*).

While the low-temperature limit in [20] had to be investigated with quite elaborate means such as the 'dilogarithm trick', the result is simply given by the universal (1.1). In contrast to the investigation [20], in the present work on the gapped system simple means such as saddle point integrations are fully sufficient, leading however to complex results such as (4.22) exhibiting crossover phenomena.

4.2. High-temperature limit

Here we analyse the high-temperature behaviour. In this limit the NLIEs (3.7) linearize and hence can be analytically solved. Using identities like

$$\frac{\partial}{\partial\beta}\ln\mathfrak{a} = \frac{\mathfrak{A}}{\mathfrak{a}}\frac{\partial}{\partial\beta}\ln\mathfrak{A} \tag{4.23}$$

$$\frac{\partial^2}{\partial\beta^2}\ln\mathfrak{a} = -\frac{\mathfrak{A}}{\mathfrak{a}^2}\left(\frac{\partial}{\partial\beta}\ln\mathfrak{A}\right)^2 + \frac{\mathfrak{A}}{\mathfrak{a}}\frac{\partial^2}{\partial\beta^2}\ln\mathfrak{A} \tag{4.24}$$

and the limiting behaviour $\mathfrak{a} = 1, \mathfrak{A} = 2$ for $\beta = 0$, we find the linearized integral equations

$$\begin{aligned}\frac{\partial}{\partial\beta}\ln\mathfrak{A}(v) &= -\frac{1}{2}\varepsilon(v) + \frac{1}{2}\kappa * \frac{\partial}{\partial\beta}\ln\mathfrak{A}(v) - \frac{1}{2}\kappa * \frac{\partial}{\partial\beta}\ln\overline{\mathfrak{A}}(v+2\mathrm{i}-\mathrm{i}\epsilon)\\ \frac{\partial}{\partial\beta}\ln\overline{\mathfrak{A}}(v) &= -\frac{1}{2}\varepsilon(v) + \frac{1}{2}\kappa * \frac{\partial}{\partial\beta}\ln\overline{\mathfrak{A}}(v) - \frac{1}{2}\kappa * \frac{\partial}{\partial\beta}\ln\mathfrak{A}(v-2\mathrm{i}+\mathrm{i}\epsilon)\end{aligned} \tag{4.25}$$

and integral equations linear in $(\partial/\partial\lambda)^2\ln\mathfrak{A}$ (with $\lambda := \lambda_n$)

$$\begin{aligned}\left(\frac{\partial}{\partial\lambda}\right)^2\ln\mathfrak{A}(v) &= \left(\frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v)\right)^2 + \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2\ln\mathfrak{A}(v) - \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2\ln\overline{\mathfrak{A}}(v+2\mathrm{i}-\mathrm{i}\epsilon)\\ \left(\frac{\partial}{\partial\lambda}\right)^2\ln\overline{\mathfrak{A}}(v) &= \left(\frac{\partial}{\partial\lambda}\ln\overline{\mathfrak{A}}(v)\right)^2 + \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2\ln\overline{\mathfrak{A}}(v) - \frac{1}{2}\kappa * \left(\frac{\partial}{\partial\lambda}\right)^2\ln\mathfrak{A}(v-2\mathrm{i}+\mathrm{i}\epsilon).\end{aligned} \tag{4.26}$$

The current correlator (3.1) is found from (3.4)

$$\begin{aligned}\left(\frac{\partial}{\partial\lambda}\right)^2\ln\Lambda\bigg|_{\lambda=0} &= \int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}} K(v)\left(\frac{\partial}{\partial\lambda}\right)^2\ln\mathfrak{A}(v)\overline{\mathfrak{A}}(v)\bigg|_{\lambda=0}\mathrm{d}v\\ &= -\frac{1}{\pi A}\int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}}\frac{\partial}{\partial\beta}\ln\mathfrak{A}(v)\left(\frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v)\right)^2\bigg|_{\lambda=0}\mathrm{d}v + \text{c.c.}\end{aligned} \tag{4.27}$$

where in the last line we have used the dressed function formalism. With the high temperature asymptotics $\mathfrak{a}(v), \overline{\mathfrak{a}}(v) = 1$ for $\beta = 0$ we find

$$\left(\frac{\partial}{\partial\lambda}\right)^2\ln\Lambda\bigg|_{\lambda=0} = -\frac{1}{8\pi A}\int_{-\frac{\pi}{\gamma}}^{\frac{\pi}{\gamma}}\frac{\partial\mathfrak{a}(v)}{\partial\beta}\left(\frac{\partial\mathfrak{a}(v)}{\partial\lambda}\right)^2\bigg|_{\lambda=0}\mathrm{d}v + \text{c.c.} \tag{4.28}$$

The integrands in the above equation are found analytically. First, from (4.25) we obtain

$$\frac{\partial\mathfrak{a}(v)}{\partial\beta}\bigg|_{\lambda=0} = \frac{J\sinh^2\gamma}{2\sin\frac{\gamma}{2}(v+\mathrm{i})}\left(\frac{1}{\sin\frac{\gamma}{2}(v+3\mathrm{i})} - \frac{1}{\sin\frac{\gamma}{2}(v-\mathrm{i})}\right) \tag{4.29}$$

and $\overline{\mathfrak{a}}$ is the complex conjugate.

Similar to the reasoning at the beginning of this section we obtain linear integral equations for the derivatives with respect to λ

$$\begin{aligned}\frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v) &= \frac{(AD)^{n-1}}{2}\varepsilon(v) + \frac{1}{2}\kappa * \frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v) - \frac{1}{2}\kappa * \frac{\partial}{\partial\lambda}\ln\overline{\mathfrak{A}}(v+2\mathrm{i})\\ \frac{\partial}{\partial\lambda}\ln\overline{\mathfrak{A}}(v) &= \frac{(AD)^{n-1}}{2}\varepsilon(v) + \frac{1}{2}\kappa * \frac{\partial}{\partial\lambda}\ln\overline{\mathfrak{A}}(v) - \frac{1}{2}\kappa * \frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v-2\mathrm{i}).\end{aligned} \tag{4.30}$$

Hence we find in the high-temperature limit

$$\frac{\partial}{\partial\lambda}\ln\mathfrak{A}(v)\bigg|_{\lambda=0} = -(AD)^{n-1}\frac{\partial}{\partial\beta}\ln\mathfrak{A}(v)\bigg|_{\lambda=0} \tag{4.31}$$

$$\frac{\partial}{\partial\lambda}\mathfrak{a}(v)\bigg|_{\lambda=0} = -(AD)^{n-1}\frac{\partial}{\partial\beta}\mathfrak{a}(v)\bigg|_{\lambda=0}. \tag{4.32}$$

Using these explicit expressions for $n = 2$ we obtain the high-temperature limit of $D_{\rm th}(T)$

$$D_{\rm th}(T) = \frac{J^4(2+\cosh 2\gamma)}{2}\frac{1}{T^2} + O\left(\frac{1}{T^3}\right) \tag{4.33}$$

which is consistent with the result in [20][7] after changing the parameter $\gamma \to {\rm i}\gamma$.

5. Summary and discussion

In this paper we have discussed the thermal transport properties in the massive regime for the spin-1/2 *XXZ* chain. The thermal current operator is expressed as a conserved quantity resulting into an anomalous thermal transport. The thermal Drude weight at finite temperatures was calculated by a path integral formulation. Due to finite temperature effects, non-dissipative thermal transport was observed even in the massive regime of the model. At low temperatures ($T \ll 1$), $D_{\rm th}(T)$ can be written in a universal form: $D_{\rm th}(T) \sim {\rm e}^{-\delta/T}/\sqrt{T}$, where δ is the one-spinon (respectively one-magnon) gap for the antiferromagnetic (respectively ferromagnetic) regime.

Finally, we would like to remark some generalizations of our results. (i) As mentioned in section 2, the conservation law of the thermal current is not limited to the present model. Therefore, the present approach is directly applicable to more general models such as the *XYZ* and the integrable higher-spin or higher-rank chains. (ii) It is quite interesting to consider the system in an external magnetic field h: $H = \mathcal{H} + h\sum_j \sigma_j^z/2$. From definition (2.4), it is observed that the energy current $\mathcal{J}_{\rm E}$ includes the spin current $\mathcal{J}_{\rm s}$ proportional to h. Namely

$$\mathcal{J}_{\rm E} = \mathcal{J}_{\rm th} + h\mathcal{J}_{\rm s} \qquad \mathcal{J}_{\rm s} = {\rm i}J\sum_{j=1}^{L}\left(\sigma_j^+\sigma_{j+1}^- - \sigma_{j+1}^+\sigma_j^-\right) \tag{5.1}$$

where the explicit form of $\mathcal{J}_{\rm th}$ is given by (2.5). Despite the fact that the thermal current is still conserved $[H, \mathcal{J}_{\rm th}] = 0$, the energy current is no longer a conserved quantity because $[H, \mathcal{J}_{\rm s}] \neq 0$. To evaluate the thermal conductivity at $h > 0$, we should carefully take into account thermomagnetic effects, which does not matter when $h = 0$ (being equivalent to half-filling) because $\langle \mathcal{J}_{\rm s}\mathcal{J}_{\rm th}\rangle = 0$. The correct thermal Drude weight at $h > 0$ is determined from the linear response theory (see [30] for example):

$$D_{\rm th}(T,h) = \beta^2\left\langle\mathcal{J}_{\rm th}^2\right\rangle_h - \frac{1}{\beta}S(T,h)^2 D_{\rm s}(T,h) \qquad S(T,h) = \beta^2\frac{\langle\mathcal{J}_{\rm s}\mathcal{J}_{\rm th}\rangle_h}{D_{\rm s}(T,h)} \tag{5.2}$$

where $\langle\cdots\rangle_h$ denotes the thermal expectation value per site for the system H; $S(T,h)$ is the thermomagnetic power and $D_{\rm s}(T,h)$ is the Drude weight of the spin stiffness $\sigma(\omega)$:

$$\operatorname{Re}\sigma(\omega) = \pi D_{\rm s}(T,h)\delta(\omega) + \sigma_{\rm reg}(\omega)$$

$$D_{\rm s}(T,h) = \frac{1}{L}\left\{\langle -K\rangle_h - 2\sum_{E_n\neq E_m} p_n\frac{|\langle n|\mathcal{J}_{\rm s}|m\rangle|^2}{E_m^h - E_n^h}\right\} \qquad p_n = \frac{{\rm e}^{-\beta E_n^h}}{\sum_k {\rm e}^{-\beta E_k^h}}. \tag{5.3}$$

Here, K and E_n^h denote the kinetic energy and the energy eigenvalues of the Hamiltonian H, respectively. The first term in (5.2) can be evaluated by an extension of the present method. The Drude weight $D_{\rm s}(T,h)$ in the second term may be calculated by the approach given in [11]. In fact, in the massless regime ($\Delta \leqslant 0$) with zero external field, $D_{\rm s}(T,0)$ has been already calculated by Zotos [10]. As mentioned in the preceding section, however, the validity of the resultant Drude weight is presently debated (see [1, 12–14] for example). In this respect, a rigorous study of the Drude weight together with the thermomagnetic power is highly desired to investigate the thermal transport in finite magnetic fields.

[7] There is a misprint in (4.18) in [20]: on the rhs of (4.18) a factor π is missing.

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