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Thermal conductivity of one-dimensional spin-1/2 systems

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Abstract

We analyze the thermal conductivity of frustrated spin-1/2 chains within linear-response theory focusing on its frequency dependence at finite temperatures. Using exact diagonalization, the low-frequency limit of the thermal conductivity is discussed in the high-temperature regime.

Key words: Low-dimensional quantum magnets, transport properties

The recent interest in thermal transport properties of one-dimensional spin-1/2 systems is motivated by the experimental observation of significant contributions to the thermal conductivity of quasi-one dimensional materials originating from magnetic excitations (see, e.g., Refs. [1,2] and further examples mentioned in Ref. [3]). A number of recent theoretical papers have either focused on the integrable XXZ model [3–7] or on generic spin models like frustrated chains or spin ladders [3,6,8–12]. When analyzing transport properties, the real part of the conductivity is usually decomposed into a singular part at zero frequency $\omega = 0$ with weight D_{th} and a regular part

$$\mathrm{Re}\,\kappa(\omega) = D_{\mathrm{th}}(T)\delta(\omega) + \kappa_{\mathrm{reg}}(\omega)\,. \qquad (1)$$

Here, κ denotes the thermal conductivity, D_{th} is the thermal Drude weight, T is the temperature, and $\delta(\omega)$ is the δ-function.

The XXZ model shows ballistic thermal transport properties due to the exact conservation of the energy-current operator [4]. A complete understanding of the temperature and magnetic field dependence of the relevant quantity, the thermal Drude weight D_{th}, has recently been established [3,5–7].

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Regarding spin ladders and frustrated chains, both numerical [3,6,12] and field theoretical studies [3,11] indicate normal transport behavior, characterized by a vanishing thermal Drude weight in the thermodynamic limit. Thus, the information relevant for the interpretation of experiments is encoded in the low-frequency behavior of the thermal conductivity.

This paper focuses on the example of the frustrated chain in the massive regime (see Ref. [12] for a similar study of spin ladders). The Hamiltonian reads

$$H = \sum_{l=1}^{N} h_l = J \sum_{l=1}^{N} [\vec{S}_l \cdot \vec{S}_{l+1} + \alpha\, \vec{S}_l \cdot \vec{S}_{l+2}]\,. \qquad (2)$$

h_l is the local energy density; $\vec{S}_l$ is a spin-1/2 operator acting on site l. N denotes the number of sites and periodic boundary conditions are imposed. αJ is the next-nearest neighbor coupling; for $\alpha = 0$, we obtain the spin-1/2 Heisenberg chain. In the following, we will consider the case of $\alpha = 1$. The energy-current operator corresponding to this Hamiltonian is chosen such that the equation of continuity $-\partial_t h_l = \mathrm{div}\, j_{\mathrm{th},l}$ is fulfilled [6]

$$j_{\mathrm{th}} = i \sum_{l=1}^{N} j_{\mathrm{th},l} = i \sum_{l=1}^{N} \sum_{r,s=0}^{1} [h_{l-r-1}, h_{l+s}]\,. \qquad (3)$$

Following linear-response theory, the thermal conductivity can be written as [13]

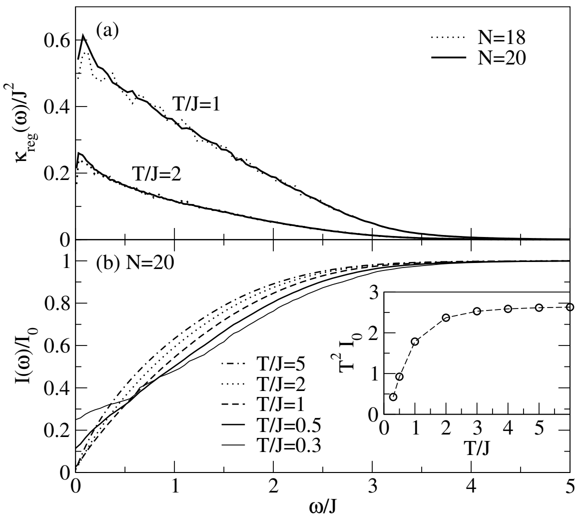

Fig. 1. Thermal conductivity of frustrated chains with $\alpha = 1$ [see Eq. (1)]. Panel (a): regular part of $\mathrm{Re}\,\kappa(\omega)$ vs ω for $T/J = 1, 2$ for $N = 18$ and $N = 20$ sites. Panel (b): integrated weight $I(\omega)$ [see Eq. (5)] vs ω for various temperatures. Inset of (b): $T^2 \cdot I_0$ vs temperature T.

$$\kappa_{\rm reg}(\omega) = \frac{\pi\, g(\omega)}{N\,T} \sum_{E_n \neq E_m} p_n\, |\langle m|j_{\rm th}|n\rangle|^2 \delta(\omega - \Delta E) \quad (4)$$

with $p_n = \exp(-E_n/T)/Z$ being the Boltzmann weight, Z the partition function, $\Delta E = E_m - E_n$, and $g(\omega) = [1 - e^{-\omega/T}]/\omega$. E_n are eigen-energies and $|n\rangle$ eigen-states of the Hamiltonian Eq. (2). Another useful quantity is the integral of $\mathrm{Re}\,\kappa(\omega)$ over frequency ω

$$I(\omega) = D_{\rm th}(T) + 2 \int_{0^+}^{\omega} d\omega'\, \kappa_{\rm reg}(\omega'); \quad I_0 = \lim_{\omega\to\infty} I(\omega)\,. (5)$$

Applying standard numerical techniques allows us to study systems with $N \leq 20$ sites. The dimension of the largest subspace is 9250 after exploiting translational invariance and conservation of total S^z.

Let us now turn to the discussion of the results presented in Fig. 1. Panel (a) contains the regular part $\kappa_{\rm reg}(\omega)$ for $T/J = 1, 2$ and $N = 18$ and $N = 20$. In this plot, $\kappa_{\rm reg}(\omega)$ has been binned with $\Delta E/J \sim 10^{-2}$.

First, note that $\kappa_{\rm reg}(\omega)$ is a structureless function of frequency ω. Depending on temperature, the data are well converged down to frequencies $\omega/J \lesssim 0.25$ while deviations between $N = 18$ and $N = 20$ sites become visible for lower frequencies. Furthermore, we observe a characteristic down-turn of $\kappa_{\rm reg}(\omega)$ at low frequencies which is also present for spin ladders [12]. This feature is less pronounced on larger systems because spectral weight is transferred from the Drude weight to finite frequencies as the system size increases. Moreover, we have to keep in mind that the Drude weight is excluded in the curves displayed in Fig. 1. Note that the Drude weight amounts to less than 3% of the total weight I_0 from Eq. (5) for $N = 20$ sites and $T/J = 1$. Thus, the scenario of ballistic thermal transport is unlikely for frustrated chains. We refer the reader to Refs. [3,6] for a detailed scaling analysis of the Drude weight. While the down-turn at low frequencies renders it difficult to draw precise conclusions about the functional form of the frequency dependence, we can, however, fairly well estimate the absolute value of $\kappa = \lim_{\omega\to 0} \kappa_{\rm reg}(\omega)$. For instance, the data shown in Fig. 1 (a) indicates $\kappa/J^2 \approx (0.27 \pm 0.3)$ for $T/J = 2$.

Next we comment on the integrated spectral weight $I(\omega)$, Eq. (5), which is shown as $I(\omega)/I_0$ in Fig. 1 (b) for $N = 20$ sites and various temperatures $T/J \geq 0.3$. Here, we see that first, $I(\omega)/I_0$ approaches 1 the faster the larger T is. Second, the curve for $T/J = 0.3$ is less smooth than the others indicating the limitations of an exact diagonalization study with respect to the accessible temperature range. A smooth curve $\mathrm{Re}\,\kappa(\omega)$ is obtained for $T/J > 0.5$ for $N = 20$. Finally, we mention that $I_0 \sim T^{-2}$ for high temperatures, as expected for thermal transport [see inset of Fig. 1 (b)].

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References

[1] A. Sologubenko, K. Giannò, H. R. Ott, U. Ammerahl, and A. Revcolevschi, Phys. Rev. Lett. 84 (2000) 2714.

[2] C. Hess C. Baumann, U. Ammerahl, B. Büchner, F. Heidrich-Meisner, W. Brenig, and A. Revcolevschi, Phys. Rev. B 64 (2001) 184305.

[3] F. Heidrich-Meisner, A. Honecker, D.C. Cabra, and W. Brenig, Phys. Rev. B 68 (2003) 134436.

[4] X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B 55 (1997) 11029.

[5] A. Klümper and K. Sakai, J. Phys. A 35 (2002) 2173; K. Sakai and A. Klümper, J. Phys. A 36 (2003) 11617.

[6] F. Heidrich-Meisner, A. Honecker, D.C. Cabra, and W. Brenig, Phys. Rev. B 66 (2002) 140406(R); Phys. Rev. Lett 92 (2004) 069703; J. Mag. Mag. Mat. 272-276 (2004) 890-891.

[7] F. Heidrich-Meisner A. Honecker, and W. Brenig, in preparation.

[8] J. V. Alvarez and C. Gros, Phys. Rev. Lett. 89 (2002) 156603; C. Gros and J. V. Alvarez, Phys. Rev. Lett. 92 (2004) 069704.

[9] E. Orignac, R. Chitra, and R. Citro, Phys. Rev. B 67 (2003) 134426.

[10] K. Saito, Phys. Rev. B 67 (2003) 064410.

[11] E. Shimshoni, N. Andrei, and A. Rosch, Phys. Rev. B 68 (2003) 104401.

[12] X. Zotos, Phys. Rev. Lett. 92 (2004) 067202.

[13] G. D. Mahan, *Many-Particle Physics*, Plenum Press, New York, 1990.