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

\[
\text{Re} \kappa(\omega) = D_{th}(T)\delta(\omega) + \kappa_{\text{reg}}(\omega).
\]

Here, \( \kappa \) denotes the thermal conductivity, \( D_{th} \) is the thermal Drude weight, \( T \) is the temperature, and \( \delta(\omega) \) is the \( \delta \)-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

\[
H = \sum_{l=1}^{N} h_l = J \sum_{l=1}^{N} [S_l \cdot S_{l+1} + \alpha S_l \cdot S_{l+2}].
\]

\( h_l \) is the local energy density; \( S_l \) is a spin-1/2 operator acting on site \( l \). \( N \) denotes the number of sites and periodic boundary conditions are imposed. \( \alpha J \) 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 \( -\partial_t h_l = \text{div} j_{th,l} \) is fulfilled

\[
j_{th} = i \sum_{l=1}^{N} j_{th,l} = i \sum_{l=1}^{N} \sum_{r,s=0}^{1} [h_{l-r-1}, h_{l+s}].
\]

Following linear-response theory, the thermal conductivity can be written as [13]
presented in Fig. 1. Panel (a) contains the regular part of Re\(\kappa(\omega)\) vs \(\omega\) for \(T/J = 1.2\) for \(N = 18\) and \(N = 20\) sites. Panel (b) integrated weight \(I(\omega)\) vs \(\omega\) for various temperatures. Inset of (b): \(T^2\cdot I_0\) vs temperature \(T\).

\[
\kappa_{\text{reg}}(\omega) = \frac{\pi g(\omega)}{N^2 T} \sum_{E_n \neq E_m} p_n |\langle m|\hat{j}_{\text{hh}}|n\rangle|^2 \delta(\omega - \Delta E) \tag{4}
\]

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 Re\(\kappa(\omega)\) over frequency \(\omega\)

\[
I(\omega) = D_{1\text{h}}(T) + 2 \int_0^\omega d\omega' \kappa_{\text{reg}}(\omega'); \quad I_0 = \lim_{\omega \to \infty} I(\omega). \tag{5}
\]

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 \(S\).

Let us now turn to the discussion of the results presented in Fig. 1. Panel (a) contains the regular part \(\kappa_{\text{reg}}(\omega)\) for \(T/J = 1.2\) and \(N = 18\) and \(N = 20\). In this plot, \(\kappa_{\text{reg}}(\omega)\) has been binned with \(\Delta E/J \approx 10^{-2}\).

First, note that \(\kappa_{\text{reg}}(\omega)\) is a structureless function of frequency \(\omega\). 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 \(\kappa_{\text{reg}}(\omega)\) 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 \(I_0\).

References


