Thermal transport properties of disordered spin-1/2 systems

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Abstract

This work studies heat transport of bond-disordered spin-1/2 chains. As an example, the XX case is analyzed, which corresponds to a model of noninteracting spinless fermions. Within the fermion representation, the single-particle eigenenergies are determined numerically, which allow one to compute transport coefficients. Since the ballistic transport properties of a clean chain are destroyed by disorder, the focus is on the frequency dependence of the thermal conductivity and on a qualitative comparison with the spin conductivity, both at finite temperatures.

Key words: Quantum spin systems, Transport properties, Disorder

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Motivated by recent experiments on transport properties of transition metal oxides [1], intense theoretical work has recently been devoted to the study of heat conduction in one-dimensional spin-1/2 systems such as the Heisenberg chain, frustrated chains, and spin ladders [2]. Among these systems, the anisotropic spin-1/2 chain exhibits ballistic thermal transport properties at all temperatures \(T\) due to its integrability [3]. The thermal conductivity diverges in the homogeneous case, signaled by a finite thermal Drude weight [4]. Here, the usual decomposition of the real part of the thermal conductivity \(\kappa\) into the Drude weight \(D_{\text{th}}\) and the regular part is utilized: \(\text{Re} \kappa(\omega) = D_{\text{th}} \delta(\omega) + \kappa_{\text{reg}}(\omega)\), \(\omega\) being the frequency. Ballistic transport is expected to be destroyed by randomness in the exchange couplings, resulting in a vanishing Drude weight. Therefore, one is interested in the regular part \(\kappa_{\text{reg}}(\omega)\), from which the dc-conductivity can be extracted by extrapolating to \(\omega = 0\).

In this contribution, the effect of bond disorder on the thermal conductivity of XX chains is studied numerically. This limiting case of the anisotropic spin-1/2 chain corresponds to free spinless fermions by means of a Jordan-Wigner transformation [5]. While particle transport in disordered fermion systems is a long-studied problem, closely related to the subject of localization (see, e.g., Ref. [6]), the thermal conductivity \(\kappa\) in these models has attracted less attention. Using bosonization, predictions were made for the concentration dependence of the thermal conductivity of spin-1/2 chains [7], and it could be very interesting to compare this to numerical results. Here, results for the frequency dependence of \(\kappa\) are presented for the case of off-diagonal disorder at finite temperatures.

The Hamiltonian in terms of spin-1/2 operators \(S_i^±, z\) acting on site \(i\) and with periodic boundary conditions (PBC) reads:

\[
H = \frac{1}{2} \sum_{i=1}^{N} J_i (S_i^+ S_{i+1}^- + h.c.),
\]

where \(N\) is the number of sites. It can equivalently be written in terms of fermionic operators \(c_i^\dagger\):

\[
H = \frac{1}{2} \sum_{i=1}^{N} J_i (c_i^\dagger c_{i+1} + h.c.).
\]
In principle, a subtlety arises since the PBCs for the spin operators give rise to a nontrivial boundary term for the fermions, which depends on the number $N$ of fermions [8]. This dependence, however, is neglected here, and PBC are imposed for all $N$, since boundary effects can be expected to vanish for large system sizes.

Introducing a spinor $\psi = (c_1^\dagger, \ldots, c_N^\dagger)$, the Hamiltonian can be written as $H = \psi^\dagger \mathcal{A} \psi$, where $\mathcal{A}$ is a symmetric $N \times N$ band matrix, with nonzero elements $A_{i,i+1} = J_i/2$ and $A_{i,N} = J_i/2$. Randomness in the $J_i$ is therefore called off-diagonal disorder, while a spatially varying magnetic field realizes diagonal disorder.

While a transformation to momentum space diagonalizes $H$ for the translationally invariant case ($J_i = J$), the computation of single-particle eigenvalues is still straightforward for random couplings (see, e.g., [8]). By means of a unitary transformation $U$ with $c_i = \sum_{\mu} U_{i\mu} \eta_\mu$ that diagonalizes the matrix $\mathcal{A}$, the Hamiltonian can be written as $H = \sum_{\mu} \epsilon_\mu \eta_\mu^\dagger \eta_\mu$, where $\epsilon_\mu$ are the single-particle eigenvalues.

The energy current operator corresponding to Eq. (2) is $J = (i/4) \sum_i (c_i^\dagger c_{i+1} - h.c.) = i \sum_{\mu}\eta_{\mu}^\dagger J_{\mu\nu} \eta_{\nu}$. Within linear response theory, $\kappa_{\text{reg}}(\omega)$ is given by [6]:

$$\kappa_{\text{reg}}(\omega) = \frac{\beta}{\omega} \sum_{\epsilon_\mu \neq \epsilon_\nu} |J_{\mu\nu}|^2 \left[ f(\epsilon_\mu) - f(\epsilon_\nu) \right] \delta(\omega - \Delta \epsilon), \quad (3)$$

where $f(\epsilon) = 1/(\exp(\beta \epsilon) + 1)$ denotes the Fermi-function, $\beta = 1/T$, and $\Delta \epsilon = \epsilon_\mu - \epsilon_\nu$.

As an example, a Gaussian distribution of random couplings is considered: $P(J_i) \propto e^{-(J_i-J)^2/w^2}$, with $J = 1$ and $w = 0.2$. The choice of the distribution does not affect the results, quantitatively consistent results for $\kappa(\omega)$ are obtained with other $P$ (e.g. box or binary distribution) by fixing the first moments of the distribution function. Figure 1 shows results for $\kappa_{\text{reg}}(\omega)$ [panel(b)] and, for comparison, $\sigma_{\text{reg}}(\omega)$ [panel(a)], which is the spin conductivity corresponding to the current operator $J = (i/2) \sum_i (c_i^\dagger c_{i+1} - h.c.)$. The parameters are $T/J = 0.5$ and $N = 1000, 5000$. An imaginary broadening of $10^{-4}$ was used. The overall form of both quantities is quite similar and resembles that known for $\sigma_{\text{reg}}(\omega)$ [9]. Moreover, both curves exhibit a maximum at roughly the same frequency ($\omega/J \approx 0.015$ for the parameters of Fig. 1). Both finite-size effects and statistical fluctuations are small in the low-frequency limit.

The behavior of $\kappa_{\text{reg}}(\omega)$ at low frequencies is of particular interest as it determines the dc-conductivity (see Refs. [10] for the case of clean spin systems). While the Drude weights vanish in the presence of disorder, the results of this work indicate finite dc-conductivities for both spin and thermal transport at finite temperatures. This is illustrated in the inset of Fig. 1. A more detailed analysis of the finite-size scaling as well as the temperature dependence will be presented elsewhere.

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