

Finite-temperature transport in disordered Heisenberg chains

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Using numerical diagonalization techniques, we explore the effect of local and bond disorder on the finite-temperature spin and thermal conductivities of the one-dimensional anisotropic spin-1/2 Heisenberg model. High-temperature results for local disorder show that the dc conductivities are finite, apart from the uncorrelated XY case where dc transport vanishes. Moreover, at strong disorder, we find finite dc conductivities at all temperatures T except at $T=0$. The low-frequency conductivities are characterized by a nonanalytic cusp shape. Similar behavior is found for bond disorder.

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The effect of correlations on localized states in disordered system¹ is a long standing problem² that is attracting renewed theoretical and experimental interests.³⁻⁷ While it is clear that in a one-dimensional (1D) noninteracting disordered system all states are localized, the introduction of correlations might lead to different possible scenario. First, at zero temperature, $T=0$, numerical results for fermions with repulsive interaction in a disordered system reveal that localization persists in spite of correlations,^{8,9} although some types of interactions might destroy the localized states leading the system to a normal diffusive state or even one with diverging low-frequency conductivity.¹⁰ Even if the system remains localized at $T=0$, an arbitrary low temperature could delocalize it or a finite critical temperature^{4,5} might be needed to drive it to a normal state at high temperatures. There are also indications that in the presence of large disorder even at high T many-body states can appear effectively localized.^{6,11}

To explore this issue, the 1D (in general) anisotropic spin-1/2 Heisenberg chain is a minimal model that allows us to investigate the interplay of disorder and correlations on transport. In the XY limit, mapped by the Jordan-Wigner transformation to a system of noninteracting spinless fermions,¹² it is expected to have all single-particle states localized under any amount of local or bond disorder consistent with the Anderson localization phenomenon.¹ The spin (in fermionic representation equivalent to charge) conductivity as well as the thermal dc conductivities are expected to vanish at all T , while ac conductivities are finite but nontrivial.¹³

Without disorder, the anisotropic XXZ model is a strongly correlated spin system, with nearest-neighbor interaction in the fermion picture. It is integrable using the Bethe ansatz method for any value of the anisotropy and it is known to show ideal spin/charge (in the easy-plane case) and thermal (for any anisotropy) conductivities at all temperatures.¹⁴

Besides the theoretical interest of this model quasi-1D magnetic compounds have recently been synthesized which are described exceedingly well by the 1D isotropic spin-1/2 Heisenberg model and show unusually high thermal conductivity due to a magnetic transport mode contribution.¹⁵ Rel-

evant to this work, experiments are underway to study the effect of disorder by nonmagnetic as well as magnetic impurities.

In this work, we will use state of the art numerical diagonalization techniques—the exact diagonalization (ED), the finite-temperature Lanczos method (FTLM) (Ref. 16), and the microcanonical Lanczos method (MCLM) (Ref. 17)—to see what they can offer to this issue of disorder and correlations. While we will study the spin and thermal conductivity of the spin-1/2 anisotropic Heisenberg model, the spin conductivity maps directly to that of the charge conductivity of a spinless fermion model.

We first consider the 1D anisotropic spin-1/2 Heisenberg model in the presence of a random local magnetic field,

$$H = \sum_l J(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) + \sum_l b_l S_l^z, \quad (1)$$

where S^α , $\alpha=x, y, z$ are spin-1/2 operators, J is the magnetic exchange coupling, Δ is the anisotropy parameter, and $-W/2 < b_l < +W/2$ are random local fields from a uniform distribution. We assume periodic boundary conditions, $\hbar = \kappa_B = 1$, and take J as the unit of energy.

Our analysis will be based on standard linear-response theory. The spin conductivity is given by

$$\sigma(\omega) = \frac{1}{\omega L} \Im \int_0^{+\infty} dt e^{izt} \langle [j(t), j] \rangle, \quad (2)$$

$$j = \sum_l j_{l,l+1} = J \sum_l (S_l^x S_{l+1}^y - S_l^y S_{l+1}^x)$$

with j representing the spin current. The corresponding thermal conductivity is given by

$$\kappa(\omega) = \frac{\beta}{\omega L} \Im \int_0^{+\infty} dt e^{izt} \langle [j^\epsilon(t), j^\epsilon] \rangle, \quad (3)$$

where $\beta=1/T$. The energy current j^ϵ in an inhomogeneous system can be defined via the dipole operator as¹⁸

$$P^\epsilon = \sum_l r_l h_l, \quad j^\epsilon = i \sum_{lm} r_l [h_m, h_l], \quad (4)$$

whereby h_l are local energy operators and r_l are the corresponding coordinates. Taking into account that locations of local-field energies are on sites and exchange energies on bonds, respectively, one arrives at

$$j^\epsilon = J^2 \sum_l j_l^\epsilon + \frac{b_l + b_{l+1}}{2} j_{l,l+1},$$

$$j_l^\epsilon = (S_{l+1}^x S_l^y S_{l-1}^y - S_{l+1}^y S_l^x S_{l-1}^x) + \Delta(x \rightarrow y, z; y \rightarrow z, x; z \rightarrow x, y). \quad (5)$$

For vanishing random fields, $W=0$, the energy current j^ϵ commutes with the Hamiltonian for all values of the anisotropy Δ and thus the system is an ideal thermal conductor¹⁴ at all T . It has also been shown that the uniform, $W=0$, system exhibits ballistic spin transport in the XY regime, $\Delta < 1$, at all temperatures although j does not commute with H .¹⁹

Let us start the analysis with the high- T limit, $T \rightarrow \infty$, which exhibits nontrivial $\sigma(\omega)$ and $\kappa(\omega)$, being in fact quite generic for all $T > 0$. The difference between spin and thermal transport can be realized already from the spin $M_n^s = \int \omega^n \sigma(\omega) d\omega = \pi \beta m_n^s$ and corresponding energy $M_n^\epsilon = \pi \beta^2 m_n^\epsilon$ frequency moments. Moments can be evaluated analytically at $T \rightarrow \infty$, e.g., $m_0^s = \langle jj \rangle / L$, $m_2^s = \langle [H, j][H, j] \rangle / L$, etc. One gets $m_0^s = J^2/8$ and

$$m_2^s = \frac{J^2}{16} [J^2 \Delta^2 + 4 \langle b^2 \rangle],$$

$$m_0^\epsilon = \frac{J^2}{32} [(1 + 2\Delta^2)J^2 + 2 \langle b^2 \rangle],$$

$$m_2^\epsilon = \frac{J^4}{64} (3 + 10\Delta^2) \langle b^2 \rangle + \frac{J^2}{16} (\langle b^4 \rangle - \langle b^2 \rangle^2), \quad (6)$$

where $\langle b^2 \rangle = W^2/12$ and $\langle b^4 \rangle = W^4/80$. Equation (6) reveals the difference between spin and thermal transport since the finite dispersion $\delta^\epsilon = \sqrt{m_2^\epsilon / m_0^\epsilon}$ of $\kappa(\omega)$ is induced solely by $W > 0$ whereas $\delta^s = \sqrt{m_2^s / m_0^s}$ remains finite even for $W=0$.

Although the lowest-frequency moments can serve as a reference, they are insufficient to reveal the most challenging $\omega \rightarrow 0$ behavior. For the latter we have to rely on numerical calculations. The most favorable case for simulations on a finite-size lattice is the strong disorder limit where we expect the localization length ξ to be shortest. In the following we consider $W=2$, where an estimate of $T=0$ localization length ξ exists in the literature,⁹ which suggests that ξ is less than ten sites in the cases we are studying.

In Figs. 1 and 2 we present results for $\sigma(\omega)$ and $\kappa(\omega)$, respectively. The data for $L=14$, with a Hilbert-space dimension of 3432 states in the $S^z=0$ subsector, were obtained by exact (full) diagonalization. The δ peaks at the excitation frequencies are binned in windows $\delta\omega=0.01$, which also gives the frequency resolution of the spectra. There is an average over $N_r=10$ random-field configurations. For L

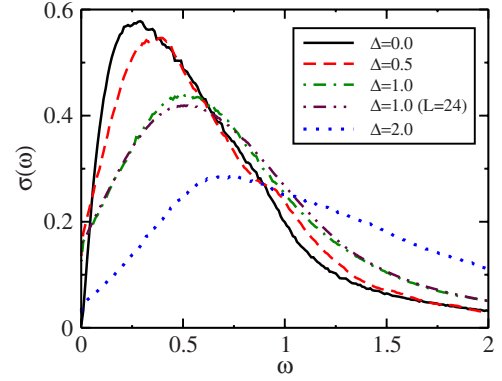


FIG. 1. (Color online) Dynamical spin conductivity $\sigma(\omega)$ at $T \rightarrow \infty$ for local disorder $W=2$ and various Δ (curves normalized to unity) evaluated via ED ($L=14$) and for $\Delta=1$ also via MCLM ($L=24$).

= 16–24 the MCLM (Ref. 17) is used, which is particularly suitable for high $T (\gg J)$, with typically 2000 Lanczos steps and random-configuration sampling $N_r > 100$. In the same plots, we show the noninteracting case for $L=1000$ and averaging $N_r=1000$, where we expect the dc conductivities $\sigma_{dc} = \sigma(\omega \rightarrow 0)$ and $\kappa_{dc} = \kappa(\omega \rightarrow 0)$ to vanish. All the spectra are normalized to a unit integral.

Data for various sizes L indicate a convergence of the finite-size effects at moderate sizes $L > 16$ (at least for $\Delta > 0.5$) for the chosen rather strong disorder $W=2$. In particular, we show in Fig. 1 the comparison of $L=14$ and $L=24$ results for $\Delta=1$. In Fig. 2, for the same parameters, the curves are also nearly indistinguishable for L between 14 and 24 sites.

These results clearly reveal that apart from the XY limit, $\Delta=0$, the system is conducting, i.e., both spin σ_{dc} and thermal κ_{dc} dc conductivities are finite. Nevertheless, due to the large disorder W the dynamics is non-Drude type since the maximum of $\sigma(\omega)$ as well as of $\kappa(\omega)$ appears at a finite $\omega^* > 0$, in analogy with the localization at $\Delta=0$. Hence, at $\Delta > 0$ and large W we are dealing with pseudolocalized dynamics.^{6,11} Another feature of this regime appears to be a generic (nonanalytic) cusplike behavior at low frequencies, $\sigma(\omega) \simeq \sigma_{dc} + \alpha|\omega|$ and $\kappa(\omega) \simeq \kappa_{dc} + \gamma|\omega|$, for which so far we

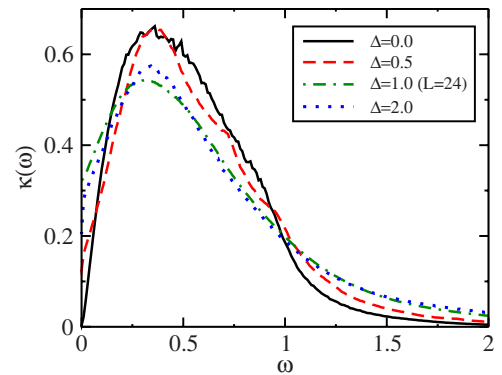


FIG. 2. (Color online) Dynamical thermal conductivity $\kappa(\omega)$ at $T \rightarrow \infty$ for $W=2$ and various Δ (curves normalized to unity) evaluated via ED ($L=14$) and MCLM ($L=24$).

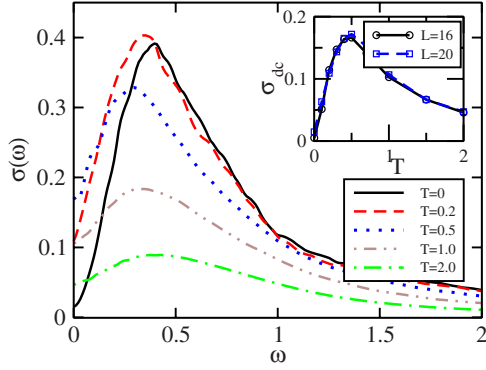


FIG. 3. (Color online) Spin conductivity $\sigma(\omega)$ for $\Delta=1$ and $W=2$ for various T .

cannot offer an analysis. It might be attributed to long-time tail effects although, in such a case, the low-frequency drop of the conductivity was found to be only a few percent²⁰ and not by an order of magnitude as in our case. Such a frequency dependence is strongly reminiscent of the behavior in strongly disordered two-dimensional (2D) system as has been analyzed theoretically and observed experimentally.²¹

Apart from a qualitative similarity between $\sigma(\omega)$ and $\kappa(\omega)$ in Figs. 1 and 2 there are also some differences. $\sigma(\omega)$ is more sensitive to Δ , as it is already evident from the moments [Eqs. (6)] and the corresponding \mathcal{S} . They originate from the fact that even at $W=0$ $\sigma(\omega \rightarrow 0)$ changes qualitatively at $\Delta=1$, not being the case for $\kappa(\omega \rightarrow 0)$.¹⁴

As our numerical simulations indicate, a similar qualitative behavior persists by decreasing the disorder to $W=1.0$ (not shown). With decreasing W the pseudolocalized form gives way to a more Drude-type form with $\omega^* \rightarrow 0$ and strongly increased σ_{dc} and κ_{dc} . However, reducing the disorder further we are running to long localization lengths (for $\Delta=0$) and in general less controllable finite-size effects preventing reliable conclusions.

The next issue is the temperature dependence of the dynamical (in particular dc) conductivity and the eventual existence of a critical temperature T_c below which the system becomes insulating.^{4,5} To study this question we employed the ED method for $L=14$ (using $N_r=10$) and the FTLM for $L=16-20$ with 200–400 Lanczos steps for high-frequency resolution and $N_r \sim 100$. The results are qualitatively similar whereby the FTLM, properly interpolating between the $T=0$ (ground-state) Lanczos method and $T>0$ behavior, is more reliable for small $T<0.5$ due to larger L and denser low-energy spectra. Results for $\sigma(\omega)$ and $\kappa(\omega)$ in the isotropic case $\Delta=1$ and at fixed $W=2$ are shown in Figs. 3 and 4 for various $T=0-2$ and $L=20$ (being essentially equal to the results obtained for $L=16$). The data again indicate that σ_{dc} and κ_{dc} remain finite at all $T>0$ and vanish only at $T=0$. A rather abrupt drop of σ_{dc} appears at $T \sim 0.1$ which is however in the range of finite-size temperature T_{fs} (for available $L=20$) below which the FTLM results are not to be trusted.¹⁶ These data suggest a zero critical temperature of localization-delocalization transition, although of course we cannot exclude an exponentially small one, which is beyond the reach of actual numerical simulations.

In connection with existing 1D magnetic compounds¹⁵

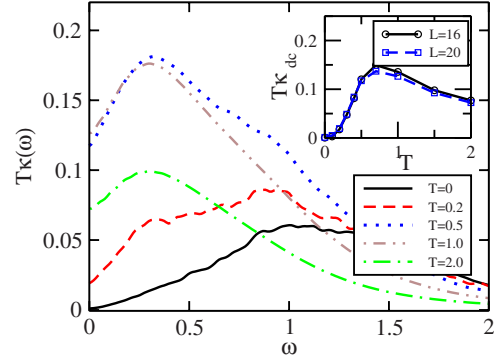


FIG. 4. (Color online) Thermal conductivity $\kappa(\omega)$ for $\Delta=1$ and $W=2$ for various T .

more relevant appears to be the spin-1/2 (anisotropic) Hamiltonian with bond disorder, i.e., disorder in exchange couplings,

$$H = \sum_l J_{l,l+1} (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z), \quad (7)$$

where $J_{l,l+1} = J(1 - s_{l,l+1})$ and we assume $-W/2 < s_{l,l+1} < W/2$ uniformly distributed random numbers. Such disorder can be induced, e.g., by coupling to static lattice displacements.²² The local spin current is now $j_{l,l+1} = J_{l,l+1} (S_l^x S_{l+1}^y - S_l^y S_{l+1}^x)$ while the energy current is given by

$$j^\epsilon = \sum_l J_{l-1,l} J_{l,l+1} j_l^\epsilon. \quad (8)$$

An open question is whether a 1D spin chain with bond disorder¹⁰ behaves qualitatively different to the site disorder discussed above. Our results indicate that it is not the case.

In Figs. 5 and 6 we present $T \rightarrow \infty$ results for $\sigma(\omega)$ as well as $\kappa(\omega)$ for $\Delta=1$ and different bond disorder strengths $W=0.5, 1, 1.5$. Results were obtained using the MCLM method on $L=20$ sites. Results for larger $W=1, 1.5$ are well converged with size and clearly indicate that we are again dealing with finite dc limits $\sigma_{dc} > 0$ and $\kappa_{dc} > 0$. With respect to the site disorder case in Figs. 1 and 2 there are similarities and also differences as follows: (a) for bond disorder we are restricted to $W < 2$ to have a meaningful model without a possibility of a broken bond, (b) the pseudolocalization is

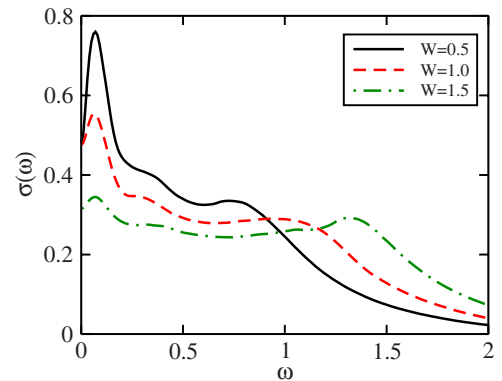


FIG. 5. (Color online) $T \rightarrow \infty$ results for $\sigma(\omega)$ and for $\Delta=1$ and different disorder W (curves are normalized).

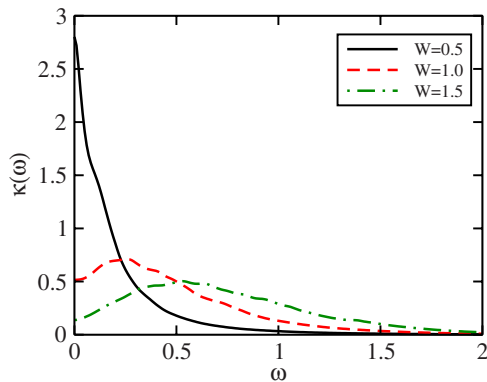


FIG. 6. (Color online) $T \rightarrow \infty$ results for $\kappa(\omega)$ for $\Delta=1$ and different W (curves are normalized).

less pronounced at least for $\sigma(\omega)$ and shows up only closer to $W=2$, e.g., for $\kappa(\omega)$ at $W=1.5$, (c) $\kappa(\omega)$ in Fig. 6 reveals a quite abrupt crossover with disorder strength from a Drude-type response (at $W=0.5$) to a localized-like one with $\omega^* > 0$ at $W=1.0$, and (d) at least for $\sigma(\omega)$ two energy scales are evident in Fig. 5 which are not present in the random-field case.

In conclusion, our results of numerical simulations on the interplay of disorder and correlations in the spin and thermal transport within Heisenberg spin chains can be summarized

by the following scenario: (a) finite random-field disorder $W > 0$ induces localization and vanishing dc transport at any T in the XY limit, corresponding to noninteracting fermions,¹ and as well generally at $T=0$ (Refs. 8 and 9) (for $\Delta > 0$ considered here); (b) apart from the latter two limits the system appears to behave as a normal conductor with finite $\sigma_{dc} > 0$ and $\kappa_{dc} > 0$ both for various $\Delta > 0$ and $T > 0$; in particular, we do not find any evidence for a phase transition by varying T or W ; (c) dynamical transport (at least for larger disorder) reveals a generic cusplike nonanalytic behavior for ω , analogous to long-time tails in classical dynamical systems in low-dimensional²³ or 2D strongly disordered systems; (d) with increasing disorder the system reveals a crossover from the Drude-type to a pseudolocalized dynamics with very low dc σ_{dc} and κ_{dc} (Ref. 11); and (e) similar conclusions seem to hold for the bond disorder.

Clearly, several caveats are in order. The considered cases mostly correspond to substantial disorder, where the finite-size effects are well under control and results converged within available L , at least for $T > T_{fs}$ and not too small $\Delta > 0$. Also, numerical results cannot exclude the localization on a very long scale $\xi \gg L$ although we do not find any signature of such a development.

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