Heat Conductivity of the Heisenberg Spin-1/2 Ladder: From Weak to Strong Breaking of Integrability

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We investigate the heat conductivity \( \kappa \) of the Heisenberg spin-1/2 ladder at finite temperature covering the entire range of inter-chain coupling \( J_\perp \), by using several numerical methods and perturbation theory within the framework of linear response. We unveil that a perturbative prediction \( \kappa \propto J_\perp^{-2} \), based on simple golden-rule arguments and valid in the strict limit \( J_\perp \to 0 \), applies to a remarkably wide range of \( J_\perp \), qualitatively and quantitatively. In the large \( J_\perp \)-limit, we show power-law scaling of opposite nature, namely, \( \kappa \propto J_\perp^2 \). Moreover, we demonstrate the weak and strong coupling regimes to be connected by a broad minimum, slightly below the isotropic point at \( J_\perp = J_\parallel \). As a function of temperature \( T \), this minimum scales as \( \kappa \propto T^{-2} \) down to \( T \) on the order of the exchange coupling constant. These results provide for a comprehensive picture of \( \kappa(J_\perp,T) \) of spin ladders.

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Introduction. Thermodynamic properties of quantum many-body systems are well understood, particularly in the vicinity of integrable points [1]. In contrast, the vast majority of dynamical questions in these systems remain a challenge to theoretical and experimental physics as well, in the entire range from weak to strong breaking of integrability. These questions consist of several timely and important issues such as eigenstate thermalization [2,3] in cold atomic gases and, as studied in this Letter, quantum transport and relaxation in condensed-matter materials. In this context, a fundamental system is the one-dimensional (1D) spin-1/2 Heisenberg model. It is relevant to the physics of quasi-1D quantum magnets [4,5], cold atoms in optical lattices [6,7], and nanostructures [8], as well as to physical situations in a much broader context [6,8].

As typical for integrable systems, the energy current in the spin-1/2 Heisenberg chain is a strictly conserved quantity [9,10]. This strict conservation implies purely ballistic flow of heat at any temperature and provides the theoretical basis for explaining the colossal magnetic heat conduction observed experimentally in quasi-1D cuprates [11,12]. In contrast to heat flow, the dynamics of spin, including the existence of ballistic [13,21] and diffusive transport channels [28,33], is theoretically resolved only partially, and also under ongoing experimental scrutiny [34,38].

Because of strict energy-current conservation in this model, the heat conductivity \( \kappa \) is highly susceptible to breaking of integrability by, e.g., spin-phonon coupling [39,41], dimerization or disorder [42,44], and interactions between further neighbors [43,45]. One of the most important perturbations is inter-chain coupling, i.e. \( J_\perp \), which is the key ingredient to spin-ladder compounds [11,12]. Early on, perturbation theory (PT) to lowest order, i.e., a simple golden-rule argument [47,48], has suggested dissipative heat flow with a scaling \( \kappa \propto J_\perp^{-2} \), as illustrated on the l.h.s. of Fig. 1. However, the relevance of such scaling is unclear off the strict limit \( J_\perp \to 0 \), as is the radius of convergence of the PT. Understanding \( \kappa \) over a wider range of \( J_\perp \) has been hampered by the lack of sufficiently accurate nonperturbative methods. In particular, state-of-the-art numerical methods have been restricted to the regime \( J_\perp = \mathcal{O}(1) \), where finite-size effects are moderate and spectral structures are broad, i.e., time scales are short [49]. Thus, heat transport in the transition from weakly coupled chains to strongly coupled ladders is understood only in few and narrow regions.

In this Letter, we lift these restrictions and study the

![FIG. 1. (Color online) Thermal conductivity \( \kappa \) (per chain) versus \( J_\perp/J_\parallel \) and \( \beta \). PT: known perturbative regime. Issues clarified in this Letter: extent of power-law scaling (dashed line) close to PT and sum-rule (SR) regimes, nonperturbative numerical treatment for entire \( J_\perp \)-range, location of minimal conductivity, and variation with temperature.](image-url)
heat conductivity $\kappa$ over the entire range of the inter-chain coupling $J_\perp$. Using several methods within the framework of linear response theory, we (a) quantitatively connect to PT in the small-$J_\perp$ limit and (b) unveil its validity for a remarkably wide range of $J_\perp$. In addition to the PT, scaling as $\kappa \propto J_\perp^{-2}$, we (c) demonstrate a qualitatively different power-law scaling $\kappa \propto J_\perp^\alpha$ in the large $J_\perp$-limit. As a consequence, we (d) find a broad minimum of $\kappa$ in the region $J_\perp \lesssim 1$. This minimum (e) scales as $\kappa \propto T^{-2}$ down to temperatures $T$ on the order of the exchange coupling constant. Thus, we are able to provide a comprehensive picture of $\kappa(J_\perp, T)$, beyond the known results sketched as part of Fig. 1.

**Ladder and Energy Current.** We study the dynamics of the energy current in a Heisenberg spin-1/2 ladder of length $N/2$ with periodic boundary conditions, where $N$ is the total number of sites. The full Hamiltonian reads $H = H_\parallel + H_\perp$ and consists of a leg part $H_\parallel$ and a rung part $H_\perp$, given by ($\hbar = 1$)

$$H_\parallel = J_\parallel \sum_{k=1}^{N/2} \sum_{i=1}^{\left\lfloor \frac{N}{2} \right\rfloor} S_{i,k} \cdot S_{i+1,k}, \quad H_\perp = J_\perp \sum_{i=1}^{N/2} S_{i,1} \cdot S_{i,2}, \quad (1)$$

where $S_{i,k}$ are spin-1/2 operators at site $(i,k)$, $J_\parallel > 0$ is the antiferromagnetic exchange coupling constant along the legs, and $J_\perp > 0$ is the rung-interaction. $z = 2$ is the number of legs. For $J_\perp = 0$, the ladder splits into two integrable chains and, for $J_\parallel = 0$, it simplifies to a set of uncoupled dimers. In the case of $J_\perp \neq 0$ and $J_\parallel \neq 0$, the ladder is nonintegrable. Generally, the model in Eq. (1) preserves the total magnetization $S^z$ and is translationally invariant due to periodic boundary conditions. While we focus on the $S^z = 0$ sector (canonical ensemble) to reduce computational effort, all results presented in this Letter do not depend on this specific choice, as demonstrated later in detail.

The energy current directly follows from the continuity equation once the local energy density is defined. Using a spatially symmetric definition for this density $49$, the energy current has the well-known form $j = j_\parallel + j_\perp$,

$$j_\parallel = J_\parallel^2 \sum_{k=1}^{z} \sum_{i=1}^{\left\lfloor \frac{N}{2} \right\rfloor} S_{i-1,k} \cdot (S_{i,k} \times S_{i+1,k}), \quad (2)$$

$$j_\perp = \frac{J_\perp}{2} \sum_{k=1}^{z} \sum_{i=1}^{\left\lfloor \frac{N}{2} \right\rfloor} (S_{i-1,k} - S_{i+1,k}) \cdot (S_{i,k} \times S_{i,3-k}), \quad (3)$$

where $j_\parallel$ and $j_\perp$ represent the contributions arising from the legs and rungs, respectively. $j$ and $H$ commute only at the integrable point $J_\perp = 0$. Within linear response theory, we investigate the autocorrelation function at the inverse temperatures $\beta = 1/T$ ($k_B = 1$),

$$C(t) = \text{Re} \left( \frac{i(t)j(t)}{N} \right) = \text{Re} \left( \frac{\text{Tr}\{e^{-\beta H}j(t)j\}}{N \text{Tr}\{e^{-\beta H}\}} \right), \quad (3)$$

where the time argument of $j(t)$ refers to the Heisenberg picture, $j = j(0)$, and $C(0) = 3(J_\parallel^2 + J_\perp^2 J_\perp^2/2)/32$ in the high-temperature limit $\beta J_\parallel \to 0$.

From $C(t)$, we first determine the Fourier transform $C(\omega)$ and then the conductivity via the low-frequency limit $\kappa/\omega = \beta^2 C(\omega \to 0)$. Additionally, we can extract the conductivity directly by $\kappa/\omega = \beta^2 \int_0^\infty dt C(t)$. Here, the cut-off time $t_1$ has to be chosen much larger than the relaxation time $\tau$, where $C(\tau)/C(0) = 1/e$.

**Methods.** We calculate $C$ by complementary numerical methods, with a particular focus on dynamical quantum typicality (DQT) $23, 26, 51$ [see also Refs. $52, 60$ for typicality]. DQT is most conveniently formulated in the time domain and relies on the relation

$$C(t) = \text{Re} \left( \frac{\Phi_\beta(t)|j\varphi_\beta(t)\rangle}{N \langle \varphi_\beta(0)|\Phi_\beta(0)\rangle} + \epsilon, \quad (4)$$

where $\varphi_\beta(t) = e^{-iHt-\beta H/2} |\varphi\rangle$, $|\varphi_\beta(t)\rangle = e^{-iHt} j \epsilon e^{-\beta H/2} |\psi\rangle$, where $|\psi\rangle$ is a single pure state drawn at random and $\epsilon$ scales inversely with the partition function, i.e., $\epsilon$ is exponentially small in the number of thermally occupied eigenstates $23, 26, 51$. The great advantage of Eq. (4) is that it can be calculated without any diagonalization by the use of forward-iterator algorithms. In this Letter, we use a fourth-order Runge-Kutta iterator with a discrete time step $\delta t J_\parallel = 0.01 \ll 1$. Using this iterator, together with sparse-matrix representations of operators, we can reach systems sizes as large as $N = 32$. For more details on the method, see Ref. $26$.

In addition, we confirm our DQT results with numerical methods based on Lanczos diagonalization $63$. Results of the latter are typically given in the frequency domain, with the frequency resolution $\delta \omega$ crucially depending on the number of Lanczos steps $M$, $\delta \omega \propto 1/M$. At low temperatures, where physics is dominated by a small number of low-lying eigenstates, we choose the finite-temperature Lanczos method (FTLM) with $M \sim 200$. At high temperatures $\beta J_\parallel \to 0$, we also use the micro-canonical Lanczos method (MCLM) with $M \sim 2000$, significantly improving $\delta \omega$.

**Results.** We begin with strong rung exchange couplings $J_\perp/J_\parallel \geq 1$ and high temperatures $\beta J_\parallel \to 0$. In Fig. 2(a) we summarize our DQT results on the time-dependent energy-current autocorrelation function $C(t)$ for different $J_\perp/J_\parallel = 1, 1.5, 2$ in the sector $S^z = 0$. Several comments are in order. First, the initial value $C(0)$ agrees with the high-temperature sum rule and therefore increases with $J_\perp$. Second, all $C(t)$ depicted decay to zero on a time scale $5\tau \sim 10/J_\parallel$. Third, the $C(t)$ curves do not change when the number of sites is increased from $N = 22$ to $N = 32$. Thus, we observe very little finite-size effects, i.e., we can safely consider our results as results on $C(t)$ in the thermodynamic limit $N \to \infty$. Note that for the largest system sizes $N \geq 30$ we restrict ourselves to a single translation subspace $k$ since, for these $N$, $C(t)$ is independent of $k$ at high temperatures $23, 26$. 


Next, we discuss the spectrum $C(\omega)$. To this end, we show in Fig. 2 for $J_{\perp}/J_{\parallel} = 1.2$ the Fourier transform of our DQT data for times $t \leq 10\tau \sim 20/J_{\parallel}$. These times correspond to a frequency resolution $\delta \omega \sim 0.15 J_{\parallel}$. Apparently, for this resolution, the Fourier transform is a smooth function of $\omega$ and displays a well-behaved limit for $\omega \to 0$, i.e., $C(\omega \to 0) = C(\omega = 0)$. Moreover, this limit and $C(\omega)$ in general do not depend on system size for $N \geq 22$. The inset of Fig. 2 clarifies the impact of the $\omega$ resolution by displaying additional Fourier transforms of DQT data, evaluated for shorter ($t \leq 5\tau$) and longer ($t \leq 50\tau$) times at $J_{\perp}/J_{\parallel} = 1$ and for the largest $N = 32$. Clearly, the low-$\omega$ limit is independent of the $\omega$ resolution resulting from the specific choice of $t$. This robustness, together with the independence from $N$, allows us to reliably extract a quantitative value for the dc heat conductivity at $J_{\perp}/J_{\parallel} = 1$, $\kappa/J_{\parallel}^3 = 0.29$. Note that for the largest $N = 32$, significant finite-size effects set in only when choosing unphysical $t \gg 50\tau$.

![Figure 3](https://via.placeholder.com/150)

**FIG. 3.** (Color online) (a) The $t$ dependence of $C$ for various small $J_{\perp}/J_{\parallel} = 0.15, . . . , 0.75$, obtained from DQT for high $T$ ($\beta J_{\parallel} \to 0$) and different $N \leq 32$. (b) Spectrum for a single $J_{\perp}/J_{\parallel} = 0.25$, obtained by Fourier transforming finite-$t$ data $t \leq 5\tau \sim 80/J_{\parallel}$ (symbols); Inset: Low-$\omega$ limit for the largest $N = 32$ and $t \leq 5\tau$ (diamonds), $10\tau$ (crosses); Main panel: Spectrum from $N = 22$ and 28 MCLM and a Lorentzian fit are shown for comparison (curves).

To additionally demonstrate the validity of our DQT approach, we compare to our FTLM results and to existing MCLM spectra from the literature [49] in Fig. 2(b). Obviously, the agreement is very good. In Fig. 2(c) we repeat the calculation of Fig. 2(b) but for $S^z = 0$, i.e., taking into account all $S^z$ sectors (grandcanonical ensemble). The overall agreement of the two figures proves that $S^z = 0$ and $\langle S^z \rangle = 0$ yield the same physics.

Now, we turn to the limit of small rung exchange couplings $J_{\perp}/J_{\parallel} < 1$. In Fig. 3(a) we depict our DQT results on $C(t)$ for various $J_{\perp}/J_{\parallel} = 0.15, . . . , 0.75$. The initial value $C(0)$ approaches the $J_{\perp} = 0$ sum rule when $J_{\perp}$ is reduced. Furthermore, the decay is slower for smaller $J_{\perp}$ and finite-size effects are naturally stronger in the vicinity of the integrable point $J_{\perp} = 0$. For the smallest $J_{\perp}/J_{\parallel} = 0.15$ depicted, these finite-size effects are still moderate when comparing $C(t)$ for $N = 22$ and $N = 30$ lattice sites. In Fig. 3(b) we show the Fourier transform of $C(t \leq 5\tau \sim 80J_{\parallel})$ for $J_{\perp}/J_{\parallel} = 0.25$. For the largest $N = 32$, this Fourier transform is well described by a Lorentzian line shape and, again, the low-$\omega$ limit does not depend on the specific choice of $t$. Since $C(\omega)$ has a very narrow spectrum, MCLM with a very high $\omega$ resolution ($M = 2000$) is a better choice for comparison than FTLM and agrees well with our DQT data.

Next, we discuss the scaling of the dc heat conductivity $\kappa$ over the entire range of $J_{\perp}$. In Fig. 4(a) we summarize $\kappa(J_{\perp})$ as inferred from DQT data for $C(t \leq 5\tau)$. Here,
we observe a broad minimum of $\kappa(J_{\perp})$, centered between two regimes with power-law scaling at large and small $J_{\perp}$. The scaling $\propto J_{\perp}^2$ in the large $J_{\perp}$ limit is a direct consequence of the static sum rule for $C(0)$, noted following Eq. 8. The scaling $\propto J_{\perp}^{-2}$ for small $J_{\perp}$, however, is a dynamical feature of the energy current. In particular, we find this scaling to hold over a remarkably wide range of $0.07 \leq J_{\perp}/J_{\parallel} \leq 0.35$. This finding is a central result of this Letter. Below $J_{\perp}/J_{\parallel} < 0.07$, computational efforts for 5τ data are very high and finite-size effects are too large, even for the systems accessible to DQT.

To gain further insight into the scaling at small $J_{\perp}$, we calculate the scattering rate $\gamma = 1/\tau$ to lowest order in $J_{\perp}$, i.e., $J_{\perp}^2$, following the PTs in Refs. 47, 48, 61, and 62. This rate reads ($\beta J_{\parallel} \to 0$)

$$\gamma = \lim_{t_{\parallel} \to \infty} \int_{0}^{t_{\parallel}} dt_{\parallel} \frac{\text{Tr}\{j_{\parallel} H_{\parallel}(t) j_{\parallel} H_{\parallel}\}}{\text{Tr}\{j_{\parallel}^2\}} \propto J_{\perp}^2, \quad (5)$$

where $t_{\parallel}$ refers to the Heisenberg picture of $H_{\parallel}$. Figure 4 (b) shows the rate $\gamma$ evaluated by DQT applied to Eq. 5 for $N \leq 30$. We find good agreement with previous evaluation of $\gamma$ in Ref. 47 based on smaller systems. Most notably, however, $\gamma$ well agrees with the scattering rate $\gamma'$ as extracted directly from $\kappa$ in Fig. 4 (a) via the relation $\gamma' = z\beta^2 C(0)/\kappa$. This agreement is another main result of our Letter. Note that PT holds up to $J_{\perp}/J_{\parallel} \sim 1$ for the simplified current $j = j_{\parallel}$, see Fig. 4 (a).

Now we turn to temperatures $\beta J_{\parallel} \neq 0$, focusing on a rung exchange coupling of $J_{\perp}/J_{\parallel} = 1$. In Fig. 5 (a) we depict our DQT results for the energy-current autocorrelation function $C(t)$ for a temperature range $\beta J_{\parallel} = 0.5, \ldots, 1.5$. While the sum rule $C(0)$ decreases as $\beta$ is increased, the relaxation time shows the tendency to increase with $\beta$. However, significant finite-size effects appear as nondecaying Drude weights. Since these Drude weights exceed 20% of $C(0)$ at $\beta J_{\parallel} \sim 1.5$, we restrict ourselves to $\beta J_{\parallel} \leq 1$. For such temperatures, once again, FTLM agrees with the Fourier transform of our DQT data, which also shows a $N$-independent dc limit for large $N \sim 30$, see Fig. 4 (b). Finally, in the inset of Fig. 5 (a) we show the temperature dependence of the dc heat conductivity $\kappa$. Remarkably, in the temperature range accessible to our methods, we observe no significant deviations from the high-temperature behavior $\kappa \propto \beta^2$. We hence expect that $\kappa$ further increases down to some low temperature, consistent with the large $\kappa$ measured experimentally.

**Conclusion.** We have studied the heat conductivity $\kappa$ of the Heisenberg spin-1/2 ladder at finite temperature and over the entire range of the rung exchange coupling $J_{\perp}$, using several methods within the framework of linear response theory. We have detailed the power-law scalings $\kappa \propto J_{\perp}^{-2}$ and $\kappa \propto J_{\parallel}^2$ at weak and strong $J_{\parallel}$, respectively. We have found a broad minimum of $\kappa$ in the region $J_{\perp} \sim 1$, with a scaling of its temperature dependence as $\kappa \propto T^{-2}$ down to $T$ on the order of the exchange coupling constant. Thus, we have provided a...
comprehensive picture of $\kappa(J_\perp, T)$.

Note added. After completion of our work we became aware of a related work by C. Karrasch, D. M. Kennes, and F. Heidrich-Meisner [64], which focuses on strong rung exchange couplings $J_\perp/J_\parallel = \mathcal{O}(1)$ using both, a different ensemble ($\mathcal{S}^2$) = 0 and a different method.

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