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 κ of the Heisenberg spin-1/2 ladder at finite temperature covering the *entire* range of interchain 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 $J_\perp = J_\parallel$. Reducing temperature T, starting from $T = \infty$, 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 [2–4] 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 spin-1/2 Heisenberg model. It is relevant to the physics of quasi-1D quantum magnets [1], cold atoms in optical lattices [5], nanostructures [6], and to physical situations in a much broader context [7,8].

As is typical for integrable systems, the energy current in the spin-1/2 Heisenberg chain is a strictly conserved quantity [9,10]. This 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 [11–14]. In contrast to heat flow, spin dynamics, including the existence of ballistic [15–27] and diffusive transport channels [28–33], is theoretically resolved only partially, and is also under ongoing experimental scrutiny [34–38].

Because of strict energy-current conservation in this model, the heat conductivity κ 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 [45,46]. One of the most important perturbations is interchain coupling, i.e., $J_\perp$, which is the key ingredient to spin-ladder compounds [11,12]. Since the discovery of the discontinuous transition from one to two dimensions in quantum magnets [47], spin ladders are a cornerstone of correlated electron systems. They display quantum confinement [48], transforming gapless spinons of simple spin chains into new massive triplons [49,50]. They provide insights into fractionalization, quantum phase transitions [51], Bose-Einstein condensation [52], and disorder-induced magnetism [53]. They are paradigmatic to high-T_C superconductors, undoped [54] and doped [55]. They serve as models in other fields, e.g., cold atomic gases [56], quantum information theory [57], and carbon nanotubes [58].

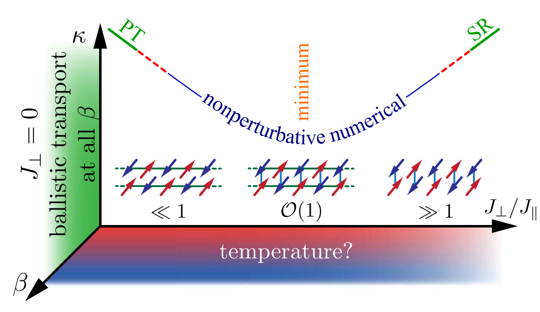

FIG. 1. Thermal conductivity κ (per chain) versus $J_\perp/J_\parallel$ and β. PT, known perturbative regime. Issues clarified in this Letter are as follows: extent of power-law scaling (dashed line) close to PT and sum-rule (SR) regimes, nonperturbative numerical treatment for entire $J_\perp$ range, location of minimal conductivity, and temperature variation.

Early on, perturbation theory (PT) to lowest order, i.e., a simple golden-rule argument [59,60], suggested *dissipative* heat flow with a scaling $\kappa \propto J_\perp^{-2}$, as illustrated on the lhs 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 κ over a wider $J_\perp$ range 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 [61]; i.e., time scales are short [62]. 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 heat conductivity κ over the *entire* range of the interchain coupling $J_\perp$. Using several methods within linear response, 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 $\kappa \propto J_\perp^2$ in the large-$J_\perp$ limit. Consequently, we (d) find a broad *minimum* of κ in the region $J_\perp \lesssim 1$. Reducing temperature T, starting from $T = \infty$, this minimum (e) scales as $\kappa \propto T^{-2}$ down to T on the order of the exchange coupling. Thus, we provide a comprehensive picture of $\kappa(J_\perp, T)$, beyond the known results sketched as part of Fig. 1.

Model.—We study a Heisenberg spin-1/2 ladder of length $N/2$ with periodic boundary conditions. The Hamiltonian $H = H_\parallel + H_\perp$ consists of a leg part $H_\parallel$ and a rung part $H_\perp$,

$$H_\parallel = J_\parallel \sum_{k=1}^{z} \sum_{i=1}^{N/2} \mathbf{S}_{i,k} \cdot \mathbf{S}_{i+1,k}, \qquad H_\perp = J_\perp \sum_{i=1}^{N/2} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}, \tag{1}$$

where $\mathbf{S}_{i,k}$ are spin-1/2 operators at site (i, k), $J_\parallel > 0$ is the antiferromagnetic leg coupling, and $J_\perp > 0$ is the rung interaction. $z = 2$ is the number of legs. For $J_\perp = 0$, the ladder splits into integrable chains, with a gapless ground state and spinon excitations. For $J_\parallel = 0$, it simplifies to uncoupled dimers, with a gapped ground state and triplon excitations. For $J_\perp$, $J_\parallel \neq 0$, the ladder is nonintegrable. Generally, the model in Eq. (1) preserves the total magnetization S^z and is translationally invariant. We focus on the representative sector $S^z = 0$ [63].

The energy current has the well-known form $j = j_\parallel + j_\perp$ [61],

$$j_\parallel = J_\parallel^2 \sum_{k=1}^{z} \sum_{i=1}^{N/2} \mathbf{S}_{i-1,k} \cdot (\mathbf{S}_{i,k} \times \mathbf{S}_{i+1,k}),$$

$$j_\perp = \frac{J_\parallel J_\perp}{2} \sum_{k=1}^{z} \sum_{i=1}^{N/2} (\mathbf{S}_{i-1,k} - \mathbf{S}_{i+1,k}) \cdot (\mathbf{S}_{i,k} \times \mathbf{S}_{i,3-k}). \tag{2}$$

j and H commute only at the integrable point $J_\perp = 0$. We investigate the autocorrelation function at inverse temperatures $\beta = 1/T$,

$$C(t) = \mathrm{Re} \frac{\langle j(t) j \rangle}{N} = \mathrm{Re} \frac{\mathrm{Tr}\{e^{-\beta H} j(t) j\}}{N \mathrm{Tr}\{e^{-\beta H}\}}, \tag{3}$$

where the time argument of $j(t)$ refers to the Heisenberg picture, $j = j(0)$, and $C(0) = 3(J_\parallel^4 + J_\parallel^2 J_\perp^2/2)/32$ for $\beta J_\parallel \to 0$.

From $C(t)$, we first determine the Fourier transform $C(\omega)$ and then the conductivity via the low-frequency limit $\kappa/z = \beta^2 C(\omega \to 0)$. Additionally, we can extract the conductivity directly by $\kappa/z = \beta^2 \int_0^{t_1} dt C(t)$. Here, the cutoff time t_1 has to be chosen much larger than the relaxation time τ, where $C(\tau)/C(0) = 1/e$ [64].

Methods.—We calculate C by complementary numerical methods, with a particular focus on dynamical quantum typicality (DQT) [25,26,65] (see also Refs. [66–74]). DQT relies on the time-domain relation

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

$|\Phi_\beta(t)\rangle = e^{-\imath H t - \beta H/2} |\psi\rangle$, $|\varphi_\beta(t)\rangle = e^{-\imath H t} j e^{-\beta H/2} |\psi\rangle$, where $|\psi\rangle$ is a *single* pure state drawn at random and ϵ scales inversely with the partition function; i.e., ϵ is exponentially small in the number of thermally occupied eigenstates [25,26,65]. The great advantage of Eq. (4) is that it can be calculated without any diagonalization by the use of forward-iterator algorithms. We use a fourth-order Runge-Kutta iterator with a discrete time step $\delta t J_\parallel = 0.01 \ll 1$. Together with sparse-matrix representations of operators, we can reach systems sizes as large as $N = 32$. For more details on the method and its accuracy, see Refs. [26,63].

Additionally, we confirm our DQT results with numerical methods based on Lanczos diagonalization in the frequency domain [75], with the frequency resolution $\delta\omega$ crucially depending on the number of Lanczos steps M, $\delta\omega \propto 1/M$. At low T, we choose the finite-T Lanczos method (FTLM) with $M \sim 200$ [63]. At high T, we also use the microcanonical Lanczos method (MCLM) with $M \sim 2000$, significantly improving $\delta\omega$.

Results.—We begin with $J_\perp/J_\parallel \geq 1$ and $\beta J_\parallel \to 0$. In Fig. 2(a) we summarize our DQT results on $C(t)$ for different $J_\perp/J_\parallel = 1, 1.5, 2$. Several comments are in order. First, the initial value $C(0)$ agrees with the high-T 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 32. Thus, we observe very little finite-size effects; i.e., we can safely consider our results as results on $C(t)$ for $N \to \infty$. Note that for $N \geq 30$ we consider a single

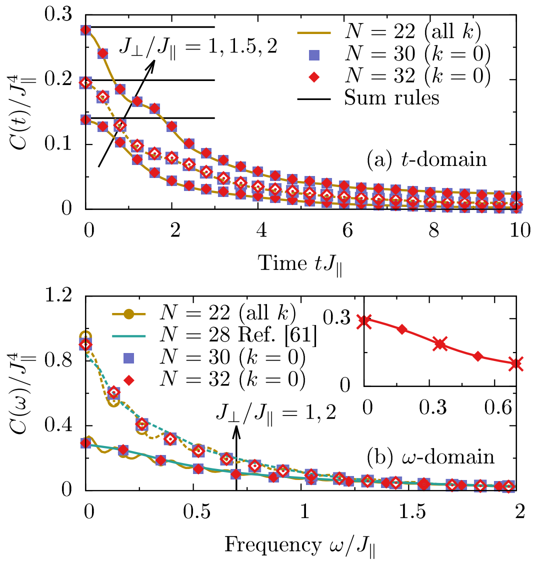

FIG. 2. (a) t and (b) ω dependence of the autocorrelation C for strong $J_\perp/J_\parallel \geq 1$, $\beta J_\parallel \to 0$, and $N \leq 32$, as obtained from DQT. Spectra in (b) are obtained by Fourier transforming finite-t data $t \leq 10\tau \sim 20/J_\parallel$ (symbols). Inset: Low-ω limit for $J_\perp/J_\parallel = 1$, the largest $N = 32$, and $t \leq 5\tau$ (crosses), 10τ (other symbols), 50τ (curves). Main panel: Spectra from Lanczos methods ($N = 28$ MCLM of Ref. [61], $N = 22$ FTLM) are shown (curves). Note that method-related errors are negligibly small [63].

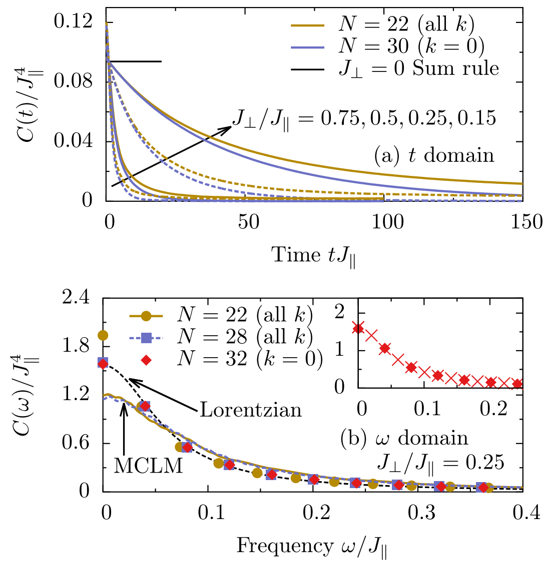

FIG. 3. (a) The t dependence of C for various small $J_\perp/J_\parallel = 0.15, \ldots, 0.75$, obtained from DQT for $\beta J_\parallel \to 0$ and $N \leq 30$. (b) Spectrum for $J_\perp/J_\parallel = 0.25$, obtained by Fourier transforming finite-t data $t \leq 5\tau \sim 80/J_\parallel$ (symbols). Inset: Low-ω limit for the largest $N = 32$ and $t \leq 5\tau$ (diamonds), 10τ (crosses). Main panel: Spectrum from $N = 22$ and 28 MCLM and a Lorentzian fit are shown (curves).

translation subspace k since, for these N, $C(t)$ is k independent at $\beta \to 0$ [25,26].

Next, we discuss the spectrum $C(\omega)$. To this end, we show in Fig. 2(b) 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 $\delta\omega \sim 0.15 J_\parallel$. For this resolution, the Fourier transform is a smooth function of ω 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(b) clarifies the impact of the ω 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-ω limit is independent of the ω resolution resulting from the specific choice of t. This robustness, together with the N independence, allows us to reliably extract a quantitative value for the dc conductivity at $J_\perp/J_\parallel = 1$, $\kappa/z\beta^2 J_\parallel^3 = 0.29$.

To additionally demonstrate the validity of our DQT approach, we compare to our FTLM results and to existing MCLM spectra from the literature [61] in Fig. 2(b). Obviously, the agreement is very good.

Now, we turn to small $J_\perp/J_\parallel < 1$. In Fig. 3(a) we depict our DQT results on $C(t)$ for various $J_\perp/J_\parallel = 0.15, \ldots, 0.75$. 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 $N = 22$, 30. In Fig. 3(b) we show the Fourier transform of $C(t \leq 5\tau \sim 80 J_\parallel)$ 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-ω limit does not depend on t. Since $C(\omega)$ has a narrow spectrum, MCLM with a high ω resolution ($M = 2000$) is a better choice for comparison than FTLM ($M = 200$) [63], and agrees well with DQT. Note that resolving narrow spectral features by DQT is a new concept of our Letter, which can be applied in a much broader context.

Next, we discuss the scaling of the conductivity κ 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 $C(0) \propto J_\perp^2$, noted following Eq. (3). The scaling $\propto J_\perp^{-2}$ for small $J_\perp$, however, is not simply related to $C(0)$ since $C(0) \approx$ const for such $J_\perp$. Particularly, we find this scaling to hold over a remarkably wide range of $0.07 \leq J_\perp/J_\parallel \lesssim 0.35$. 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 N 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 $J_\perp$,

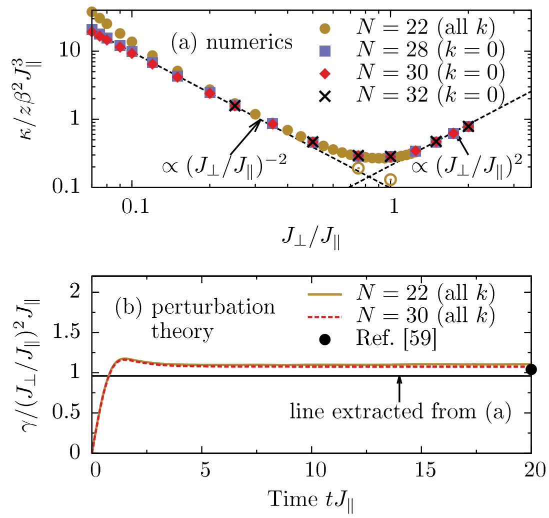

FIG. 4. (a) Scaling of the conductivity κ with $J_\perp$, obtained from DQT and finite-t data $t \leq 5\tau$ for $\beta J_\parallel \to 0$ and $N \leq 32$ (closed symbols). Results for the simplified operator $j' = j_\parallel$ are also depicted at $J_\perp/J_\parallel \sim 1$ (open symbols). Additionally, power laws $0.097(J_\perp/J_\parallel)^{-2}$ and $0.21(J_\perp/J_\parallel)^2$ are shown (lines). (b) PT for the scattering rate γ, carried out using DQT. The PT of Ref. [59] is also depicted (bullet).

i.e., $J_\perp^2$, following the PTs in Refs. [59,60,76,77]. This rate reads ($\beta J_\parallel \to 0$)

$$\gamma = \lim_{t_1\to\infty} \int_0^{t_1} dt_\parallel \frac{\mathrm{Tr}\{\imath[j_\parallel, H_\perp](t_\parallel)\imath[j_\parallel, H_\perp]\}}{\mathrm{Tr}\{j_\parallel^2\}} \propto J_\perp^2, \quad (5)$$

where $t_\parallel$ refers to the Heisenberg picture of $H_\parallel$. Figure 4(b) shows γ evaluated by DQT applied to Eq. (5) for large $N \leq 30$. Note that this application of DQT is a new concept of our Letter [63]. As shown in Fig. 4, we find good agreement with previous evaluation of γ in Ref. [59] based on smaller systems. Most notably, however, γ well agrees with the scattering rate γ' as extracted directly from κ 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), which is the regime where the system is Markovian, i.e., has no memory. For the explicit calculation of the memory kernel, see Ref. [63].

Now we turn to $\beta J_\parallel \neq 0$, focusing on $J_\perp/J_\parallel = 1$. In Fig. 5(a) we depict our DQT results for $C(t)$ for $\beta J_\parallel = 0.5, \ldots, 1.5$. While $C(0)$ decreases as β is increased, the relaxation time shows the tendency to increase with β. 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 β, 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. 5(b). Finally, in the inset of Fig. 5(a) we show the T

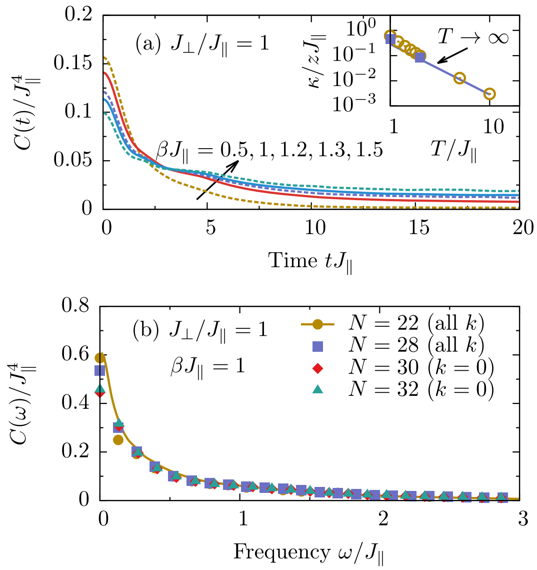

FIG. 5. (a) The t dependence of C for $\beta J_\parallel = 0.5, \ldots, 1.5$, obtained from DQT for $J_\perp/J_\parallel = 1$ and $N = 28$. (b) Spectrum for $\beta J_\parallel = 1$, obtained by Fourier transforming finite-t data $t \leq 5\tau \sim 12/J_\parallel$ for $N \leq 32$. Additionally, a spectrum from $N = 22$ FTLM is depicted (curve). Inset: T dependence of the conductivity κ, calculated by $N = 32$ DQT (closed symbols, curve) and $N = 22$ FTLM (open symbols).

dependence of the conductivity κ. Remarkably, in the T range accessible to our methods, we observe no significant deviations from the high-T behavior $\kappa \propto \beta^2$. While these T are low from a numerical point of view, they are still too high for a comparison to experiments on yet available materials, where the exchange coupling constant is large.

Conclusion.—We studied the heat conductivity κ of the Heisenberg spin-1/2 ladder at finite temperature and over the entire range of the rung interaction $J_\perp$, using several methods within linear response. We detailed the power-law scalings $\kappa \propto J_\perp^{-2}$ and $\kappa \propto J_\perp^2$ at weak and strong $J_\perp$, respectively. We found a broad minimum of κ 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. Thus, we provided a comprehensive picture of $\kappa(J_\perp, T)$.

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