

Low-Temperature Transport in Heisenberg Chains

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A technique to determine accurately transport properties of integrable and nonintegrable quantum-spin chains at finite temperatures by quantum Monte Carlo is presented. The reduction of the Drude weight by interactions in the integrable gapless regime is evaluated. Evidence for the absence of Drude weight in the gapless regime of a nonintegrable system with longer-ranged interactions is presented. We estimate the effect of the nonintegrability on the transport properties and compare with recent experiments on one-dimensional quantum-spin chains.

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Introduction.—During the last few years several families of materials containing well characterized quasi-one-dimensional spin-1/2 structures have been synthesized. The charge-transfer gap is in many cases large and the spin excitations contribute significantly to the thermal and magnetization transport at low temperatures. For example, ^{63}Cu NMR studies [1] in Sr_2CuO_3 have measured a spin diffusion coefficient (equivalent to diffusive magnetization transport) several orders of magnitude larger than the value for conventional diffusive systems, and thermal transport measurements in Sr_2CuO_3 and SrCuO_2 indicate [2] quasi-ballistic transport with a mean-free path of several thousands of Å.

These unusual results have been related to the peculiar physics of one-dimensional quantum chains. It is known that the spin transport in the XXZ chain

$$H^{(xxz)} = \sum_i \left[\frac{J_{xx}}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + J_z S_i^z S_{i+1}^z \right]$$

is not diffusive, even for $T \gg J_{xx}$ [3,4]. A connection between integrability and transport [5–9] enlightens the situation. In a generic integrable model such as $H^{(xxz)}$, the spin current is not conserved, but it has a nonvanishing “component” with respect to the projection onto a conserved operator. As a consequence, the current-current correlation functions do not decay to zero for large times.

The Hamiltonian appropriate for real compounds such as Sr_2CuO_3 and SrCuO_2 correspond to $H^{(xxz)}$ only in first approximation. A crucial question is therefore: How do small deviations from integrability change the picture described above? Extending an earlier analysis by Giamarchi [10], Rosch and Andrei concluded recently within a memory-matrix approach [11], that deviations from integrability lead to an exponentially large conductivity in Hubbard-like models away from commensurability.

Despite the ongoing effort devoted to this problem, the fundamental difference between integrable and nonintegrable models has not yet shown up in quantum Monte Carlo (QMC) simulations [12,13], presumably due to the demanding numerical requirements. In this Letter, we develop the techniques and tools for the data analysis necessary for extracting the Drude weight for integrable and

the lifetime, mean-free path and the diffusion constant for nonintegrable quantum-spin models from correlation functions obtained by QMC simulations using the loop algorithm [14]. We present extensive comparison with exact results obtained by Bethe ansatz and compare for a nonintegrable system with recent experiments on Sr_2CuO_3 .

Drude weight.—QMC simulations yield in general correlations functions on the imaginary-time axis. We therefore consider the Kubo formula for the dynamical conductivity $\sigma(\omega_n) = \lim_{q \rightarrow 0} \sigma(q, \omega_n)$

$$\sigma(q, \omega_n) = \frac{-\langle K \rangle - \Lambda(q, \omega_n)}{\omega_n} \equiv \frac{D(q, \omega_n)}{\omega_n} \quad (1)$$

on the imaginary axis, where $\langle K \rangle$, for the models we will consider, is the expectation value of the kinetic energy per site and where Λ is the current-current correlation as a function of the Matsubara frequency

$$\Lambda(q, \omega_n) = \frac{1}{L} \int_0^\beta e^{i\omega_n \tau} \langle j^z(q, \tau) j^z(-q, 0) \rangle d\tau. \quad (2)$$

Equation (1) leads via $\sigma(\omega) = \pi D(T) \delta(\omega) + \sigma_{\text{reg}}(\omega)$ to the conventional relation [12] between the current-current correlation function and the Drude weight (we are borrowing the terminology of electrical responses) $D(T) = \lim_{\omega_n \rightarrow 0} \lim_{q \rightarrow 0} D(q, \omega_n)$

$$D(T) = -\langle K \rangle - \Lambda(q \rightarrow 0, \omega_n \rightarrow 0). \quad (3)$$

Note that $\Lambda(q, \omega + i\delta)$ is analytic in the upper half of the complex ω plane and the extrapolation along the imaginary axis can be reliably performed at low temperatures, when many Matsubara frequencies $\omega_n = 2\pi Tn$ are available close to $\omega = 0$ for the extrapolation [13].

The continuity equation $\frac{\partial}{\partial t} S_i^z(t) + \frac{\partial}{\partial x} j_i^z(t) = 0$ leads to the expression

$$j_i^z = -iJ_{xx}(S_i^+ S_{i+1}^- - S_i^- S_{i+1}^+)/2 \quad (4)$$

for the current operator $j_i(t)$ in the XXZ model. In Fourier space, the continuity equation takes the form

$$\frac{d}{d\tau} S_q^z(\tau) = [H, S_q^z] = i(1 - e^{iq}) j_q^z. \quad (5)$$

$\Lambda(q, \omega_n)$ is a nondiagonal four-site operator. In principle nondiagonal operators can be computed using the loop

algorithm [15] but, as discussed recently [16], the algorithm to compute two-site correlation functions is more efficient than the algorithms that compute operators involving three or more sites. To obtain high quality data we measure directly the dynamical susceptibility in imaginary time

$$S(q, \omega_n) = \frac{1}{L} \int_0^\beta e^{i\omega_n \tau} \langle S_q^z(\tau) S_{-q}^z(0) \rangle, \quad (6)$$

a simple diagonal two-site correlation function. The Drude peak is computed by using Eq. (3) and the relation

$$\omega_n^2 S(q, \omega_n) = 4 \sin^2(q/2) D(q, \omega_n). \quad (7)$$

This relation can be derived by a twofold partial integration of the right-hand side of Eq. (6) with respect to τ , which leads to

$$S(q, \omega_n) = \frac{-1}{\omega_n^2} \langle \langle [H, S_q^z], S_{-q}^z \rangle \rangle - \frac{4 \sin^2(q/2)}{\omega_n^2} \Lambda(q, \omega_n),$$

where we have used Eq. (5) for the imaginary-time derivatives of S_q^z and S_{-q}^z and definition (2). Evaluation of the double commutator ($[H, S_q^z], S_{-q}^z$), which is the boundary term from the partial integration, then leads to Eq. (7). Note that this double commutator occurs here for the Matsubara correlation functions and does not occur for a related real-frequency correlation function [8].

Data analysis.—At low temperatures and frequencies, the scaling of $D(q, \omega_n)$ can be obtained by simply invoking the conformal symmetry of the model emerging in the gapless regime $J_z < J_{xx}$. $S(q, \omega_n)$ at small q then takes the form $S(q, \omega_n) = D_1(T) q^2 / [(c q)^2 + \omega_n^2]$. This expression and Eq. (7) suggest the form

$$D(q, \omega_n) = \frac{D_1(T) \omega_n^2}{\Delta^2(q) + \omega_n^2}. \quad (8)$$

Alternatively, Eq. (8) can be viewed as the first term of the exact representation for $D(q, \omega_n)$ containing an infinite number of terms [13].

The XXZ model maps to an interacting 1D spinless fermionic system at half filling. For the noninteracting case (the XX chain) we can compute exactly $D(q, \omega_n)$ and we obtain $D(0) = J_{xx}/\pi$, and $\Delta(q) = J_{xx} \sin(q) \sim J_{xx} q$. For $J_z < J_{xx}$ the umklapp term remains marginally irrelevant and one expects Luttinger liquid like correlation functions [10] such as Eq. (8).

In the ideal Luttinger liquid the bosonic excitations are arbitrarily well defined at low temperatures and low frequencies. The conductivity is necessarily infinite in that case, and ansatz (8), being invariant under time reversal, reflects that property. Nevertheless, we are also interested in the study of more general situations in which the bosons can decay, become quasiparticles, and memory effects can be taken into account. To this end we use the formalism of the memory matrices which has been successfully applied to study how one-dimensional electron liquids can gain a resistivity [10,11].

This is achieved by taking the following fitting function for $D(q, \omega_n > 0)$:

$$D(q, \omega_n) = \sum_{j=1}^2 \frac{D_j(q) \omega_n^2}{\Delta_j^2(q) + 2\gamma_j(q) \omega_n + \omega_n^2}. \quad (9)$$

$D(q, \omega_n)$ is analytic in the upper complex plane for $\gamma_j(q) \geq 0$. For $\Delta_i(0) = \lim_{q \rightarrow 0} \Delta_i(q)$ we find either a (i) gapless regime: $\Delta_1(0) = 0$ and $\Delta_2(0) > 0$, or a (ii) gap-full regime: $\Delta_1(0) > 0$ and $\Delta_2(0) > \Delta_1(0)$. The first term in Eq. (9) dominates the low-frequency behavior in both cases and we have set generally $\gamma_2 \equiv 0$ in order to keep the number of parameters to a minimum.

In the gapless regime the optical conductivity (1) takes for small frequencies the Drude form

$$\text{Re} \sigma(\omega) = \frac{2D_1(0)\gamma_1(0)}{\omega^2 + 4\gamma_1^2(0)} \equiv \frac{\sigma_0}{1 + (\omega\tau)^2}, \quad (10)$$

where we introduced the dc conductivity $\sigma_0 = D_1(0)/[2\gamma_1(0)]$ and the quasiparticle lifetime $\tau = [2\gamma_1(0)]^{-1}$. For $\tau \rightarrow \infty$ Eq. (10) reduces to $\text{Re} \sigma(\omega) = \pi D_1(0) \delta(\omega)$. At high frequencies

$$\lim_{\omega_n \rightarrow \infty} D(0, \omega_n) = -\langle K \rangle \equiv D_1(0) + D_2(0), \quad (11)$$

and a finite $D_2(0)$ results in a reduction of the Drude weight $D(T)$ with respect to the kinetic energy; see Eq. (3). A finite $D_2(0)$ measures therefore the amount of decay experienced by the *total* current due to the interactions. We note that the ansatz Eq. (9) for $D(q, \omega_n)$, together with Eq. (11), is consistent with the f -sum rule [17] $\int_0^\infty \text{Re} \sigma(\omega) = -\frac{\pi}{2} \langle K \rangle$ for the optical conductivity.

Ballistic transport.—In Fig. 1 we show the values for $D_1(q)$ and $\Delta_1(q)$ for the XX chain for different system sizes as obtained by QMC [18], $D_2(q)$ and $\gamma_1(q)$ optimize to zero for this model. The different system sizes collapse at the smallest momenta and in this way the thermodynamic limit and the $q \rightarrow 0$ limit are performed simultaneously. Our prescription to extract $D_1(0)$ as the limiting

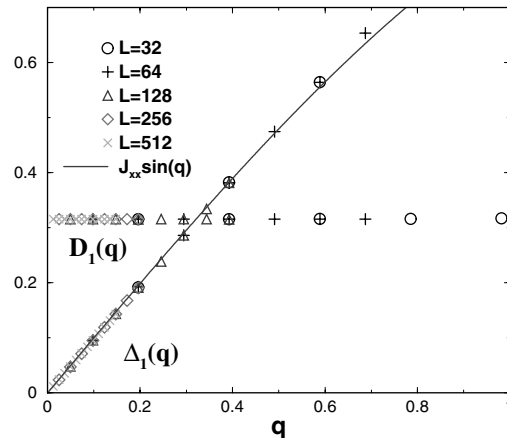


FIG. 1. The parameters $D_1(q)$ and $\Delta_1(q)$ from Eq. (9) as a function of momenta q , for the XX model ($J_z = 0$) and various system sizes at $T = 0.004J_{xx}$. Statistical error bars are of the order of the symbol size [18].

value $D_1(0) = \lim_{q \rightarrow 0} D_1(q)$ is more involved than previous $q \equiv 0$ calculations [13], but we believe it to be necessary in order to avoid substantial finite-size effects due to the fact that $D(q \rightarrow 0, \omega_n)$ becomes a step function at $\omega_n = 0$ in the thermodynamic limit; compare Eq. (8).

For finite interaction J_z we find in the gapless regime $J_z \leq J_{xx}$, that $\Delta_1(q) \approx c(J_z)q$, where $c(J_z)$ is the velocity

$$c(J_z) = \frac{\pi}{2} \frac{\sqrt{J_{xx}^2 - J_z^2}}{\arccos(J_z/J_{xx})} \quad (12)$$

of the des Cloiseaux-Pearson spectrum [19]. In Fig. 2 we compare the measured value of $c(J_z)$ with the Bethe-ansatz result (12) for $J_z/J_{xx} = 1/2, 1$. $\Delta_1(q)$ is fitted well in the gapped phase by $\varepsilon(q) = \sqrt{\Delta_0^2 + (cq)^2}$. We find $\Delta_0 = 0.191J_{xx}$, which is close to twice the one-magnon gap of $0.091J_{xx}$ [19].

The damping $\gamma_1(q)$ is vanishingly small for $J_z < J_{xx}$ and acquires a finite value in the gapped phase which can be fitted phenomenologically by the relation $\gamma_1(q)\Delta_1(q) \approx \text{const}$, independent of q .

In Fig. 3 (inset) we present values obtained by QMC for the Drude weight in the gapless regime, $J_z < J_{xx}$ at $T = 0.004J_{xx}$. We find good agreement with the $T = 0$ Bethe ansatz result [20]

$$D(0) = \frac{J_{xx}\nu^2}{4\pi} \frac{\sin(\pi/\nu)}{\nu - 1}, \quad J_z = J_{xx} \cos(\pi/\nu), \quad (13)$$

especially at the smaller values of J_z . In this region the correlation function is expected to satisfy more accurately the scaling law (8). The $S(q, \omega_n)$ in the isotropic Heisenberg model does not follow strictly the Luttinger liquid form. It presents multiplicative logarithmic corrections, that should be observed also for values of J_z slightly smaller than

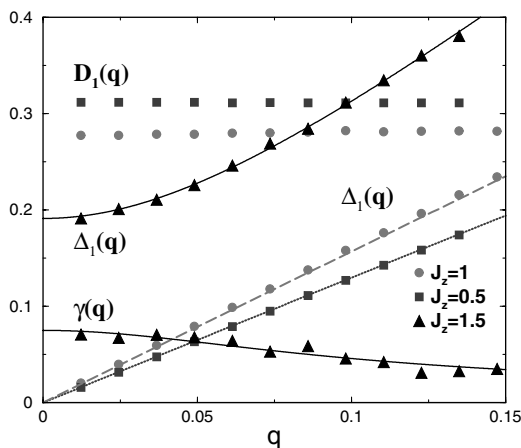


FIG. 2. $D_1(q)$, $\Delta_1(q)$, and $\gamma_1(q)$ from Eq. (9) as a function of momenta q for the XXZ model, $L = 512$ and for various J_z at $T = 0.004J_{xx}$. $\gamma_1(q)$ is too small for $J_z \leq J_{xx}$ to show up on this scale. The lines are the Bethe-ansatz result (12) for the velocity $c(J_z)$ (no fit, for $J_z \leq J_{xx}$). For the discussion of the fit for $J_z = 1.5J_{xx}$, see the text.

J_{xx} when finite temperatures and system sizes impose a cutoff for the RG equation of the umklapp coupling constant [10].

We study now the behavior of the Drude weight at finite temperatures for models free from strong multiplicative corrections. The main conclusion of Zotos [21] is the fast decay of the Drude weight when the temperature increases, $D(T) - D(0) \sim -\kappa T^{2/(\nu-1)}$ where κ is a constant and ν defined by Eq. (13). This rapid decrease with increasing temperature is consistent with exact diagonalization studies at high temperatures [9]. Klümper *et al.* have found, on the other hand [22], with an alternative Bethe-ansatz approach, a functionally different behavior for $D(T)$; see Fig. 4. For a numerical probe of $D(T)$ we focus on $\nu = 6$ and consider several small temperatures. In Fig. 4 we show a comparison of our data with the two available analytical results [21,22]. Our results agree with the temperature dependence predicted by Klümper *et al.*, suggesting in particular a finite Drude weight also at the isotropic point [22].

Diffusive transport.—We consider now a perturbation of $H^{(xxz)}$ that breaks the integrability but keeps the z component of the magnetization conserved:

$$H' = J'_z \sum_i S_i^z S_{i+3}^z. \quad (14)$$

The expression (4) for the spin current remains valid. For this model, $H = H^{(xxz)} + H'$, we predict a transition to a gapped phase around $J'_z \cong 0.3J_{xx}$ (for $\nu = 6$); see Fig. 3. We find the relaxation time $\tau = 1/2\gamma_1(0) = \lim_{q \rightarrow 0} 1/2\gamma_1(q)$ to be finite within numerical accuracy (due to finite q and ω_n resolution), leading to a finite dc conductivity in the gapless phase.

For $1/\omega \gg \tau$ the optical conductivity takes [for small $cq/\gamma_1(0)$] the diffusion form

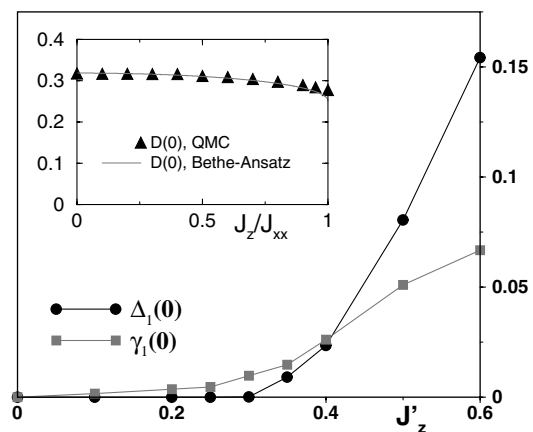


FIG. 3. For $L = 512$ and $T = 0.004J_{xx}$ the QMC results for the gap $\Delta_1(0)$ and the relaxation rate $\gamma_1(0)$ as a function of J'_z for $H^{(xxz)} + H'$ with $J_z = J_{xx} \cos(\pi/6)$. Inset: The QMC results for the Drude weight for $J'_z = 0$ and $T = 0.004J_{xx}$ and $L = 512$ in comparison with the Bethe-ansatz result at $T = 0$, Eq. (13). Note that $D(T)$ is smooth for low T (see Fig. 4).

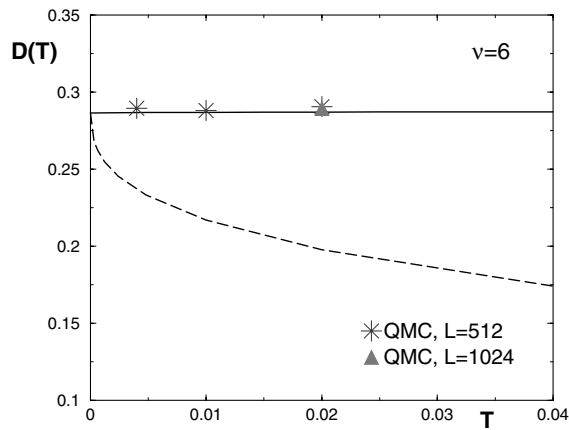


FIG. 4. QMC results for the Drude weight for $L = 512, 1024$ and $J_z = J_{xx} \cos(\pi/6)$ as a function of temperature (in units of J_{xx}) in comparison with two (solid lines: Ref. [22]; dashed lines: Ref. [21]) Bethe-ansatz results.

$$\sigma(q, \omega) = \frac{\sigma_0 \omega}{\omega + iD_s q^2}, \quad D_s = \frac{c^2}{2\gamma_1(0)} \equiv c^2 \tau. \quad (15)$$

D_s is the spin-diffusion constant. Equation (15) is consistent with $D_s = c\lambda_s$, where $\lambda_s = c\tau$ is the mean free length.

We have evaluated $\sigma(T)$, in addition to the data presented in Fig. 3, for $\nu = 6$, $J'_z = 0.3J_{xx}$ and find $\sigma(T = 0.004J_{xx}) = 13.6 \pm 0.9$, $\sigma(T = 0.008J_{xx}) = 12.1 \pm 1.0$, and $\sigma(T = 0.012J_{xx}) = 10.1 \pm 0.8$.

We now take $J_{xx} = 2000$ K, which is appropriate for Sr_2CuO_3 and evaluate the transport coefficients for $J'_z = 0.3J_{xx}$, $\nu = 6$, $T = 0.004J_{xx}$. We find $\lambda \approx 88$ lattice constants and $D_s \approx 6 \times 10^{15} \text{ sec}^{-1}$. We do not expect this model to be directly relevant for Sr_2CuO_3 . But if we ask ourselves now the question of whether the experimental results for λ and D_s being large (but finite) could be explained within a pure spin model with a small deviation from integrability, we might expect $H = H^{(xxz)} + H'$ to show the characteristic behavior of a nonintegrable quantum-spin chain. If we now change the deviation from integrability (controlled by J'_z) such that $\gamma_1(0)$ decreases by a factor of about 10, then both λ and D_s would increase by the same factor and would be consistent with the experimentally measured values [1,2].

Discussion.—We have shown that certain transport properties of quantum-spin chains can be evaluated directly from two-point correlations functions using a relation between $S(q, \omega_n)$ and the dynamical conductivity which we have derived. For the integrable chains we support the original suggestion by Zotos *et al.* [5–7] of a finite Drude weight at finite temperatures and settle a recent dispute regarding the functional form of $D(T)$. In addition we present results suggesting the absence of

ballistic transport (i.e., zero Drude weight) for a nonintegrable model, for which we are able to estimate the magnitude of the dc conductivity. We have shown that the experiments on quasi-one-dimensional spin compounds [1,2] are, in principle, consistent with the notion that they probe directly nonintegrability effects, though we cannot rule out at this point that disorder or the coupling to phonons [3] would lead to the observed finite values for the transport coefficients.

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