Conductivity of quantum spin chains: A quantum Monte Carlo approach

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We discuss zero-frequency transport properties of various spin-1/2 chains. We show that a careful analysis of quantum Monte Carlo data on the imaginary axis allows to distinguish between intrinsic ballistic and diffusive transport. We determine the Drude weight, current-relaxation lifetime, and the mean free path for integrable and nonintegrable quantum spin chains. We discuss, in addition, some phenomenological relations between various transport-coefficients and thermal response functions.

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I. INTRODUCTION

The role of spin excitations on the transport properties of quasi-one-dimensional Mott insulators has been the subject of extensive experimental research over the last few years. A recent ^{17}O NMR investigation[1] of Sr_2CuO_3, extending an earlier ^{63}Cu NMR study,[2] measured a $q=0$ spin-diffusion coefficient (equivalent to diffusive magnetization transport) several orders-of-magnitude larger than the value for conventional diffusive systems. Thermal transport measurements in Sr_2CuO_3 and $SrCuO_2$ indicate at the same time, quasiballistic transport with a mean free path of several thousands[3] angstrom.

It is well known from structural considerations[4] and from studies of the magnetic excitation spectrum[4,5] that Sr_2CuO_3 and $SrCuO_2$ can be accurately described by the XXZ chain:

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

Evidence for ballistic (or quasiballistic) magnetization transport has been found in recent exact diagonalization studies[6] of $H^{(xxz)}$ at high temperatures.[7,8] A connection between integrability, conservation laws, and ballistic transport has been proposed by Zotos and co-workers.[7,9–12] If the current-current correlation does not decay to zero for long times, i.e., when part of the current operator is conserved, and when a certain (nonzero) projection of the (here, magnetic) current operator commutes with the Hamiltonian, the transport is ballistic even at finite temperatures. This seems to be the case, in general, for Bethe-ansatz solvable models like $H^{(xxz)}$, although a formal proof for this connection is still outstanding.

At present it is unclear whether there exist nonintegrable models which exhibit ballistic transport; none have been found so far. Real compounds like Sr_2CuO_3 and $SrCuO_2$ correspond to $H^{(xxz)}$ in any case only in first approximation. It is therefore important to examine whether general, nonintegrable, quantum spin chains show ballistic or diffusive transport properties at finite temperatures. This question has been studied by Rosch and Andrei[13] within a short-time approximation (a memory-matrix approach, extending an earlier analysis by Giamarchi[14]) for Luttinger liquids with higher-order umklapp scattering. They found only exponentially small deviations from ballistic transport away from commensurability. An alternative route to diffusive transport, spin-phonon coupling, has been studied by Narozhny.[15]

In his seminal paper[16] in 1964, Kohn proved that the existence of a delta peak at zero frequency (the Drude peak) in the conductivity is the essential difference between ground states with localized and extended electronic states. A simple extension of this idea to the spin transport can be used to distinguish, without other explicit information about the excitation spectrum, a spin insulator, such as spin-Peierls compounds, from a spin conductor such as Sr_2CuO_3. Despite ongoing efforts[17,18] devoted to this problem, the fundamental difference between models with ballistic and diffusive transport properties has shown up only recently in quantum Monte Carlo (QMC) simulations.[19] The purpose of this paper is to explain in detail how this important issue can be tackled numerically by QMC methods.

The organization of the paper is as follows. Section II contains the basic definitions and sets the notation that we will use throughout the paper. In Sec. III we deduce the connection between the spin current-current and density-density correlation functions emphasizing the role of boundary terms that occur in Matsubara formalism, and in Sec. IV we discuss how to exploit that connection to compute the conductivity in imaginary frequency using quantum Monte Carlo cluster algorithms in an efficient way. In Sec. V we describe a procedure to extract transport coefficients (Drude weight and the diffusion coefficient) from QMC data in general one-dimensional (1D) interacting systems, either integrable or nonintegrable. In Sec. VI we apply this method to the XXZ chain and we obtain the Drude weight at finite temperatures. We then discuss several phenomenological relations between transport and thermal coefficients in Sec. VII. Section VIII is devoted to the computation of diffusion constants, mean free paths, and lifetimes in a nonintegrable spin chain. In Sec. IX we present our conclusions.

II. SPIN CONDUCTIVITY

QMC simulations yield, in general, correlation functions on the imaginary-time axis. We therefore consider the Kubo formula for spin conductivity in the Matsubara formalism.

The spin conductivity in one-dimensional spin chains can be defined as the response of the current to a homogeneous and time-dependent twist $\Phi=\Sigma_l \phi_l$ in the quantization axis:

$$H^{(xxz)}(\Phi)=\sum_l \left[k_l\cos(\phi_l)+j_l^z\sin(\phi_l)+J_z S_l^z S_{l+1}^z\right], \tag{1}$$

where

$$k_l=\frac{J_{xx}}{2}(S_l^+S_{l+1}^-+S_l^-S_{l+1}^+) \tag{2}$$

and

$$j_l^z=\frac{J_{xx}}{2i}(S_l^+S_{l+1}^--S_l^-S_{l+1}^+). \tag{3}$$

Formally, Eq. (1) is the Hamiltonian of an XXZ chain in which the quantization axis of the local spin operators has been rotated by a site-dependent angle ϕ_l along the z axis. To obtain the expression of the Kubo formula for the spin conductivity we expand $H^{(xxz)}(\Phi)$ in a Taylor series:

$$H^{(xxz)}(\Phi)=H^{(xxz)}+\sum_l j_l^z\phi_l+\frac{k_l}{2}\phi_l^2, \tag{4}$$

and we obtain the *total* spin-density current by differentiating with respect to ϕ_l,

$$\frac{\partial H^{(xxz)}(\Phi)}{\partial\phi_l}=(j_l^z)^T=j_l^z+k_l\phi_l. \tag{5}$$

The first term is the paramagnetic part of the current. If the z component of the magnetization is conserved, it can also be deduced using the discretized continuity equation

$$\frac{\partial}{\partial t}S_l^z(t)+[j_l^z(t)-j_{l-1}^z(t)]=0, \tag{6}$$

where the second term is the discrete version of the divergence in one dimension. If we combine it with the equation of motion,

$$\frac{\partial}{\partial t}S_l^z(t)=i[H,S_l^z], \tag{7}$$

we obtain the expression (3). The second term in Eq. (5), proportional to the magnetic flux, is called the diamagnetic current. The expectation value of the total current is

$$\langle j^T(q,\omega_n)\rangle=-[\langle K\rangle+\Lambda(q,\omega_n)]\phi_l, \tag{8}$$

where $\langle K\rangle=\langle\Sigma_l k_l\rangle$ is the expectation value of the kinetic energy per site and Λ is the current-current correlation as a function of the Matsubara frequency,

$$\Lambda(q,\omega_n)=\frac{1}{L}\int_0^\beta e^{i\omega_n\tau}\langle j^z(q,\tau)j^z(-q,0)\rangle d\tau. \tag{9}$$

The response to the time-integrated twist is then obtained from Eq. (8) and the dynamical conductivity takes the usual form

$$\sigma(q,\omega_n)=\frac{-\langle K\rangle-\Lambda(q,\omega_n)}{\omega_n}\equiv\frac{D(q,\omega_n)}{\omega_n}. \tag{10}$$

Equation (10) leads, via analytical continuation $i\omega_n\rightarrow\omega+i\delta$ and $\delta\rightarrow 0$, using $\sigma(\omega_n)=\lim_{q\rightarrow 0}\sigma(q,\omega_n)$, to the usual representation of the dynamical conductivity

$$\sigma(\omega)=\pi D(T)\,\delta(\omega)+\sigma_{reg}(\omega,T), \tag{11}$$

where $D(T)$ is the Drude weight[20] that can be computed via $D(T)=\lim_{\omega_{n\rightarrow 0}}\lim_{q\rightarrow 0}D(q,\omega_n)$:

$$D(T)=-\langle K\rangle-\Lambda(q\rightarrow 0,\omega_n\rightarrow 0). \tag{12}$$

It can be proved[11] that this limit is consistent with the definition introduced by Kohn[16] at $T=0$,

$$D=L\left(\frac{d^2E}{d^2\Phi}\right)_{\Phi=0}, \tag{13}$$

where E is the ground-state energy and Φ the total external flux. Recently D has been extended by Zotos, Naef, and Prevlošek[11] to finite T:

$$D(T)=L\sum_\alpha\frac{\exp(-\beta E_\alpha)}{Z}\left(\frac{d^2E_\alpha}{d^2\Phi}\right)_{\Phi=0}. \tag{14}$$

It is important to note that the limits $\lim_{q\rightarrow 0}$ and $\lim_{\omega\rightarrow 0}$ do not commute. When the limits are taken in the opposite order one obtains the conventional spin stiffness which represents the response to a *static* twist:

$$\rho_s=\lim_{q\rightarrow 0}\lim_{\omega_n\rightarrow 0}D(q,\omega_n). \tag{15}$$

A nonzero value of the Drude weight implies that the total magnetic current does not decay to zero when $t\rightarrow\infty$ (i.e., the transport is ballistic). The most simple example to illustrate this situation is the XX chain. In that case $[H_{XX},j^z(q)]=0$. Taking the spectral representation of $\Lambda(q,\omega_n)$ for $\omega_n>0$ we have

$$\Lambda(q,\omega_n)=\frac{1}{ZL}\sum_{m,n}^{E_m\neq E_n}\frac{e^{-\beta E_m}|\langle m|j^z(q)|n\rangle|^2}{i\omega_n-(E_m-E_n)}. \tag{16}$$

Note that degenerated states are explicitly excluded from the sum and therefore $|\langle m|j^z(q)|n\rangle|=0$ and the conductivity reduces to $\sigma=-\pi\langle K\rangle\delta(\omega)$, which saturates the f sum rule. Interactions spoil the commutation of spin current and Hamiltonian but, if the umklapp part of the interaction is irrelevant and the system remains gapless, the Drude weight remains finite and the current-current correlation functions can reduce the Drude peak from the kinetic energy. This situation is indeed realized in the gapless regime of the XXZ chain but the integrable nature of the interaction in this case plays, as we will see, a definitive role. The regular part of the conductivity is in any case (integrable or nonintegrable systems) enhanced to fulfill the f sum rule.

III. RELATION BETWEEN CORRELATION FUNCTIONS AT $T \neq 0$

Now we will derive a connection in between the current-current correlation function $D(q,\omega_n)$ and the dynamical susceptibility $S(q,\omega_n)$; in the next section we will explain how to exploit this connection in QMC calculations. The spin-spin correlation function is defined by

$$S(q,\omega_n)=\frac{1}{L}\int_0^\beta e^{i\omega_n\tau}\langle S_q^z(\tau)S_{-q}^z(0)\rangle. \tag{17}$$

In Fourier space, the continuity Eq. (6) takes the form

$$\frac{d}{d\tau}S_q^z(\tau)=[H,S_q^z]=i(1-e^{iq})j_q^z. \tag{18}$$

We integrate the right-hand side of Eq. (17) with respect to τ twice, use Eq. (18), and obtain

$$S(q,\omega_n)=\frac{-1}{\omega_n^2}\langle[[H,S_q^z],S_{-q}^z]\rangle-\frac{4\sin^2(q/2)}{\omega_n^2}\Lambda(q,\omega_n), \tag{19}$$

where we have used the definition (9). The double commutator in the right-hand side of Eq. (19) is the boundary term of the partial integration and is evaluated to read

$$\langle[[H,S_q^z],S_{-q}^z]\rangle=4\sin^2(q/2)\langle K\rangle. \tag{20}$$

Recalling the definition of $D(q,\omega_n)$ we arrive at

$$D(q,\omega_n)=\frac{\omega_n^2}{4\sin^2(q/2)}S(q,\omega_n). \tag{21}$$

Note, that the double commutator in Eq. (19) occurs for the Matsubara correlation functions and does not occur for a related real-frequency correlation function.[12]

IV. QMC EVALUATION OF THE CONDUCTIVITY

In this section we will discuss the usefulness of Eq. (21) in the context of QMC simulation, comparing two different possibilities to compute the conductivity using quantum cluster algorithms. Cluster algorithms for QMC simulations allow for global updates of the configuration by flipping simultaneously spin-clusters whose typical sizes are of the order of the correlation length of the system. The loop algorithm[21] we used in the present study gives an efficient prescription to construct clusters. The resulting autocorrelation time is in general of the order of one Monte Carlo step (see Ref. 22 for an excellent review).

The current-current correlation function in real space and imaginary time takes the form

$$\Lambda(l,\tau)=\frac{1}{LN_T}\sum_{l',\tau'} j_{l+l'}^z(\tau'+\tau)j_{l'}^z(\tau'), \tag{22}$$

where N_T is the number of Trotter slices. The contributions to $\Lambda(l,\tau)$ are nondiagonal four-site operators, typically $(J_{xx}/4)S_{l_1}^+(\tau_1)S_{l_1+1}^-(\tau_1)S_{l_2}^-(\tau_2)S_{l_2+1}^+(\tau_2)$. In principle, nondiagonal operators can be computed using the loop algorithm.[23] When these nondiagonal operators are two-point-like, only one-loop terms contribute to the correlation function. In that case it is possible to design efficient improved estimators, meaning that a given magnitude is evaluated not only in one configuration but in all configurations related by loop flippings. The evaluation of a four-point correlation function is more involved.[24] In that case there are two-loop terms and one-loop terms which contribute in different ways depending on the specific shape of the loop, see Fig. 1 for an illustration. As a consequence the improved estimators are much less efficient. The dynamical susceptibility in $S(q,\omega_n)$ is, on the other hand, a two-point diagonal operator that can be evaluated efficiently using improved estimators, and it is related to the conductivity using the Kubo formula (10) and the relation (21).

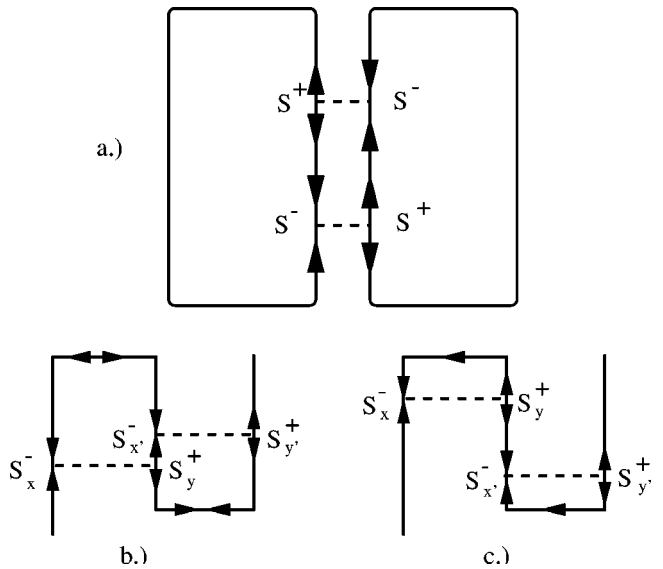

FIG. 1. (a) Two-loop contribution to the current-current correlation function; an S^+ and S^- operator must be applied in each loop to close it consistently in terms of the loop orientation. (b) and (c) Two kinds of one-loop contributions to the current-current correlation function. The ordering of the S^+ and S^- in terms of loop time is crucial to evaluate the contribution of these terms.

In particular, one can compute within each loop α the magnitude:

$$W(q,\omega_n,\alpha)=\frac{\beta}{N_T}\sum_{(x,\tau)\in\alpha} S_l^z(\tau)e^{i(ql+\omega_n\tau)}. \tag{23}$$

The dynamical structure factor is then

$$S(q,\omega_n)\sim\sum_\alpha W(q,\omega_n,\alpha)W(-q,-\omega_n,\alpha), \tag{24}$$

where α runs over all loops constructed. In particular we want to emphasize the importance of relation (21), because only using it we obtained the high-quality data (large set of uncorrelated measurements with small statistical error bars) that is necessary in order to extract dc-transport coefficients.

Finally we mention a few numerical details. We used the discrete imaginary-time version of the loop algorithm with a Trotter decomposition of typically $N_T=800-2000$ and on

the average 6×10^6 full MC updates in the grand-canonical ensemble. Test runs within a canonical ensemble were also performed to exclude any influence of the ensemble in the transport properties. The error bars (either the statistical ones or those derived from the fitting) are of the order of the symbol size in all the figures presented.

V. DATA ANALYSIS

QMC simulations yield results on the imaginary axis and the analytic continuation $i\omega_n\rightarrow\omega+i\delta$ is a numerically ill-conditioned problem. This is a subtle issue, since the existence of a finite Drude peak at $\omega=0$ cannot be obtained reliably by a numerical analytic continuation. The dynamical conductivity is, however, analytic in the upper half of the complex plane; its low ω_n behavior can therefore be used to determine its low ω behavior when (i) a general expression, correct at low frequencies, for $\sigma(z)$ (for complex z) is known and (ii) if one works at low enough temperatures in the QMC simulations such that the spacing of the Matsubara frequencies $\omega_n=2\pi T$ allows the numerical results for $\sigma(i\omega_n)$ to determine reliably the parameters of the general fitting functions. We will use this procedure here.

At low temperatures and frequencies, the scaling of $D(q,\omega_n)$ can be obtained simply invoking the conformal symmetry of the model emerging in the gapless regime $J_z<J_{xx}$. $S(q,\omega_n)$ at small q takes the form

$$S(q,\omega_n)=\frac{D_1(T)q^2}{(cq)^2+\omega_n^2}. \tag{25}$$

Note that, unlike near $q=\pi$, the dynamical susceptibility about $q=0$ does not show power laws. 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 $D_1(q,\omega_n)$ and we obtain $D_1(0)=J_{xx}/\pi$, and $\lim_{q\rightarrow0}J_{xx}\sin(q)=J_{xx}q\equiv cq$.

Expression (25) and Eq. (21) suggest the form

$$D(q,\omega_n)=\frac{D_1(T)\omega_n^2}{\Delta^2(q)+\omega_n^2}. \tag{26}$$

Alternatively, Eq. (26) can be viewed as the first term of the exact representation for $D(q,\omega_n)$ containing an infinite number of terms:[18]

$$D(q,\omega_n)=\sum_{j=1}^{2}\frac{D_j(q)\omega_n^2}{\Delta_j^2(q)+2\gamma_j(q)\omega_n+\omega_n^2}. \tag{27}$$

The choice of this fitting function is essential to distinguish the transport properties of ballistic and diffusive systems; indeed it allows the correct computation of the Drude weight and the diffusion coefficient. We discuss now in detail the properties of Eq. (27):

(i) For $\gamma_j(q)\geqslant0$, $D(q,\omega_n)$ is analytic in the upper half of the complex plane.

(ii) For the zero-q gaps $\Delta_i(0)=\lim_{q\rightarrow0}\Delta_i(q)$ we find two possibilities: $\Delta_1(0)=0$ and $\Delta_2(0)>0$, i.e., Eq. (27) describes a gapless phase, and $\Delta_1(0)>0$ and $\Delta_2(0)>\Delta_1(0)$, i.e., Eq. (27) describes a gapped phase. In the first case, Eq. (27) reproduces the correct ω and q dependencies for the scaling form of the Luttinger liquid (26). The first term in Eq. (27) dominates the low-frequency behavior in both cases and we have set generally $\gamma_2\equiv0$ in order to keep the number of parameters to a minimum.

(iii) At high frequencies

$$\lim_{\omega_n\rightarrow\infty}D(0,\omega_n)=-\langle K\rangle\equiv D_1(0)+D_2(0), \tag{28}$$

and a finite $D_2(0)$ results in a reduction of the Drude weight $D(T)$ with respect to the kinetic energy, see Eq. (12). A finite $D_2(0)$ measures the amount of decay experienced by the *total* current due to the interactions, see discussion below. We note also that the ansatz Eq. (27) for $D(q,\omega_n)$, together with Eq. (28), is consistent with the f sum rule[25]

$$\frac{1}{\pi}\int_0^\infty \mathrm{Re}\,\sigma(\omega)d\omega=-\langle K\rangle \tag{29}$$

for the optical conductivity.

(iv) In the gapless regime $D(q,\omega_n)/\omega_n$ can describe a normal conductor with finite dc conductivity whenever the damping $\gamma_1(0)$ is finite. Using the analytic continuation $i\omega_n\rightarrow\omega+i\delta$ we find for a term $n=1,2$, contributing the optical conductivity $D(q,\omega_n)/\omega_n$,

$$\lim_{\omega\rightarrow0}\left.\frac{-i\omega D_n(0)}{\Delta_n^2(0)-2i\omega\gamma_n(0)-\omega^2}\right|_{\Delta_n(0)>0}=0. \tag{30}$$

We find in general that $\Delta_2(q)>0$, as illustrated in Fig. 3 below, and hence $D_2(0)$ does not contribute to the Drude weight.

The real part of the optical conductivity (10) takes then, for small frequencies, the Drude form:

$$\mathrm{Re}\,\sigma(\omega)=\frac{2D_1(0)\gamma_1(0)}{\omega^2+4\gamma_1^2(0)}\equiv\frac{\sigma_0}{1+(\omega\tau)^2}, \tag{31}$$

where we introduced the dc conductivity

$$\sigma_0=D_1(0)/[2\gamma_1(0)] \tag{32}$$

and the quasiparticle lifetime

$$\tau=[2\gamma_1(0)]^{-1}. \tag{33}$$

For $\tau\rightarrow\infty$ Eq. (31) reduces to $\mathrm{Re}\,\sigma(\omega)=\pi D_1(0)\delta(\omega)$.

If we consider now the q dependence for $1/\omega\gg\tau$, the optical conductivity takes [for small $cq/\gamma_1(0)$] the diffusion form

$$\sigma(q,\omega)=\frac{\sigma_0\omega}{\omega+iD_sq^2},\quad D_s=\frac{c^2}{2\gamma_1(0)}\equiv c^2\tau. \tag{34}$$

D_s is the spin-diffusion constant. Equation (34) is consistent with $D_s=c\lambda_s$, where $\lambda_s=c\tau$ is the mean free length.

(v) The uniform spin stiffness $\rho_s=\lim_{q\rightarrow0}\lim_{\omega_n\rightarrow0}D(q,\omega_n)$ is always zero, as expected for a quantum critical antiferromagnetic chain.

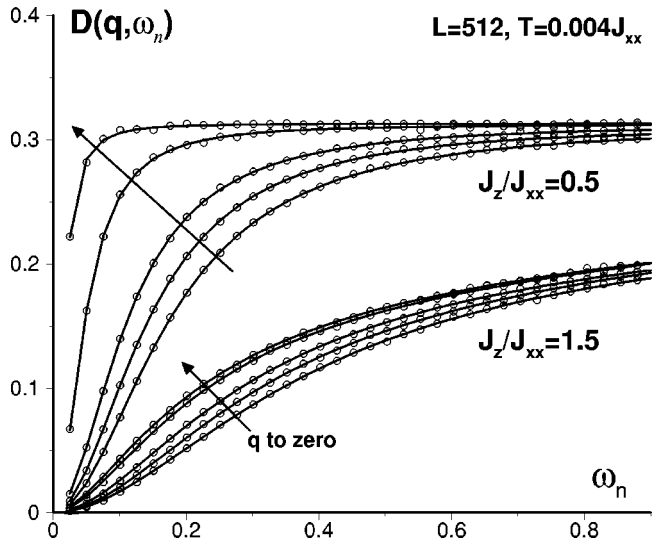

FIG. 2. $D(q,\omega_n)$ as a function of ω_n for various momenta q, $T=0.004J_{xx}$, and $J_z/J_{xx}=0.5$ and 1.5. The lines are fits by Eq. (27). Statistical errors are of the order of the symbol size. Note the different limiting behavior of $D(q\to 0,\omega_n)$ for $J_z/J_{xx}=0.5$ and $J_z/J_{xx}=1.5$.

(vi) The quality of the fit to $D(q,\omega_n)$ by Eq. (27) is, in general, excellent, as illustrated in Fig. 2 for $J_z=0.5J_{xx}$ and $J_z=1.5J_{xx}$. Note that the $q\to 0$ limiting curve for $D(q,\omega_n)$ is singular in the gapless phase ($J_z=0.5J_{xx}$), but well defined in the gapped phase ($J_z=1.5J_{xx}$).

VI. BALLISTIC TRANSPORT

In this section we will apply the procedure described in Sec. IV to the XXZ chain. We will compare with exact known results and study the controversial finite temperature behavior of $\sigma(\omega=0)$ for this model.

We present in Fig. 3 selected values for $D_{1,2}(q)$, $\Delta_1(q)$, and $\gamma_1(q)$ for $J_z/J_{xx}=1.0$ and 1.5 as obtained by fitting $D(q,\omega_n)$ with Eq. (27), see Fig. 2. We have included (no fit) in Fig. 3 the linearized Bethe-ansatz result for the magnon dispersion $\lim_{q\to 0}\Delta_1(q)=c(J_z)q$, which is valid in the gapless regime $J_z\leqslant J_{xx}$. The magnon velocity $c(J_z)$ is given by[26]

$$c(J_z)=\frac{\pi}{2}\frac{\sqrt{J_{xx}^2-J_z^2}}{\arccos(J_z/J_{xx})}=\frac{\pi}{2}\frac{\sin(\theta)}{\theta}, \tag{35}$$

where $J_z=\cos(\theta)J_{xx}$. In the gapped phase we used the standard ansatz $\Delta_1(q)=\sqrt{\Delta_0^2+(cq)^2}$ for a gapped dispersion relation, finding $\Delta_0=0.191J_{xx}$, which is close to twice the one-magnon gap of $0.091J_{xx}$.[26]

We find that the damping $\gamma_1(q)$ is very small for $J_z<J_{xx}$ and reduces for $q\to 0$. Within numerical accuracy we conclude that $\gamma_1(0)=0$ and that Re $\sigma(\omega)$ diverges for $\omega\to 0$. In the gapped phase, on the other side, we have found finite values for the damping with $\gamma_1(q)$, slightly increasing for $q\to 0$, see Fig. 3. Phenomenologically the relation $\gamma_1(q)\Delta_1(q)\approx$const holds for $J_z>J_{xx}$, independent of q.

In Fig. 4 we present values obtained by QMC simulations

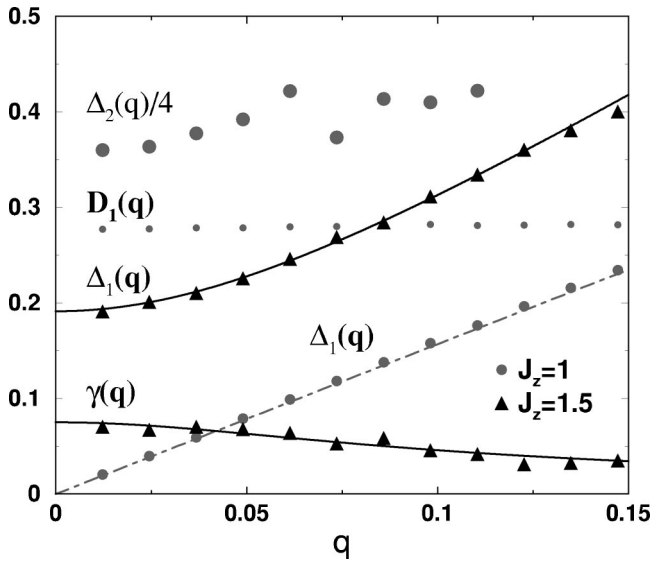

FIG. 3. $D_1(q)$, $\Delta_{1,2}(q)$, and $\gamma_1(q)$ from Eq. (27) as a function of momenta q for the XXZ model, $L=512$, and for various J_z at $T=0.004J_{xx}$. $\gamma_1(q)$ is too small for $J_z\leqslant J_{xx}$ to show up on this scale. The lines are the Bethe-ansatz result (35) for the velocity $c(J_z)$ (no fit, for $J_z\leqslant J_{xx}$). For the discussion of the fit for $J_z=1.5J_{xx}$, see the text.

for the q-dependent Drude weight for $J_z=J_{xx}$ at $T=0.004J_{xx}$. We find good convergence for small but finite q, but slow convergence for $q\to 0$ as a function of system size, due to the multiplicative logarithmic corrections present at the isotropic point. We have indicated by the horizontal arrow the $T=0$, $q=0$ Bethe-ansatz result.[27] For $J_z<J_{xx}$ the agreement between low-T QMC and $T=0$, $q=0$ Bethe-ansatz results is excellent.[19]

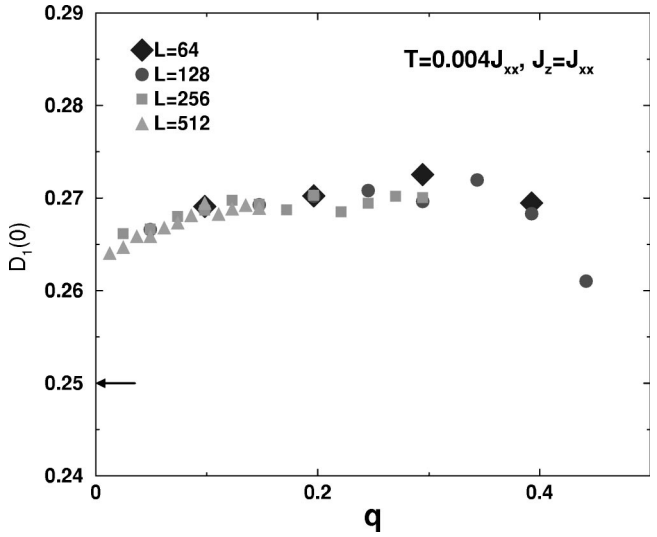

FIG. 4. The q-dependent Drude weight $D_1(q)$ for the isotropic Heisenberg chain at $T=0.004J_{xx}$ for various system sizes $L=64,\ldots,512$. The $T=0$, $q=0$ result given by Eq. (41) is indicated by the arrow. The convergence with system size is slow for $q\to 0$, due to the logarithmic corrections present at the isotropic point $J_z=J_{xx}$.

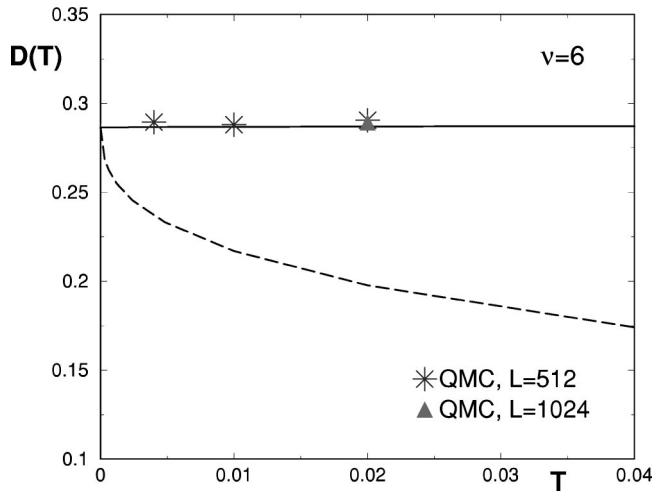

FIG. 5. QMC results for the Drude weight for $L=512$ and 1024 and $J_z=J_{xx}\cos(\pi/6)=0.866J_{xx}$ as a function of temperature (in units of J_{xx}) in comparison with two (solid lines: Ref. 29, dashed lines: Ref. 28) Bethe-ansatz results.

In order to obtain reliable data for the thermodynamic limit it is very helpful to avoid the problems apparent in Fig. 4 present in models with strong multiplicative corrections. This can be achieved by considering $J_z<J_{xx}$. Here we consider $J_z=J_{xx}\cos(\pi/6)$, see Fig. 5, since (i) Bethe-ansatz results have been presented for this ratio of J_z/J_{xx}, (ii) numerical problems due to multiplicative logarithmic corrections are absent for this value of J_z/J_{xx} (see Fig. 6), and (iii) J_z is large enough that substantial effects due to the ''interaction term'' J_z can be observed.

A fast decay of the Drude weight at low temperatures has been found by a Bethe-ansatz calculation by Zotos.[28] This result is in the high-temperature limit in agreement with exact diagonalization studies which converge relatively well in the limit of infinite temperatures.[7] A functionally different behavior for $D(T)$ has been found by Klümper *et al.*,[29] with an alternative Bethe-ansatz approach, see Fig. 5. The differences between the two different Bethe-ansatz predictions are substantial. In Fig. 5 we show a comparison of our data with the two available analytical results.[28,29] Our results agree with the temperature dependence predicted by Klümper *et al.*

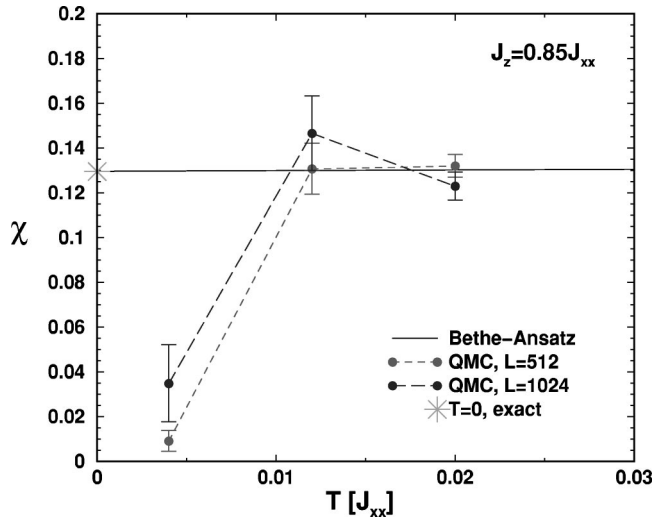

FIG. 6. QMC results for the uniform susceptibility $\chi(T)$ for $L=512$ and 1024 and $J_z=0.85J_{xx}$ together with the Bethe-ansatz result (solid line, Ref. 30), as a function of temperature. The star denotes the $T=0$ Bethe-ansatz result. Note the absence of finite-size effects for $T>0.012J_{xx}$ in the QMC data.

We have evaluated the uniform susceptibility $\chi(T)$ for $J_z=0.85J_{xx}$, and $L=512$ and 1024, and several low temperatures in order to address the following two questions: (i) Is it correct to compare $T=0$ Bethe-ansatz results with QMC results obtained for a temperature $T=0.004J_{xx}$ and $L=512$? (ii) Is $T=0.02J_{xx}$ large enough for $L=512$ and 1024 not to be affected substantially by finite-size effects? The data presented in Fig. 6 shows that $T=0.004J_{xx}$ is indeed below the finite-size gap and should be a good approximation to the $T=0$ data, and that for $T\geqslant 0.012J_{xx}$ no finite-lattice effect can be observed within the statistical error bars given. Note that the low-T dependence of the Bethe-ansatz[30] result shown in Fig. 6 for $\chi(T)$ can be fitted by $\chi(T)\sim T^x$ with $x\approx 0.867$. This exponent is very close to the exact value $x=0.858$ obtained by Eggert *et al.*[32] for $J_z=0.85J_{xx}$. Since $x<1$ the slope $d\chi(T)/dT$ diverges for $T\rightarrow 0$. This divergence is, however, not relevant for the temperature scale presented in Fig. 6.

VII. PHENOMENOLOGICAL RELATIONS BETWEEN TRANSPORT COEFFICIENTS

Let us consider a 1D system with a finite magnetization relaxation time τ, which might be due to either intrinsic relaxation processes or due to weak residual coupling to an external bath (i.e., phonons). The dc-magnetic conductivity takes then the form

$$\sigma(\omega=0)=D_1(0)\tau, \tag{36}$$

see Eqs. (32) and (33).

Let us assume that an inhomogeneous magnetic field $B^z(x)$ is applied in the chain along the z axis. In principle, this is a nonequilibrium situation but if dB^z/dx is small we can assume, after coarse-graining the chain, that we have a well-defined local magnetization $M(x)$ and all thermodynamic relations hold locally. Generalizing the usual phenomenology[31] for electric transport we write the magnetic current as

$$j(x)=v[M(x+\lambda)-M(x)]=\lambda v\frac{dM}{dx}, \tag{37}$$

where $\lambda=v\tau$ is the mean free path and v is the velocity associated to the magnetization current that we will identify later. We can express the magnetization current in terms of the gradient of the magnetic field:

$$j(x)=v^2\tau\frac{dM}{dx}=v^2\tau\frac{dM}{dB^z}\frac{dB^z}{dx}. \tag{38}$$

Using $j(x)=\sigma(dB^z/dx)$ we arrive at the expression

$$\sigma=v^2\tau\chi. \tag{39}$$

This relation is analogous to the well-known[31] phenomenological kinetic formula for the thermal conductivity $\kappa = c_V v^2 \tau$, where c_V is the specific heat and κ the thermal conductivity. τ can be eliminated if we use Eq. (36):

$$\frac{\sigma}{\chi\tau} = \frac{D_1(0)\tau}{\chi\tau} = \frac{D_1(0)}{\chi} = v^2. \tag{40}$$

This phenomenological equation is independent of the value of τ, and holds also in the limit $\tau \to \infty$, when $D_1(0)$ becomes the Drude weight. Since the derivation of Eq. (40) is based on quasiballistic arguments, it is of interest to examine whether this relation holds at low temperatures for Luttinger liquids and Bethe-solvable models. At $T=0$ both magnitudes χ and D have been computed exactly[27,32] for the XXZ chain by Bethe Ansatz:

$$D(0) = \frac{J_{xx}\pi}{4} \frac{\sin(\theta)}{\theta(\pi-\theta)}, \tag{41}$$

where we have defined $J_z = \cos(\theta) J_{xx}$ and

$$\chi(0) = \frac{\theta}{J_{xx}\pi(\pi-\theta)\sin(\theta)}. \tag{42}$$

Dividing both relations we obtain

$$\frac{D_1(0)}{\chi(0)} = \frac{\pi^2 J_{xx}^2}{4} \frac{\sin^2(\theta)}{\theta^2} \equiv c^2(J_z). \tag{43}$$

This result then allows us to identify the magnetization-transport velocity v in Eq. (40) with the spin-wave velocity $c(J_z)$: At $T=0$ Eq. (40) is then exact. The validity of Eq. (43) in a leading, low-T correction is an open question presently. The leading T corrections to $D_1(T)$ and $\chi(T)$ are $\sim T^2$ for $J_z=0$ and do not cancel; Eq. (43) is exact for the XX model only at $T=0$. The leading T corrections to the susceptibility show,[32] however, an exponent crossover for $J_z = 0.5 J_{xx}$ and Eq. (43) might hold in leading low-T order for $J_z > 0.5 J_{xx}$.

A relation similar to Eq. (40) has been discussed recently for thermal transport[33,34] experiments,[3,35] where we define[20,33] $\kappa(T) \equiv \kappa^{th}(T)\tau$, where κ^{th} is the *thermal Drude weight*. For the XXZ chain one finds[34] that both $\kappa^{th}(T)$ and $c_V(T)$ are linear in temperature for small temperatures and that

$$\lim_{T\to 0} \frac{\kappa^{th}(T)}{c_V(T)} = c^2(J_z). \tag{44}$$

Combining Eq. (40) and Eq. (44) we obtain

$$\frac{D_1(0)}{\chi(0)} = \lim_{T\to 0} \frac{\kappa^{th}(T)}{c_V(T)}. \tag{45}$$

For ballistic systems the quantity $D_1(0)$ in the above equation is identical to the Drude weight. This relation can therefore be interpreted in the framework of a Luttinger liquid. The Hamiltonian of a Luttinger liquid can be written in the diagonal form:

$$H = \sum_q v_s |q| b_q^\dagger b_q + \frac{1}{2}\frac{\pi}{L}(v_N N^2 + v_J J^2), \tag{46}$$

where the first term corresponds to the bosonic part and N and J are integer quantum numbers associated to states with nonzero charge and current, respectively. The three velocities present in the Hamiltonian, the sound velocity v_s, the charge velocity v_N, and the current velocity v_J, are not independent but restricted by an universal relation valid in all microscopic models in the Luttinger-liquid universality class:[36]

$$v_N v_J = v_s^2. \tag{47}$$

For the XXZ chain the values of these three parameters of the effective low-energy Hamiltonian (46) have been identified *independently*, v_N and v_s by Haldane[36] and v_J by Gomez-Santos,[37] using the results of different Bethe-ansatz studies.[27,38,39]

Guided by the phenomenological derivation presented above we propose the following (phenomenological) finite temperature extensions of the velocities in Eq. (46):

$$\pi v_N \to \frac{1}{\chi(T)}, \quad \frac{v_J}{\pi} \to D_1(T), \quad v_s^2 \to \frac{\kappa^{th}(T)}{c_V(T)}. \tag{48}$$

The extension to finite temperatures of v_N and v_J are in agreement with their physical meanings $\pi v_N = (dB/dM)_{B=0}$ and[20,37] $v_J/\pi = L(d^2E/d^2\Phi)_{\Phi=0}$ for Luttinger liquids. On the other hand, for the magnitudes involved in the thermal ratio, the bosonic part of the Hamiltonian does play an important role. In fact, only the bosonic degrees of freedom transport the energy in the homogeneous states (which, by definition[31] do not carry particle currents) relevant for the thermal conductivity $\kappa = \kappa^{th}\tau$ and the specific heat c_V. It is therefore justified to consider κ^{th}/c_V as the natural extension of v_s^2 to low temperatures. Recently this ratio has been computed using Bethe-ansatz techniques at all temperatures by Klümper and Sakai.[34] κ^{th}/c_V is a well-behaved function of T; even more it is very flat at low temperatures and takes the expected value $v_s^2 \equiv c^2(J_z)$ at $T=0$.

VIII. DIFFUSIVE TRANSPORT

We study now the effect of nonintegrable interaction terms in the conductivity of a 1D spin system. To be specific, we add a small perturbation to $H^{(xxz)}$, which breaks the integrability of $H^{(xxz)}$:

$$H' = J_z' \sum_i S_i^z S_{i+3}^z. \tag{49}$$

The expression (3) for the spin current remains valid, since H' does contain only S^z operators and the system remains nonfrustrated and free from sign problems. We have performed QMC simulations for the resulting model $H = H^{(xxz)} + H'$ mainly for $J_z = J_{xx}\cos(\pi/6)$. We find a transition to a gapped phase around $J_z' \cong 0.3 J_{xx}$, see Fig. 7. The exponential opening of the gap resembles a Kosterlitz-Thouless transition very similar to the one present in the XXZ chain at the isotropic point and suggests that H' does

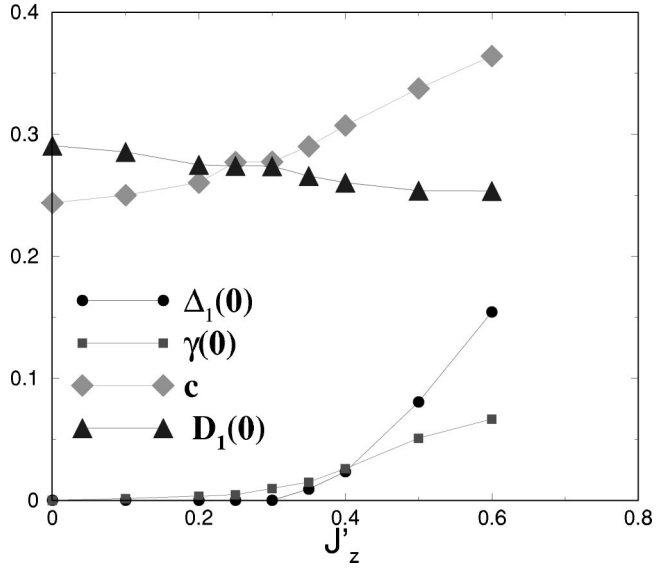

FIG. 7. For $L=512$ and $T=0.004J_{xx}$ the QMC results for the gap $\Delta_1(0)$, the relaxation rate $\gamma_1(0)$, the effective velocity c, and the parameter $D_1(0)$ as a function of J_z' for $H^{(xxz)}+H'$ with $J_z=J_{xx}\cos(\pi/6)$.

not change the universal properties of $H^{(xxz)}$, it only shifts the transition point and adds the ingredient of nonintegrability. We find the relaxation time $\tau=1/[2\gamma_1(0)]=\lim_{q\to 0}1/[2\gamma_1(q)]$ to be finite within numerical accuracy (due to finite-q and ω_n resolution), leading to a finite dc conductivity in the gapless phase.

We have examined the temperature dependence of the resulting dc conductivity. Due to our restriction to $T\ll J_{xx}$, resulting from the finite-ω_n resolution on the imaginary axis (see Sec. IV), we could not examine a large enough T range in order to determine the full T dependence of $\sigma(0)$. We found for $J_z'=0.3J_{xx}$ $\sigma(T=0.004J_{xx})=13.6\pm 0.9$, $\sigma(T=0.008J_{xx})=12.1\pm 1.0$, and $\sigma(T=0.012J_{xx})=10.1\pm 0.8$.

In agreement with our expectation of a diverging dc conductivity in a translationally invariant system at $T=0$ we find $\sigma(0.008)>\sigma(0.012)$. The increase from $\sigma(0.008)$ to $\sigma(0.004)$ is, on the other hand, only modest, presumably due to the finite-size resolution limitation illustrated in Fig. 6.

IX. CONCLUSIONS

We have shown that quantum Monte Carlo simulations of quantum spin chains are a powerful tool to obtain finite and diverging transport coefficients at very low temperatures. We have derived an useful relation between the dynamical structure factor $S(q,\omega_n)$ and the dynamical conductivity $\sigma(q,\omega_n)$, which allows to calculate $\sigma(q,\omega_n)$ to very high accuracy on the imaginary axis. For an integrable chain we support the original suggestion by Zotos *et al.*[9–11] 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., a zero Drude weight) for a nonintegrable model, for which we are able to estimate the magnitude of the dc conductivity. We have discussed our result in the framework of phenomenological relations and Luttinger-liquid theory. Connections to recent studies of the diverging thermal conductivity of quantum spin chains were made.

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