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 (QMC) data on the imaginary axis allows to distinguish between intrinsic ballistic and diffusive transport. We determine the Drude weight, current-relaxation life-time and the mean-free path for integrable and a non-integrable quantum-spin chain. We discuss, in addition, some phenomenological relations between various transport-coefficients and thermal response functions.

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I. INTRODUCTION

The role of the spin excitations on the transport properties of quasi-one dimensional Mott-insulators has been the subject of extensive experimental research in the last few years. A recent $^{17}$O NMR investigation of Sr$_2$CuO$_3$, extending an earlier $^{63}$Cu NMR study, 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$_2$CuO$_3$ and SrCuO$_2$ indicate at the same time, quasi-ballistic transport with a mean-free path of several thousands of $\AA$.

It is well known from structural considerations and from studies of the magnetic excitation spectrum, that Sr$_2$CuO$_3$ 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 quasi-ballistic) magnetization transport have been found in recent exact diagonalization studies of $H^{(xxz)}$ at high temperatures. A connection between integrability, conservation laws and ballistic transport has been proposed by Zotos and coworkers. If the current-current correlation does not decay to zero for long times, i.e when part of the current operator is conserved, i.e. when a certain (non-zero) 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 non-integrable models which do exhibit ballistic transport, none has been found so far. Real compounds like Sr$_2$CuO$_3$ and SrCuO$_2$ correspond to $H^{(xxz)}$ anyhow only in first approximation. It is therefore important to examine whether general, non-integrable, quantum spin chains show ballistic or diffusive transport properties at finite temperatures. This question has been studied by Rosch and Andrei within a short-time approximation (a memory-matrix approach, extending an earlier analysis by Giamarchi) 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, the coupling spin-phonon coupling has been studied by Narozhny.

In his seminal paper in 1960, W. Kohn proved that the existence of a the 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, like spin-Peierls compounds, from a spin conductor like Sr$_2$CuO$_3$. Despite an on-going effort devoted to this problem, the fundamental difference between models with ballistic and diffusive transport properties has shown up only recently in QMC-simulations.

The purpose of this paper is to explain in detail how this important issue can be tackled numerically by QMC.

The organization of the paper is as follows. Section II contains the basic definitions and sets the notation that we will use along the paper. In Section 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 Section 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 Section V we describe a procedure to extract transport coefficients (Drude weight and the diffusion coefficient) from QMC-data in general 1D interacting systems either integrable or non-integrable. In Section VI we apply this method to the XXZ chain and we obtain the Drude weight at finite temperatures. We then discuss several phenomenology relations between transport and thermal coefficients in Section VII. Section VIII is devoted to the computation of diffusion constants, mean-free paths and life-times in a non-integrable spin chain. In Section IX we present our conclusions.
II. SPIN CONDUCTIVITY

QMC-simulations yield in general correlations 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 \( \Phi = \sum_l \phi_l \) in the quantization axis.

\[
H^{(xxz)}(\Phi) = \sum_l \left[ k_l \cos(\phi_l) + j_z^l \sin(\phi_l) + J_z S^z_l S^z_{l+1} \right]
\]  

(1)

where

\[
k_l = \frac{J_{xx}}{2} \left( S^+_l S^-_{l+1} + S^-_l S^+_{l+1} \right)
\]  

(2)

and

\[
j_z^l = \frac{J_{zz}}{2} \left( S^+_l S^-_{l+1} - S^-_l S^+_{l+1} \right)
\]  

(3)

Formally (1) is the hamiltonian of a XXZ chain in which the quantization axis of the local spin operators has been rotated by a site-dependent angle \( \phi_l \) 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:

\[
H^{(xxz)}(\Phi) = H^{(xxz)} + \sum_l j_z^l \phi_l + \frac{k_l}{2} \phi_l^2
\]  

(4)

and we obtain the total spin-density current by differentiating with respect to \( \phi_l \).

\[
\frac{\partial H^{(xxz)}(\Phi)}{\partial \phi_l} = (j_z^l)^T = j_z^l + k_l \phi_l
\]  

(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.

\[
\frac{\partial}{\partial t} S^z_l(t) + (j_z^l(t) - j_z^{l-1}(t)) = 0
\]  

(6)

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

\[
\frac{\partial}{\partial t} S^z_l(t) = i[H, S^z_l]
\]  

(7)

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

\[
\langle j_z^l(q, \omega_n) \rangle = -\left( \langle K \rangle + \Lambda(q, \omega_n) \right) \phi_l
\]  

(8)

where \( \langle K \rangle = \sum_k k_l \) is the expectation value of the kinetic energy per site and \( \Lambda \) is the current-current correlation as a function of the Matsubara frequency,

\[
\Lambda(q, \omega_n) = \frac{1}{\beta} \int_0^\beta e^{i\omega_n \tau} \langle j_z^q(\tau) j_z^{-q}(0) \rangle \, d\tau
\]  

(9)

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

\[
\sigma(q, \omega_n) = -\frac{\langle K \rangle - \Lambda(q, \omega_n)}{\omega_n} \equiv \frac{D(q, \omega_n)}{\omega_n}
\]  

(10)

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

\[
\sigma(\omega) = \pi D(T) \delta(\omega) + \sigma_{reg}(\omega, T)
\]  

(11)

where \( D(T) \) is the Drude weight that can be computed via \( D(T) = \lim_{\omega_n \to 0} \lim_{\eta \to 0} D(q, \omega_n) \):

\[
D(T) = -\langle K \rangle - \Lambda(q \to 0, \omega_n \to 0)
\]  

(12)

It can be proved that this limit is consistent with the definition introduced by W. Kohl at \( T = 0 \),

\[
D = L \left( \frac{d^2 E}{d^2 \Phi} \right)_{\Phi=0}
\]  

(13)

where \( E \) is the ground state energy and \( \Phi \) the total external flux. Recently \( D \) has been extended by Zotos, Naef to finite \( T \)

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

(14)

It is important to note that the limits \( \lim_{q \to 0} \) and \( \lim_{\omega_n \to 0} \) 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.

\[
\rho_s = \lim_{q \to 0} \lim_{\omega_n \to 0} D(q, \omega_n)
\]  

(15)

A non-zero value of the Drude weight implies that the total magnetic-current does not decay to zero when \( t \to \infty \) (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

\[
\Lambda(q, \omega_n) = \frac{1}{ZL} \sum_{m,n} \frac{E_m - E_n}{\epsilon \omega_n - (E_m - E_n)}
\]  

(16)

Note that degenerated states are explicitly excluded from the sum and therefore \( \langle |m| j_z^2(q)|n\rangle = 0 \) and the conductivity reduces to \( \sigma = -\pi \langle K \rangle \delta(\omega) \) that 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 remain 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 non-integrable systems) enhanced to fulfill the f-sum rule.

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

where we have used the definition (13). The double commutator in the right hand side of Eq. (19) is the boundary term of the partial integration and is evaluated to

\[ \langle [H, S^z_q], S^z_{-q} \rangle = 4 \sin^2(q/2) \langle K \rangle \]

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

\[ D(q, \omega_n) = \frac{\omega_n^2}{4 \sin^2(q/2)} S(q, \omega_n) . \]

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

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

\[ S(q, \omega_n) = \frac{1}{L} \int_0^\beta e^{i\omega_n \tau} \langle S^z_q(\tau)S^z_{-q}(0) \rangle . \]

In Fourier space, the continuity equation (3) takes the form

\[ \frac{d}{d\tau} S^z_q(\tau) = [H, S^z_q] = i \left( 1 - e^{iq} \right) j^z_q . \]

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

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

where we have used the definition (13). The double commutator in the right hand side of Eq. (19) is the boundary term of the partial integration and is evaluated to

\[ \langle [H, S^z_q], S^z_{-q} \rangle = 4 \sin^2(q/2) \langle K \rangle \]

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

\[ D(q, \omega_n) = \frac{\omega_n^2}{4 \sin^2(q/2)} S(q, \omega_n) . \]

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

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 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 [22] for an excellent review).

The current-current correlation function in real space and imaginary time takes the form
\[ \Lambda(l, \tau) = \frac{1}{L N_T} \sum_{l', \tau'} j_{l+l'}^\ast (\tau' + \tau) j_{l'}^\ast (\tau') \]  

where \( N_T \) is the number of Trotter slices. The contributions to \( \Lambda(l, \tau) \) are non-diagonal four-site operators, typically \( (J_{xx}/4)S_{l_1}^+(\tau_1)S_{l_2}^+(\tau_2)S_{l_3}^+(\tau_3)S_{l_4}^+(\tau_4) \). In principle non-diagonal operators can be computed using the loop algorithm. When these non-diagonal 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. 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 \( G_{xx}^{(1)} \) and the relation \( \Sigma \). The dynamical structure factor is then

\[ S(q, \omega_n) = \sum_{\alpha} W(q, \omega_n, \alpha) W(-q, -\omega_n, \alpha), \]  

where \( \alpha \) runs over all loops constructed. In particular we want to emphasize the importance of relation \( \Sigma \), 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.

A second technical important issue is the relation between the conductivities in real and imaginary axis. As has been discussed by Kirchner, Evertz and Hanke the limit \( \omega \to 0 \) of the conductivity can be also approached from the imaginary frequency axis. Taking the analytical continuation to the real frequencies \( i\omega_n \to \omega + i\delta \) in the spectral representation of \( \Sigma(q, \omega_n) \) (Eq. \( 10 \)), we note that \( \Sigma(q, \omega + i\delta) \) is analytic in the upper half of the complex \( \omega \)-plane. Zero-frequency properties like the Drude weight or the diffusion constant can be reliably extracted by the extrapolation along the imaginary axis at low temperatures, when many Matsubara frequencies \( \omega_n = 2\pi T n \) are available close to \( \omega = 0 \) for the extrapolation. This is the case, however, only at low temperatures and will therefore present results only for \( T \ll J_{xx} \).

Finally we mention a few numerical details. We used the discrete imaginary-time version of the Loop Algorithm with a Trotter decomposition of typically \( N_T = 800 \) and on the average \( 6 \times 10^6 \) 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.

![Fig. 3](image-url)  

**FIG. 3.** \( D_1(q) \), \( \Delta_1(q) \) and \( \gamma_1(q) \) from Eq. \( 25 \) as a function of momenta \( q \) for the XXZ-model, \( L = 5 \times 10^3 \) and for various \( J_z \) at \( T = 0.004 J_{xx} \). \( \gamma_1(q) \) is too small for \( J_z \leq J_{xx} \) to show up on this scale. The lines are the Bethe-Ansatz result \( \Sigma \) for the velocity \( c(J_z) \) (no fit, for \( J_z \leq J_{xx} \)). For the discussion of the fit for \( J_z = 1.5 J_{xx} \) see the text.

**V. DATA-ANALYSIS**

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 then form

\[ S(q, \omega_n) = \frac{D_1(T) q^2}{(c q)^2 + \omega_n^2}. \]  

Note that, unlike near \( q = \pi \), the dynamical susceptibility about \( q = 0 \) do 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 \( D_1(0) = J_{xx}^2 / \pi \), and lim \( \omega_n \to 0 J_{xx} \sin(q) / J_{xx} q \equiv c q \).

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

\[ D(q, \omega_n) = \frac{D_1(T) \omega_n^2}{\Delta^2(q) + \omega_n^2}. \]  

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.

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

i.) $D(q, \omega_n)$ is analytic in the upper complex-plane for $\gamma(q) \geq 0$.

ii.) For the zero-$q$ gaps $\Delta_1(0) = \lim_{q \to 0} \Delta_1(q)$ we find to possibilities: (a) $\Delta_1(0) = 0$ and $\Delta_2(0) > 0$, i.e., Eq. (27) describes a gapless phase. (b) $\Delta_1(0) > 0$ and $\Delta_2(0) > \Delta_1(0)$ and i.e., Eq. (27) describes a gaped phase. In the first case, (27) reproduces the correct $\omega$ and $q$ dependence for the scaling form of the Luttinger liquid (28). The first term in Eq. (27) 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.

iii.) At high frequencies

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

(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. (22). A finite $D_2(0)$ measures therefore the amount of decay experienced by the total current due to the interactions. We note also that the Ansatz Eq. (27) for $D(q, \omega_n)$, together with Eq. (28), is consistent with the f-sum-rule (20).

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

(29)

for the optical conductivity.

iv.) In the gapless regime $D(q, \omega_n)$ can describe a normal conductor with finite DC-conductivity. The optical conductivity (10) takes for small frequencies the Drude form.

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

(30)

where we introduced the DC-conductivity

$$\sigma_0 = D_1(0)/(2\gamma_1(0))$$

(31)

and the quasi-particle lifetime

$$\tau = (2\gamma_1(0))^{-1}.$$ 

(32)

For $\tau \to \infty$ Eq. (30) reduces to $\text{Re} \sigma(\omega) = \pi D_1(0) \delta(\omega)$. Even more, 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

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

(33)

$D_s$ is the spin-diffusion constant. Eq. (33) is consistent with $D_s = c\lambda_s$, where $\lambda_s = c\tau$ is the mean free length.

v.) The uniform spin stiffness $\rho_s = \lim_{q \to 0} \lim_{\omega_n \to 0} D(q, \omega_n)$ is always zero, as expected for a quantum-critical antiferromagnetic chain.

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 gaped phase ($J_z = 1.5J_{xx}$).

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. (10) 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 $J_z = J_{xx}$.

VI. BALLISTIC TRANSPORT

In this Section we will apply the procedure described in Section V 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.

In Fig. 3 we show the values for $D(q)$, $\Delta_1(q)$ and $\gamma_1(q)$ for $J_z/J_{xx} = 0.5, 1.0$ and 1.5. These are the values used in Fig. 2 for fitting $D(q, \omega_n)$. We have included (no fit) in Fig. 3 for the gapless regime $J_z \leq J_{xx}$, the Bethe-Ansatz result $\lim_{q \to 0} \Delta_1(q) = c(J_z) q$ for the magnon dispersion, where $c(J_z)$ is the velocity

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

(34)

of the des Cloizeaux-Pearson spectrum (2), with $J_z = \cos(\theta)J_{xx}$. In the gaped phase we have fitted $\Delta_1(q)$ 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 $0.091J_{xx}$.

The damping $\gamma_1(q)$ is vanishing small for $J_z < J_{xx}$ and acquires a finite value in the gaped phase. We found phenomenological that $\gamma_1(q) = \text{const.}$, independent of $q$, for $J_z > J_{xx}$. In Fig. 3 we present values obtained by QMC 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. For $J_z < J_{xx}$ the agreement in between low-$T$ QMC and the $T = 0$, $q = 0$ Bethe-Ansatz result is excellent.

We study now the behavior of the Drude weight at finite temperatures for models free from strong multiplicative corrections. The main conclusion of a Bethe-Ansatz calculation by Zotos is a fast decay of the Drude weight when the temperature increases, in agreement with exact diagonalization studies in the limit of infinite temperatures. Klümper et al. have found, with an alternative Bethe-ansatz approach, a functionally different behavior for $D(T)$, see Fig. 3. For a numerical probe of $D(T)$ we focus on $J_z = J_{xx} \cos(\pi/6)$ and consider several small temperatures. For this value of $J_z/J_{xx}$ the numerical problems due to multiplicative logarithmic corrections are absent (compare Fig. 3) and the difference in 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. Our results agree with the temperature-dependence predicted by Klümper et al.

We have evaluated the uniform susceptibility $\chi(T)$ for $J_z = 0.85J_{xx}$, $L = 512$, 1024 and several low temperatures in order to address the two questions: (a) Is it correct to compare $T = 0$ Bethe-Ansatz results with QMC-results obtained for a temperature $T = 0.004J_{xx}$ and $L = 512$? (b) Is $T = 0.02J_{xx}$ large enough for $L = 512$, 1024 not to be affected substantially by finite-size effects? The data presented in Fig. 4 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 $T \geq 0.012J_{xx}$ no finite-lattice effect can be observed within the statistical error-bars given. Note that the low-$T$ dependence of the Bethe-Ansatz result shown in Fig. 4 for $\chi(T)$ can be fitted by $\chi(T) \sim T^3$ with $x \approx 0.867$. This exponent is very close to the exact value $x = 0.858$ obtained by Eggert et al. for $J_z = 0.85J_{xx}$. Since $x < 1$ the slope $\Delta \chi(T)/\Delta T$ is diverging for $T \to 0$. This divergence is, however, not relevant for the temperature-scale presented in Fig. 4.

Let us consider a 1D system system with a finite magnetization relaxation time $\tau$, 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

$$\sigma(\omega = 0) = D_1(0) \tau,$$  \hspace{1cm} (35)

see Eq. 34 and (24).

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 non-equilibrium 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 for electric transport we write the magnetic current as

$$j(x) = v(M(x + \lambda) - M(x)) = \lambda v \frac{dM}{dx},$$  \hspace{1cm} (36)

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

$$j(x) = v^2\tau \frac{dM}{dx} = v^2\tau \frac{dM}{dB^z} \frac{dB^z}{dx}.$$  \hspace{1cm} (37)

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

$$\sigma = v^2\tau \chi.$$  \hspace{1cm} (38)

This relation is analogous to the well-known phenomenological kinetic formula for the thermal conductivity $\kappa = c_V v^2\tau$, where $c_V$ is the specific heat and $\kappa$ the
thermal conductivity. \( \tau \) can be eliminated if we use Eq. (33):

\[
\frac{\sigma}{\chi \tau} = \frac{D_1(0)}{\chi \tau} = \frac{D_1(0)}{\chi} = v^2 .
\]

(39)

This phenomenological equation is independent of the value of \( \tau \), and holds also in the limit \( \tau \to \infty \), when \( D_1(0) \) becomes the Drude weight. Since the derivation of (39) is based on quasi-ballistic 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 \( \chi \) and \( D \) have been computed exactly for the XXZ chain by Bethe-Ansatz:

\[
D(0) = \frac{J_{xx} \pi}{4} \sin(\theta)\frac{\theta}{\theta(\pi - \theta)},
\]

(40)

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

\[
\chi(0) = \frac{\pi^2 J_{xx}^2 \sin^2(\theta)}{4 \theta^2} \equiv c^2(J_z).
\]

(41)

This results then allows us to identify the magnetization-transport velocity \( v \) in (33) with the spin-wave velocity \( c(J_z) \): At \( T = 0 \) Eq. (39) is then exact. The validity of (12) in leading, low-T correction is an open question presently. The leading \( T \)-correction to \( D_1(T) \) and \( \chi(T) \) are \( \sim T^2 \) for \( J_z = 0 \) and do not cancel; Eq. (12) is exact for the XX-model only at \( T = 0 \). The leading \( T \)-corrections to the susceptibility show\(^\text{12}\) however, an exponent crossover for \( J_z = 0.5J_{xx} \) and (12) might hold in leading low-T order for \( J_z > 0.5J_{xx} \).

A relation similar to (10) has been discussed recently for thermal transport experiments\(^\text{6,13}\) where we defined\(^\text{6,13}\) \( \kappa(T) \equiv \kappa^{th}(T) \tau \), where \( \kappa^{th}(T) \) is the thermal Drude weight. For the XXZ chain one finds\(^\text{6,13}\) that both \( \kappa^{th}(T) \) and \( \theta(T) \) are linear in temperature for small temperatures and that

\[
\lim_{T \to 0} \frac{\kappa^{th}(T)}{\theta(T)} = \sqrt{c^2(J_z)} .
\]

(43)

Combining Eq. (13) and Eq. (14) we obtain

\[
\frac{D_1(0)}{\chi(0)} = \lim_{T \to 0} \frac{\kappa^{th}(T)}{\theta(T)} .
\]

(44)

For ballistic systems the quantity \( D_1(0) \) in 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:

\[
H = \sum_q v_q |q| b_q^\dagger b_q + \frac{1}{2} \frac{\pi}{L} (v_N N^2 + v_J J^2) ,
\]

(45)

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.

\[
v_N v_J = v_s^2 .
\]

(46)

For the XXZ chain the values of these three parameters of the effective low-energy Hamiltonian (13) have been identified independently, \( v_N \) and \( v_s \) by Haldane\(^\text{37}\) and \( v_J \) by Gomez-Santos\(^\text{37}\) using the results of different Bethe-Ansatz studies\(^\text{11,12}\).

Guided by the phenomenological derivation presented above we propose the following (phenomenological) finite-temperature extensions of the velocities in Eq. (45).

\[
v_N \to \frac{1}{\chi(T)}, \quad v_J \to D_1(T), \quad v_s \to \frac{\kappa^{th}(T)}{\theta(T)}
\]

(47)

The extension to finite temperatures of \( v_N \) and \( v_J \) are in agreement with their physical meaning \( v_N = \left( \frac{d \Phi}{d \xi} \right)_{B=0} \) and\(^\text{11,12}\) \( v_j/\pi = L(\frac{d \tilde{E}}{d \phi})_{\phi=0} \) 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 do not carry particle currents) relevant for the thermal conductivity \( \kappa = \kappa^{th} \tau \) and the specific heat \( \theta(T) \). It is therefore justified to consider \( \kappa^{th}/\theta(T) \) as the natural extension of \( \sigma_s \) to low temperatures. Recently this ratio has been computed using Bethe-Ansatz techniques at all temperatures by Klumper and Sakai\(^\text{34}\) \( \kappa^{th}/\theta(T) \) is a well behaved function of \( T \), even more it is very flat at low temperatures and takes the value the expected value \( \sigma_s^2 \equiv c^2(J_z) \) at \( T = 0 \).
FIG. 6. QMC results for the uniform susceptibility $\chi(T)$ for $L = 512$, 1024 and $J_z = 0.1J_{xx}$ together with the Bethe-Ansatz result (solid line, Ref.[4]), 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.

VIII. DIFFUSIVE TRANSPORT

We study now the effect of non-integrable 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 $H^{(xxz)}$:

$$H' = J'_z \sum_i S^z_i S^z_{i+3}. \quad (48)$$

The expression (48) for the spin current remains valid, since $H'$ does contain only $S^z$-operators and the system remains non-frustrated 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 gaped phase around $J'_z \approx 0.3J_{xx}$, 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 $H'$ is not changing the universal properties of $H^{(xxz)}$, only shifting the transition point and adding the ingredient of non-integrability. We find the relaxation time $\tau = 1/(2\gamma_1(0)) = \lim_{q \rightarrow 0} 1/(2\gamma_1(q))$ to be finite within the numerical accuracy (due to finite-q and $\omega_n$ 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 $T < J_{xx}$, resulting from the finite-$\omega_n$ resolution on the imaginary axis (see Section [V]) 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 translational-invariant system 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.[1] 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 non-integrable 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 was made.

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