

Quantum Monte Carlo simulation for the conductance of one-dimensional quantum spin systems

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Recently, the stochastic series expansion (SSE) has been proposed as a powerful Monte Carlo method, which allows simulations at low T for quantum-spin systems. We show that the SSE allows us to compute the magnetic conductance for various one-dimensional spin systems without further approximations. We consider various modifications of the anisotropic Heisenberg chain. We recover the Kane-Fisher scaling for one impurity in a Luttinger liquid and study the influence of noninteracting leads for the conductance of an interacting system.

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I. INTRODUCTION

In general, integrable one-dimensional models show an ideally conducting behavior in contrast to most real three-dimensional materials.¹ There has been intensive investigation of the influence of the integrability on the conductivity for various model systems.¹⁻⁴ The conductance of conducting, nearly one-dimensional devices is, on the other hand, of substantial experimental interest. Over the last years it has become possible to fabricate mesoscopic devices,⁵ such as carbon nanotubes which can be viewed as a realization of systems with ballistic transport properties. Therefore the computation of dynamical transport quantities has received considerable interest.

A basic approach for the study of the conductance has been in the past via the Bosonization of appropriate model systems,⁶⁻⁸ valid in the low-temperature limit. Numerical studies have so far involved the density-matrix renormalization-group (DMRG) technique^{9,10} and Monte Carlo (MC).^{11,12} In the case of Ref. 9 a reduced set of states was used in order to evaluate the dynamics; in Ref. 10, a phenomenological formula by Sushkov¹³ was used to compute the conductance. The simulations by Refs. 11 and 12 use an effective Bosonized Hamiltonian as a starting point.

Here we will discuss how to obtain the conductance with quantum Monte Carlo (QMC) on the original lattice Hamiltonian. For this purpose the conductance will be calculated on the imaginary frequency axis. We will show that a reliable extrapolation to zero frequency can be performed at finite but low temperatures. We will thus obtain approximation-free results for the dynamics of inhomogeneous quantum-spin systems at low but finite temperatures, within a well defined numerical accuracy defined by the statistics of the MC sampling and the accuracy of the zero-frequency extrapolation.

By the Jordan-Wigner transform a one-dimensional spinless Fermionic system can be mapped to a hard-core boson model. Hence it is possible to calculate the conductance for a Fermionic system in a Bosonic one. This is vitally important since boson models can be easily analyzed by Monte Carlo simulations where the sign problem is absent. However, for an evaluation of the conductance one requires a highly efficient simulation method which performs well at low temperatures. Recently,¹⁴ such a powerful method has been proposed: the stochastic series expansion (SSE). In this paper

we will compute the conductance in a hard-core boson lattice model by the aid of this method.

II. EXPLANATION OF THE METHOD

A. Definition of the conductance

We consider the anisotropic xxz Hamiltonian

$$H_{xxz} = \sum_{n=1}^{N-1} J_x (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) / 2 + J_z S_n^z S_{n+1}^z,$$

where the $S_n^\pm = S_n^x \pm iS_n^y$ are the raising/lowering operators for spin-1/2 Heisenberg spins. The spin-current operator j_n at a given site n follows from the continuity equation and is given by (see, e.g., Ref. 4)

$$j_n = iJ_x e (S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+) / (2\hbar).$$

As a perturbation we will use a local “voltage drop.” In the hard-core boson notation this corresponds to a step in chemical potential—at site m —which is equivalent to

$$P_m = e \sum_{n>m} S_n^z,$$

in terms of the Heisenberg-spin operators.

The conductance is then defined as the dynamical response of the current operator at site x to the voltage drop at site y :

$$g := \lim_{z \rightarrow 0} \text{Re} \frac{i}{\hbar} \int_0^\infty e^{izt} \langle [j_x(t), P_y] \rangle dt. \quad (1)$$

For open boundary conditions (OBC's) the relation $i[H, P_x] = \hbar j_x$ holds and a partial integration of Eq. (1) yields

$$g = \text{Re} \left[(-iz)^{-1} \frac{i}{\hbar} \left(\langle [j_x, P_y] \rangle - \int_0^\infty e^{izt} \langle [j_x(t), j_y] \rangle dt \right) \right].$$

Using $\text{Re}(ab) = \text{Re} a \text{Re} b - \text{Im} a \text{Im} b$ in the above equation gives two contributions to the conductance. With the definition of the generalized Drude weight for two operators A and B ,

$$\langle\langle AB \rangle\rangle \equiv \lim_{z \rightarrow 0} (-iz) \int_0^\infty e^{itz} \langle \Delta A(t) \Delta B \rangle dt,$$

where $\Delta A = A - \langle A \rangle$ one can show using the Lehmann representation¹⁵ that the first contribution ($\text{Re } a \text{ Re } b$) reads

$$\langle\langle j_x j_y \rangle\rangle \text{Re}(-iz)^{-1} = \langle\langle j_x j_y \rangle\rangle \pi \delta(\text{Re } z). \quad (2)$$

The second factor in expression (2) [namely, $\text{Re}(-iz)^{-1}$] gives rise to a delta function, such that Eq. (2) should be the dominating contribution to g . The first factor of expression (2) (namely, $\langle\langle j_x j_y \rangle\rangle$) is closely related to the Drude peak $D = \langle\langle JJ \rangle\rangle / N$ where $J = \sum_n j_n$ is the total current operator.

From the discussion of the Drude peak¹⁶ we know that under OBC's the Drude peak is zero [because D can be written as the response to a static twist which can be removed by a gauge transformation of the form $\exp(i\sum_n n S_n^z)$ (see Ref. 16)] whereas it is nonzero for periodic boundary conditions (PBC's). In our case $\langle\langle j_x j_y \rangle\rangle$ is zero under OBC's [use a gauge transform $\exp(i\sum_{n>y} S_n^z)$]. Under PBC's we find, because of translational invariance and because of the continuity equation, that $\langle\langle j_x j_y \rangle\rangle$ depends neither on x nor y . This implies $D = N \langle\langle j_x j_y \rangle\rangle$. Since the Drude peak is finite (at least for the models we are interested in) we conclude that expression (2) vanishes even under PBC's in the thermodynamic limit. So we obtain

$$g = \text{Re}[(z\hbar)^{-1}] \text{Re} \int_0^\infty e^{izt} \langle [j_x(t), j_y] \rangle dt. \quad (3)$$

Restarting from Eq. (1) we may—again by partial integration—arrive at another formula,

$$g = \text{Re} \left[\frac{i}{\hbar} \left\{ -\langle [P_x, P_y] \rangle - (iz) \int_0^\infty e^{izt} \langle [P_x(t), P_y] \rangle dt \right\} \right].$$

The first term in the square brackets does not contribute—as the potentials P_x and P_y commute—and if we restrict ourselves to $\text{Re } z = 0$ we obtain

$$g = -\text{Im } z \text{Im} \left(\frac{1}{\hbar} \int_0^\infty e^{izt} \langle [P_x(t), P_y] \rangle dt \right). \quad (4)$$

The latter formula is especially useful for MC simulations as it allows the computation of the conductance in terms of the diagonal S^z - S^z correlators (under OBC's).

According to its definition as it is given by Eq. (1) the conductance might in principle depend on the actual choice of the positions of the voltage drop y and the current measurement x . Here, we point out that in the limit $z \rightarrow 0$ this is not the case. In a rather general situation one can show (using the continuity equation) that the right-hand side of Eq. (1) gives the same result for any choice of x and y (see Appendix A).

It is instructive to consider the free fermion case in detail. We denote the (formal) dependence on x and y by corresponding subscripts. Of course, in a translational invariant system g_{xy} depends only on the difference $x - y$. The conductance g as a function of $\omega = \text{Im } z$ (here and in the sequel

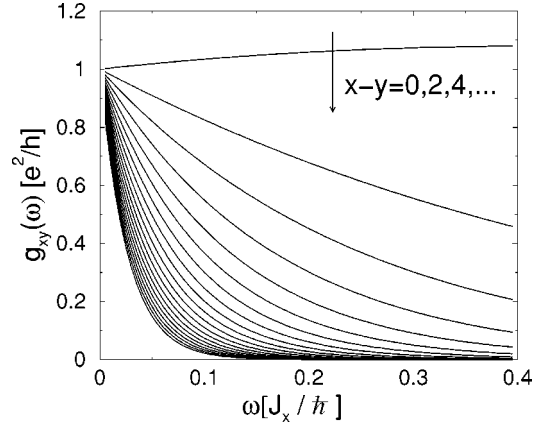


FIG. 1. The conductance of the xy chain at $T=0.01$ versus frequency on the imaginary axis for various distances ($x-y=2n$, $n \in \mathbb{N}$) between voltage drop (y) and current measurement (x).

$\text{Re } z = 0$) is plotted for the free fermion case in Fig. 1. One sees that the conductance in the limit $\omega \rightarrow 0$ approaches the universal value e^2/h . Here we emphasize that a spatial separation of voltage drop and current measurement leads to an exponential decrease in $g(\omega)$ at small ω . Therefore we will restrict our attention to the cases $|x-y| \leq 1$ for the rest of the paper.

B. Technical details of the MC method

We now turn to some technical details of our simulations. The second formula for the conductance, Eq. (4), lends itself to a study with Monte Carlo simulations (it requires OBC's). At the Matsubara frequencies $\omega_M = 2\pi M(\beta\hbar)^{-1}$, $M \in \mathbb{N}$ we may use the equivalent expression

$$g(\omega_M) = -\omega_M / \hbar \text{Re} \int_0^{\hbar\beta} \langle P_x P_y(i\tau) \rangle e^{i\omega_M \tau} d\tau.$$

We employ a standard QMC method (SSE) to compute the conductance. Since P_x is diagonal in the S^z -basis, the simulation of $\langle H^k P_x H^{L-k} P_y \rangle$ can be easily performed with the help of the SSE.^{14,17,18} Here, L is the approximation order. One may simply obtain $\langle P_x P_y(i\tau) \rangle$ as a linear combination of the terms $\langle H^k P_x H^{L-k} P_y \rangle$ with binomial weight factors $B(\tau, k)$. We found it convenient to assume a Gaussian distribution for the $B(\tau, k)$ instead of a binomial one, because the former is easier to evaluate. The error that we introduce by this replacement is smaller than the statistical error if $L > 100$. (Note that in our simulations L is typically of the order of $10^4 - 10^5$.)

What remains to be done in order to get

$$g(\omega_M) = -\omega_M / \hbar \int_0^{\hbar\beta} \cos(\omega_M \tau) \langle P_x P_y(i\tau) \rangle d\tau$$

is an integration in the final step. We performed it with the Simpson rule and a grid of 800 τ values.

We are now left with the standard problem of extrapolating $g(\omega)$ from the Matsubara frequencies ω_M to $\omega = 0$. Un-

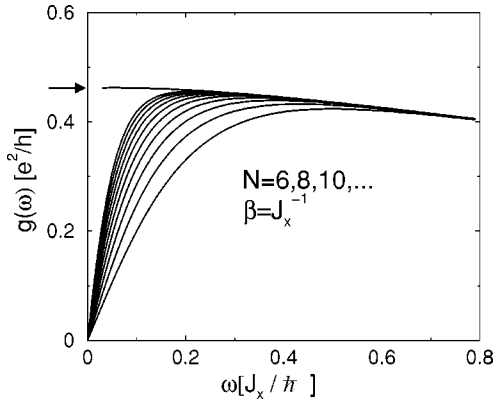


FIG. 2. Conductance g as a function of ω . The arrow indicates the result of the thermodynamic limit.

fortunately, the spacing of the Matsubara frequencies is linear in T , so our method becomes unstable when we increase T .

To see that an application of our MC method makes only sense at low temperatures we compare it to a simpler method: exact diagonalization. Figure 2 shows $g(\omega)$ for various system sizes N at $T=J_x/k_B$. One sees that convergence with N is rather fast (at high temperatures). Hence one can determine $g(\omega)$ for $\omega > J_x/\hbar$ with exact diagonalization. To compute $g(\omega)$ at some $\omega \leq J_x/\hbar$ with MC methods one needs to work at a temperature $T < J_x/(2\pi k_B)$, and even then exact diagonalization is preferable as it yields $g(\omega)$ in a continuous interval rather than on a discrete set of points. Hence at high temperatures the MC method is inferior to a simple exact diagonalization.

In our simulation we make one ‘‘MC sweep’’ between two measurements which consists of one diagonal update and several loop updates¹⁴ between two measurements. We are able to run approximately 10^5 sweeps.

C. Test with Jordan-Wigner

If $J_z=0$ then $g(\omega)$ can be exactly evaluated—for arbitrary system size—not only at $\omega=0$ (see below).

We can exploit this fact in two regards: First, we test our MC method by comparing it with the exact curve obtained by Jordan-Wigner. The result can be seen in Fig. 3.

Second, we can test which frequencies (and hence which temperatures) we need such that a linear extrapolation can be carried out without introducing a larger error than the statistical one. One sees also which system sizes are needed to determine $g(\omega)$ without detectable finite-size error. Our conclusion is that our method works for $T < 0.02$. At $T \approx 0.01$ a system size of $N \approx 200$ – 300 is appropriate.

III. CONDUCTANCE IN VARIOUS SYSTEMS

A. Results for a dimerized Jordan-Wigner chain

One may derive a simple analytical result for the conductance in the free fermion case. Here, we consider the slightly more difficult case—but also more interesting as the system has a gap¹⁹—of a dimerized chain with magnetic field B , i.e.,

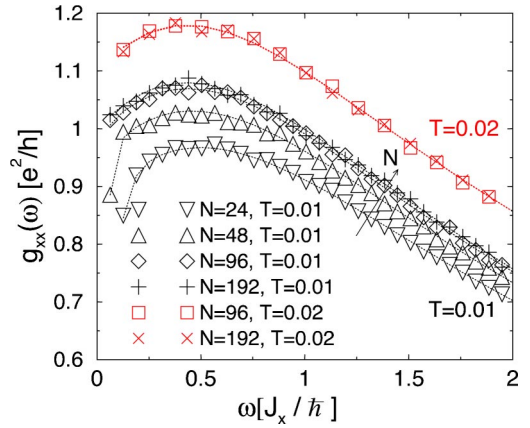


FIG. 3. Monte Carlo data (symbols) in comparison with the exact Jordan-Wigner result (dotted lines). The curves for $T=0.02$ are offset by 0.1 for clarity. (We use OBC’s.)

$J_z=0$ and the hopping parameter alternates: $(J_x)_{2n,2n+1}=J_1$ and $(J_x)_{2n+1,2n+2}=J_2$. The energy dispersion is given by

$$E_k^\pm = B \pm \sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos(2k)}/2$$

and we assume a positive dispersion $E_k=E_k^+$ if $k \in [0, \pi/2] \cup [3\pi/2, 2\pi]$ and $E_k=E_k^-$ else. The gap E_g is $E_g = E_{\pi/2}^+ - E_{\pi/2}^-$ at $k = \pm \pi/2$. The evaluation of the formula for the conductance Eq. (1) is in principle straightforward (see Appendix B). One obtains the compact result

$$g = \frac{e^2}{2h} [\tanh(E_0\beta/2) - \tanh(E_{\pi/2}\beta/2) - \tanh(E_{\pi/2}^+\beta/2) + \tanh(E_{\pi/2}^-\beta/2)]. \quad (5)$$

In the case of zero magnetic field this reduces to

$$g = \frac{e^2}{h} [\tanh(E_0\beta/2) - \tanh(E_{\pi/2}^+\beta/2)].$$

The $T=0$ value of the conductance as a function of magnetic field is quantized: It is zero if $|B|$ is smaller than the zero-field gap $E_{\pi/2}^+$ or larger than the zero-field band width E_0 , and it is 1 between these values, and precisely at these values it is $1/2$ (all values in units of e^2/h).

B. Comparison with the Apel-Rice formula

At low temperatures the xxz chain can be described by a Luttinger liquid. For this model the conductance was obtained by Apel and Rice in the 1980s.^{7,20}

$$g_{\text{ApelRice}} = \frac{e^2}{h} \frac{\pi}{2(\pi - \theta)}, \quad (6)$$

where $\cos \theta = J_z/J_x$. This formula may be derived from Eq. (4) if we use concrete expressions for $\langle S_n^z S_m^z(i\tau) \rangle$ which are available from conformal field theory.²² Figure 4 shows our QMC results for $g(\omega)$ on the imaginary axis for the xxz model; in Fig. 5 we display a comparison, as a function of

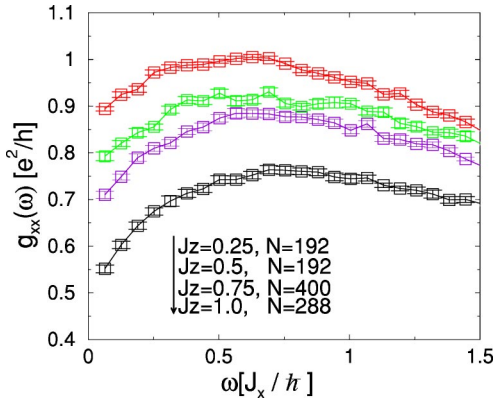


FIG. 4. Monte Carlo data (symbols) for various interaction strengths at $T=0.01J_x/k_B$ (using OBC's and 2×10^5 Monte Carlo sweeps). Shown is the conductance as a function of imaginary frequency.

J_z , between the $g(\omega=0)$ extrapolated from Fig. 4, and the exact Bosonization result, Eq. (6).

We note that the statistical error of the QMC results presented in Fig. 5 does not increase much with the parameter J_z . This is due to our using the “directed loops” as described in Ref. 21. The choice for transition probabilities which was proposed there makes the SSE algorithm more effective. Here the improvement is remarkable.

C. System with one impurity

Now, we consider the Hamiltonian

$$H = H_{xxz} + B_{\text{Imp}} S_{N/2}^z,$$

i.e., we add an impurity in the middle of the system. This model was studied in a paper by Kane and Fisher.⁸ Later, this kind of model received considerable attention by other authors.^{12,23–26} By an RG approach, Kane and Fisher found that the perturbation B_{Imp} is relevant for repulsive interactions (i.e., $J_z > 0$). This means that at zero T the chemical potential anomaly “cuts” the system into two halves, such

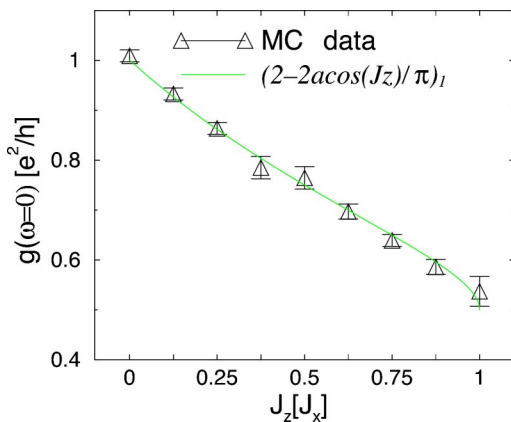


FIG. 5. Conductance of the xxz spin chain at $T=0.01J_x/k_B$ in comparison with the exact result by Apel and Rice [Eq. (6)] for a Luttinger liquid. The Monte Carlo data are obtained by extrapolating the results of Fig. 4 to $\omega=0$.

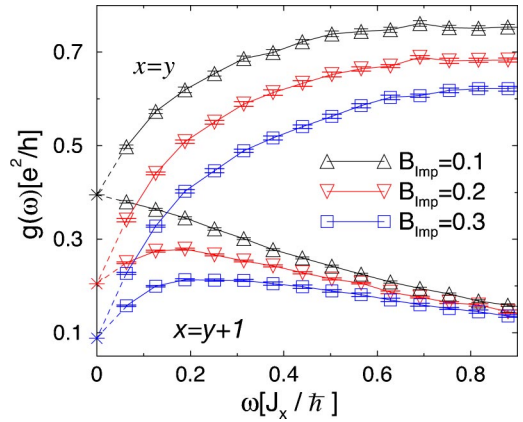


FIG. 6. Conductance of the Heisenberg chain ($N=400$ sites) with one impurity at $T=0.01J_x/k_B$ for different impurity strengths and positions of voltage drop and current measurement (using OBC's). A possible extrapolation to $\omega=0$ is proposed by the dashed lines.

that the conductance is zero. This result cannot be directly confirmed by Monte Carlo methods since these are necessarily finite-temperature methods.

Fortunately, the scaling behavior (with temperature) of the conductance is also known. For $K=1/2$ one may derive an exact formula for the conductance by a re-Fermionization technique:^{6,23}

$$g = e^2/h \left[1 - \frac{B_{\text{Imp}}^2}{2\pi^2 T} \psi' \left(1/2 + \frac{B_{\text{Imp}}^2}{2\pi^2 T} \right) \right], \quad (7)$$

where ψ is the digamma function. So we can compare our MC data once again with an exact result. In Fig. 6 we present two different QMC results for the conductance on the imaginary axis of the Heisenberg chain with one impurity, for different impurity strengths.

For the upper set of curves in Fig. 6 the position of voltage drop and the position of the current measurement are $x=y=N/2$; and for the lower set of curves they are $x=N/2$, $y=N/2-1$. The curves are not as smooth as the ones in Fig. 4, so we use a quadratic fit from the first three Matsubara frequencies instead of a linear extrapolation to estimate $g(\omega=0)$. We also note that the curves with $x-y=1$ are better suited for extrapolation than those with $x=y$ because the slope at $\omega=0$ is smaller. The statistical error is less than one percent. The result from the extrapolation is given in Fig. 7 along with the exact curves from Eq. (7). We used system sizes of $N=400$ for $T \geq 0.01J_x/k_B$ and $N=800$ for $T=0.005J_x/k_B$. We performed 2×10^5 MC sweeps. The error bars are smaller than the symbol size, so the error that we see in the figure is mainly due to our extrapolation method [and to possible logarithmic finite-temperature corrections to Eq. (7)]. We see that the quadratic fit tends to underestimate the correct value.

D. Inhomogeneous systems

Several years after the publication of Eq. (6) by Apel and Rice it was generally agreed upon^{27,28} that it does not reflect the (correct) physical behavior one would encounter in an

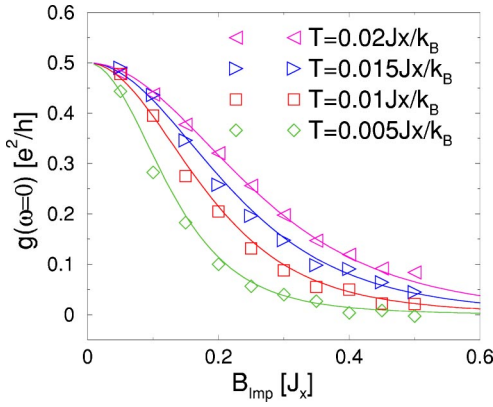


FIG. 7. Conductance of the Heisenberg chain with one impurity at various temperatures ($N=800$ for $T=0.005J_x/k_B$ and $N=400$). MC data (symbols) are drawn in comparison with the exact formula (solid lines) by Weiss *et al.* (Ref. 23) for a Luttinger liquid at the isotropic point $K=\frac{1}{2}$ (i.e., $J_z=J_x$).

experimental realization. Experiments are never performed on a closed system but on one coupled to reservoirs which make it possible for the particles to leave and enter the system. These reservoirs can be modeled by attaching two leads consisting of infinite noninteracting spin half chains to our model.

The complete Hamiltonian then reads

$$H = H_{xxz}(J_z=0) + \sum_{n=(N-N_I+1)/2}^{(N+N_I-3)/2} S_n^z S_{n+1}^z, \quad (8)$$

i.e., the interaction is confined to a small region in the middle consisting of N_I sites. This approach has been followed by many authors, e.g., in Refs. 10 and 29–31. Generally, the presence of leads yields a conductance which is independent of J_z ,^{27,28} namely,

$$g = e^2/h,$$

in sharp contrast to Eq. (6). The noninteracting semichains—which we call leads—play the role of reservoirs.

We note that the behavior of $g(\omega)$ depends on the parity of N_I a fact which was already reported in Ref. 10. (A similar effect was also found in the Hubbard model.³²) In the following we will only consider the case of N_I odd. A detailed discussion of N_I even/odd and a comparison with Ref. 10 will be presented elsewhere.

The “natural” choice for current measurement and voltage drop would be at the two ends of the interacting region. But here is caution advised. From Fig. 1—which is again for the free Fermion case—one learns two things: First, g does not depend on the choice of x and y . Second, if x and y are some distance apart, convergence with ω becomes slow, hence one needs to go to lower T and larger system sizes if one wants to extract $g(\omega=0)$ reliably. A simple phenomenological explanation for this is the following: If the place of the measurement is far from the voltage drop the particles have to travel a long distance and hence one has to wait a long time before one can determine g . We can now place both the voltage drop and our current measurement at the

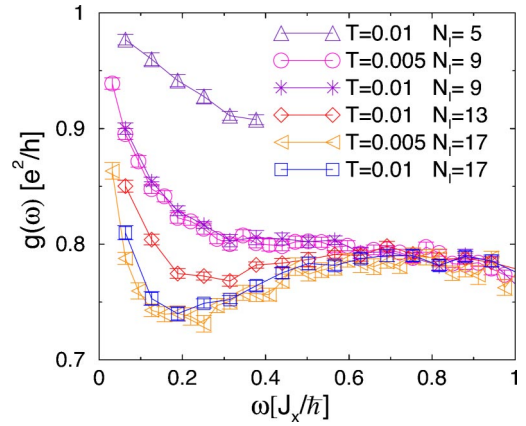


FIG. 8. Conductance, in units of e^2/h , of the Heisenberg chain with noninteracting leads; see Eq. (8). The system size is $N=320$. The values for temperature T and size of the interacting region N_I are given. (We use OBC’s, 10^5 MC sweeps, and $x=y$ for the voltage drop.)

middle of the system, but this should not help much. The problem is that the particles still have to travel a long distance until they see the leads. Hence $g(\omega)$ will be unaffected by the introduction of leads if ω is sufficiently large. This expectation is confirmed by the QMC data presented in Fig. 8. In this figure the exponential decay of $g(\omega)$ at small ω is apparent, and the curves illustrate clearly that this decay is induced by the length scale N_I —because it becomes stronger with increasing N_I . It is this decay that prevents us from discussing larger N_I . If we increase N_I the decay becomes stronger, hence we need to evaluate $g(\omega)$ for more (and smaller) frequencies in order to extract $g(\omega=0)$ reliably. But smaller frequencies are only available at smaller temperatures. As we cannot decrease T much below $0.01J_x/k_B$ we restrict ourselves to $N_I < 20$. If we considered a system with $N_I=200$ (at $T=0.01J_x/k_B$) we would not see any difference from a system without leads, because the difference occurs at small ω .

The data presented in Fig. 8 clearly indicate an upturn of $g(\omega)$ for $\omega \rightarrow 0$, indicating that $g(\omega=0)$ is unaffected by the interaction in the low-temperature limit. Our result may, however, not be totally convincing, since we can only analyze relatively small interacting regions. One might argue that the enhanced conductance is not due to the leads but simply to the reduced “mean” interaction—which is close to zero as only few sites interact. To invalidate this argument we considered another model. We have performed QMC simulation of a system where we attach a lead only at one side such that we obtain a chain which is noninteracting in one half and interacting in the other. For this system we found no deviation at all imaginary frequencies from the situation where the interacting region extends over the whole chain, even though there are as many interacting as interaction-free bonds.

E. Spin Hamiltonian with third-nearest-neighbor interaction

Monte Carlo simulations allow the inclusion of long-range hopping, and thus breaking the integrability of the pure

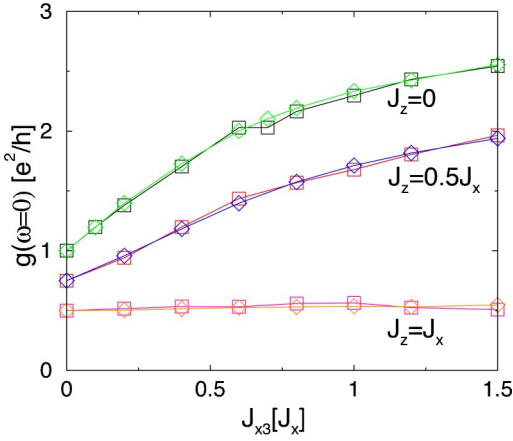


FIG. 9. Conductance of the Hamiltonian Eq. (9) (with 400 sites, $T=0.01$) as a function of J_{x3} for various anisotropies. Squares: quadratic fit from the first three Matsubara frequencies; diamonds: linear fit from the first six frequencies. (We use OBC's, 10^5 MC sweeps, and $x=y+1$ for the voltage drop.)

xxz Hamiltonian, as long as the resulting system is not frustrated. We thus consider a Hamiltonian with a third-nearest-neighbor interaction:

$$H = H_{xxz} + J_{x3} \sum_n [(S_n^+ S_{n+3}^- + S_n^- S_{n+3}^+)/2 + J_z/J_x S_n^z S_{n+3}^z]. \quad (9)$$

For simplicity we assumed that the anisotropy is independent of the hopping range (i.e., $J_{z3} = J_{x3} J_z/J_x$). In this context we emphasize that the long-range hopping in the spin system does not transform under Jordan-Wigner to a long-range hopping in a Fermionic system but to a more complicated four-sites operator.

In general, adding a new term to the Hamiltonian changes the current operator which is defined via the continuity equation, $\nabla j := (j_{n+1} - j_n) = i[S_{n+1}^z, H]/\hbar$. In a one-dimensional system with OBC's the continuity equation is solved, however, by the relation $j_x = i[H, P_x]/\hbar$ (see Sec. II A) such that Eq. (4) still applies. Nonetheless, it is useful to look at the current operator for this case. It reads

$$j_n = j_{n,1} + j_{n,3} + j_{n-1,3} + j_{n-2,3},$$

where $j_{n,k} = iJ_x e(S_n^+ S_{n+k}^- - S_n^- S_{n+k}^+)/2\hbar$. If we compare it with the current operator of the xxz chain we see that the long-range hopping J_{x3} gives rise to three additional terms which are analogous to the first one.

We compute the conductance as a function of the hopping amplitudes J_{x3}/J_x and present the result in Fig. 9. If $J_{x3} = 0$ the conductance is, of course, given by the Apel-Rice result Eq. (5). However, if $J_{x3} \gg J_x$ we may eventually neglect the nearest-neighbor-hopping term such that we end up with three uncoupled chains. Thus we conclude that the conductance will grow towards three times the Apel-Rice result when we increase J_{x3} . From the figure we see that the crossover between these two values is shifted to smaller values of J_{x3} when the anisotropy is increased. (In fact, at the isotropic point the increasing of g is barely visible.)

In conclusion we have developed a QMC technique which allows the evaluation of the dc conductance for a wide range of nonfrustrating quantum-spin chains at low but finite temperatures. We have presented several stringent tests for this technique, like the Kane-Fisher scaling for the conductance through an impurity in a Luttinger liquid.

APPENDIX A: PROOF THAT THE RIGHT-HAND SIDE OF EQ. (1) IS INDEPENDENT OF x AND y

Here we provide a general argument which relies on the (physical) assumption that some linear-response functions are finite in the thermodynamic limit.

Theorem: *In a spin system the conductance $g_{xy} \equiv g$ does not depend on x and y if the linear response of an operator S_n^z to a perturbation P_m is bounded in the thermodynamic limit.*

Proof:

First we consider $\lim_{z \rightarrow 0} z \int_0^\infty e^{izt} \langle [S_n^z(t), P_m] \rangle dt$. This expression corresponds to a plateau value of the response function $\varphi(t) := i \langle [P_m, S_n^z(t)] \rangle$, i.e.,

$$\lim_{z \rightarrow 0} z \int_0^\infty e^{izt} \langle [S_n^z(t), P_m] \rangle dt = \lim_{t \rightarrow \infty} \varphi(t).$$

The response function may be written in the following way (by Kubo's identity):³³

$$\varphi(t) = \beta(P_m, iL e^{iLt} S_n^z) =: \partial_t \Phi(t).$$

Here (\cdot, \cdot) is the Mori scalar product (for operators A and B : $\beta(B, A) = \int_0^\beta \text{Tr} B^\dagger \exp(-\tau H) A \exp[(\tau - \beta)H] d\tau / \text{Tr} \exp(-\beta H)$) and L is the Liouville operator. To prove that $\varphi(t) \rightarrow 0$ as $t \rightarrow \infty$, it is sufficient to show that Φ as a function of t is bounded.

But this is just the assumption that we made in the statement of the theorem because $(S_n^z(t), P_m)$ represents the linear response of the operator S_n^z to the perturbation P_m .

Finally, we can prove our main assertion. We want to show $g(x, y) = g(x', y') \forall x, y, x', y'$. This follows easily from $g(x, y) = g(x+1, y) \forall x, y$ and $g(x, y) = g(x, y+1) \forall x, y$. We will consider only the second equality [the proof of the first equality is analogous by the symmetric structure of Eq. (4)].

Using Eq. (4) and our previous result we see that

$$g(x, y) - g(x, y+1) = \lim_{z \rightarrow 0} \text{Im} z \int_0^\infty e^{izt} \langle [S_{y+1}^z(t), P_x] \rangle dt = 0.$$

Q.E.D.

APPENDIX B: DERIVATION OF EQ. (5)

For eigenvalues E_n and E_k the respective one-particle eigenstates will be denoted by $|n\rangle$ and $|k\rangle$, the annihilation operators by c_n and c_k , and the occupation numbers by n_n and n_k . For the current operator we find: $N\langle k, j_x k \rangle = e v_k := e/\hbar (dE/dk)$ and $\langle -k, j_x k \rangle = 0$.

In a free Fermion system one can derive a simple expression for $\langle A(i\omega_M) B \rangle = \int_0^\beta d\tau e^{i\omega_M \tau} \langle AB(i\tau) \rangle$ [with $i\omega_M = \omega$]

$+i\delta=2\pi iM/(\hbar\beta)$] when A and B are one-particle operators (i.e., $A=\sum_{n,k}A_{nk}c_n^\dagger c_k$):

$$\langle AB \rangle(i\omega_M) = \sum_{n \neq k} \frac{A_{nk}B_{kn}}{i\hbar\omega_M + E_n - E_k} f_{kn},$$

where $f_{kn} = \sinh[\beta(E_n - E_k)/2]/2 \cosh(\beta E_n/2) \cosh(\beta E_k/2) = (\langle n_k \rangle - \langle n_n \rangle)$. $\langle A(z = \omega + i\delta)B \rangle$ may then be obtained by analytic continuation. In our case A and B are local current operators; for the conductance we use Eq. (3):

$$g = \frac{1}{\omega} \text{Im} \sum_{n \neq k} \frac{\langle n, j_x k \rangle \langle k, j_y n \rangle}{i\hbar\omega_M + E_n - E_k} f_{kn} = -\frac{1}{\omega} \sum_{n \neq k} \langle n, j_x k \rangle \times \langle k, j_y n \rangle \frac{\delta}{(\hbar\omega + E_n - E_k)^2 + \delta^2} f_{kn}.$$

For $\delta \rightarrow 0$

$$\frac{\delta}{(\hbar\omega + E_n - E_k)^2 + \delta^2} \rightarrow \pi \delta(\hbar\omega + E_n - E_k).$$

In the continuum limit we replace $\sum_k N^{-1} \rightarrow \int (dk/2\pi)$ $= \int (dE_k/2\pi) |\hbar v_k|$.

Performing the integration over the variable n and then taking $\omega \rightarrow 0$ yields

$$g = \frac{e^2}{2\hbar} \int \frac{dk}{2\pi} |\hbar v(k)| \frac{\beta/2}{2 \cosh^2(\beta E_k/2)} = \frac{e^2}{\hbar} \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} \frac{\hbar v_k \text{sgn}(k) \beta/2}{4 \cosh^2(\beta E_k/2)} = \frac{e^2}{h} \int_{k=0}^{k=\pi} \frac{dE \beta/2}{2 \cosh^2(\beta E_k/2)} = \frac{e^2}{2h} \int_{E_{\pi/2}^+}^{E_0 \beta/2} dx \frac{1}{\cosh^2(x)} + \frac{e^2}{2h} \int_{E_{\pi/2}^-} dx \frac{1}{\cosh^2(x)} = \frac{e^2}{2h} [\tanh(E_0 \beta/2) - \tanh(E_{\pi/2} \beta/2) - \tanh(E_{\pi/2}^+ \beta/2) + \tanh(E_{\pi/2}^- \beta/2)].$$

Note that the conductance does not depend on the energy dispersion but only on the band width E_0 and the gap $E_{\pi/2}^+$.

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