

Density-matrix renormalization group study of the linear conductance in quantum wires coupled to interacting leads or phonons

Jan-Moritz Bischoff^{*} and Eric Jeckelmann[†]

Leibniz Universität Hannover, Institut für Theoretische Physik, Appelstraße 2, D-30167 Hannover, Germany



(Received 4 July 2019; revised manuscript received 16 August 2019; published 28 August 2019)

In a previous paper [Bischoff and Jeckelmann, *Phys. Rev. B* **96**, 195111 (2017)] we introduced a density-matrix renormalization group method for calculating the linear conductance of one-dimensional correlated quantum systems and demonstrated it on homogeneous spinless fermion chains with impurities. Here we present extensions of this method to inhomogeneous systems, models with phonons, and the spin conductance of electronic models. The method is applied to a spinless fermion wire-lead model, the homogeneous spinless Holstein model, and the Hubbard model. Its capabilities are demonstrated by comparison with the predictions of Luttinger liquid theory combined with Bethe ansatz solutions and other numerical methods. We find a complex behavior for quantum wires coupled to interacting leads when the sign of the interaction (repulsive/attractive) differs in the wire and leads. The renormalization of the conductance given by the Luttinger parameter in purely fermionic systems is shown to remain valid in the Luttinger liquid phase of the Holstein model with phononic degrees of freedom.

DOI: [10.1103/PhysRevB.100.075151](https://doi.org/10.1103/PhysRevB.100.075151)

I. INTRODUCTION

Confining electrons to one dimension results in various surprising properties because of the fermionic nature of the particles [1–3]. In practice, one-dimensional electron systems can be realized in semiconductor wires [4], atomic wires deposited on a substrate [5,6], carbon nanotubes [7], or atomic and molecular wire junctions [8–11]. In contrast to the behavior of a three-dimensional metal, which is well described by the Fermi liquid paradigm, theory predicts that one-dimensional conductors should exhibit the behavior of a Luttinger liquid [2]. In particular, the transport properties have been studied and controversially discussed for more than three decades [2,3].

In a previous paper [12] we introduced a density-matrix renormalization group method (DMRG) for calculating the linear conductance of one-dimensional correlated quantum systems with short-range interactions at zero temperature based on the Kubo formalism [13,14]. By taking advantage of the area law for the entanglement entropy [15] the DMRG method provides us with the most efficient method for calculating the properties of these systems [16–19]. Our method combines DMRG with a finite-size scaling of dynamical correlation functions to compute the conductance in the thermodynamic limit. The method was demonstrated on the homogeneous spinless fermion chains with impurities [12], for which well-established results were available [2,20–22].

In this paper we develop the method further to treat a variety of more complex models. We present extensions to wire-lead systems with different interactions in the wire and

leads, to electron-phonon models, and to spinful fermions (electrons). These extensions are necessary steps toward future studies of more realistic models that are able to describe quantitatively the experimental realizations of one-dimensional electronic conductors [4–11]. Here, we apply our method to a spinless fermion wire-lead model, the homogeneous spinless Holstein model, and the Hubbard model to demonstrate its current capabilities and limitations using the predictions of Luttinger liquid theory combined with Bethe ansatz solutions and numerical results found in the literature.

The method is summarized in the next section. The extension and results for inhomogeneous systems such as the spinless fermion wire-lead system are presented in Sec. III. The extension to systems with phonon degrees of freedom and the results for the spinless Holstein model are shown in Sec. IV. Section V describes the generalization to spinful fermion (electron) models and to the calculation of the spin conductance as well as our results for the spin conductance of the Hubbard model. Finally, Sec. VI contains our conclusion and outlook.

II. METHOD

In this section we summarize our DMRG method for calculating the conductance of one-dimensional correlated quantum systems. It is based on the approach developed by Bohr *et al.* [14]. Full details can be found in our previous paper [12]. We consider a one-dimensional lattice of M sites. It consists of left and right segments (called leads) with approximately $(M - M_W)/2$ sites each and a central segment (called the wire) of M_W sites. A current can be generated by applying a potential bias. We assume that the potential remains constant in the leads and drops linearly in the wire;

^{*}jan.bischoff@itp.uni-hannover.de

[†]eric.jeckelmann@itp.uni-hannover.de

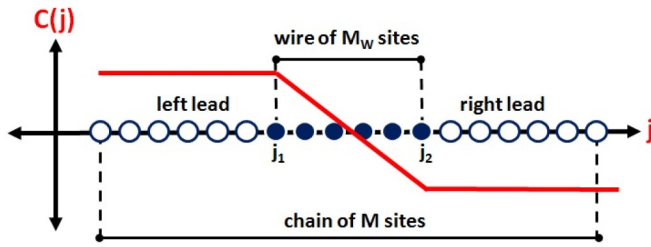


FIG. 1. Schematic of the wire-lead layout for calculating the conductance. The chain of M sites is made of left and right leads and a central wire of M_w sites. These three different sections are defined by the profile $C(j)$ of the external perturbation (e.g., applied bias voltage). Additionally, the wire and leads may include different sites, degrees of freedom, or interactions represented by the solid and empty circles, respectively.

i.e., it has the shape

$$C(j) = \begin{cases} \frac{1}{2}, & \text{for } j \leq j_1, \\ -\frac{j-j_1}{j_2-j_1} + \frac{1}{2}, & \text{for } j_1 \leq j \leq j_2, \\ -\frac{1}{2}, & \text{for } j \geq j_2, \end{cases} \quad (1)$$

where j_1 and j_2 are the first and last site in the wire, respectively. This is illustrated in Fig. 1.

The resulting linear conductance can be calculated directly from dynamical current-current correlation functions in the thermodynamic limit using Kubo's linear response theory [13]. The dynamical DMRG method [23,24] can be used to compute the imaginary part of the frequency-resolved current-current correlation functions for a finite lattice size M ,

$$G_{J,\eta}(\omega) = \langle 0 | J \frac{\eta}{(E_0 - H + \hbar\omega)^2 + \eta^2} J | 0 \rangle, \quad (2)$$

where H is the Hamilton operator, $|0\rangle$ is its ground state, E_0 is the ground-state energy, J is the current operator in the wire, and $\eta > 0$ is a small number. The Hamilton operator and the current operator depend on the system studied and thus will be given explicitly in the next sections where we present our results for specific models. We note that the conductance can also be calculated from static correlation functions with the time-independent DMRG method [25].

For the DMRG calculations presented here we used up to 400 density matrix eigenstates. The discarded weights were smaller than 10^{-6} and thus we estimate that the DMRG truncation errors are negligible compared to finite-size effects. We observed some DMRG convergence problems for the phononic systems only; see Sec. IV.

It is important to realize that the wire segment (and consequently both lead segments) is defined by the potential profile (1) and thus, in practice, by the lattice region, where the current operator J acts. It is possible but not necessary to include any information about the wire-lead layout in the Hamilton operator H , such as different interactions or different degrees

of freedom for the wire and leads. In fact, in our first work we tested our method with homogeneous systems only; i.e., the degrees of freedom and interactions were identical for all sites, but for the presence of up to two impurities (on-site potentials) in the middle of the wire.

From the DMRG data for (2) we can calculate the “finite-size conductance”

$$G(M) = \frac{q^2}{\omega} [G_{J,\eta(M)}(\omega) - G_{J,\eta(M)}(-\omega)]|_{\omega=0} \quad (3)$$

for a given system size M using the scaling $\eta(M) = C/M$, where q is the charge carried by each fermion. The constant C depends on the properties of the system investigated. For all results presented here we used $C = 48t$ or $96t$. Extrapolating $G(M)$ to infinite system length M yields our estimation of the conductance G in the thermodynamic limit. Here, we used chain lengths up to $M = 2000$.

For a noninteracting tight-binding chain it can be shown analytically that $G(M)$ converges to the exact result for $M \rightarrow \infty$, i.e., the quantum of conductance

$$G_0 = n \frac{q^2}{h}, \quad (4)$$

where $n = 1$ for spinless fermions and $n = 2$ for electrons. For correlated systems we can only compute (2) and (3) numerically. In practice, there are two main practical issues. First, DMRG must be able to calculate $G(M)$ with enough accuracy for large system sizes M . Second, $G(M)$ should converge neatly to the actual value of the conductance for $M \gg 1$. In our previous work we showed that this method yields correct results for the renormalized conductance of the one-component Luttinger liquid in the homogeneous spinless fermion chain as well as for one and two impurities added to the chain. In the next sections we will show that this approach can also be applied to inhomogeneous systems, electronic Hamiltonians, and models with phonons.

In all our numerical results and figures we use $q = 1$ and $\hbar = 1$. This yields $G_0 = \frac{n}{2\pi}$. Therefore, we show $2\pi G(M)$ in our figures.

III. INHOMOGENEOUS WIRE-LEAD SYSTEM

As mentioned above our method was demonstrated in Ref. [12] for homogeneous systems only. In real systems, however, the wire and leads are of different nature. For instance, it is often assumed that metallic leads are Fermi liquids and thus they are modeled by noninteracting tight-binding chains attached to the interacting wire [14,26–34]. Additionally, one can introduce a weaker link (hopping term) between leads and wires [14,28,29]. (We will not study this possibility here because it would require a smaller η and possibly a different scaling of η with M). More generally, one may have to consider different interactions in the leads and in the wire as well as additional degrees of freedom (such as phonons) in the wires.

Therefore, we have generalized our method to this situation and tested it on a spinless fermion model with different nearest-neighbor interactions in the wire (V_w) and in the leads

(V_L). Explicitly, this corresponds to the Hamiltonian

$$\begin{aligned}
 H = & -t \sum_{j=2}^M (c_j^\dagger c_{j-1} + c_{j-1}^\dagger c_j) \\
 & + V_W \sum_{j=j_1+1}^{j_2} \left(n_j - \frac{1}{2}\right) \left(n_{j-1} - \frac{1}{2}\right) \\
 & + V_L \sum_{j=2}^{j_1} \left(n_j - \frac{1}{2}\right) \left(n_{j-1} - \frac{1}{2}\right) \\
 & + V_L \sum_{j=j_2+1}^M \left(n_j - \frac{1}{2}\right) \left(n_{j-1} - \frac{1}{2}\right). \quad (5)
 \end{aligned}$$

The operator c_j^\dagger (c_j) creates (annihilates) a spinless fermion at position j ($= 1, \dots, M$) while $n_j = c_j^\dagger c_j$ counts the number of spinless fermions on this site. The hopping amplitude is identical for the wire and leads and sets the energy unit $t = 1$. We assume that the system has an even number of sites M and is occupied by $M/2$ spinless fermions (half filling).

From the potential profile (1) follows that the current operator is given by

$$J = \frac{1}{M_W - 1} \frac{it}{\hbar} \sum_{j=j_1+1}^{j_2} (c_j^\dagger c_{j-1} - c_{j-1}^\dagger c_j). \quad (6)$$

In principle, the wire edge sites j_1 and j_2 in the definition of the Hamiltonian (5) could be different from those used for the potential profile (and thus the current operator). Here we assume that the screening of the potential difference between source and drain occurs entirely (and linearly) in the wire and thus we use the same values for j_1 and j_2 in both the Hamilton operator (5) and the current operator (6).

Field-theoretical approaches predict that the conductance of a homogeneous Luttinger liquid is renormalized as

$$G = K G_0, \quad (7)$$

where K is the Luttinger parameter [20–22]. We could reproduce this result in our previous work for the homogeneous spinless fermion model, i.e., for $V_W = V_L$ in (5). On the contrary, field-theoretical approaches predict that the conductance through a Luttinger liquid wire connected to leads is not renormalized by interactions in the wire and is entirely determined by the lead properties [35–39]. In particular, if the leads are Luttinger liquids their Luttinger parameter K_L determines the conductance through (7) [36,38]. However, field-theoretical approaches assume perfect contacts, i.e., without any single-particle backscattering [38]. Numerical calculations for lattice models of quantum wires connected to noninteracting leads show that the conductance deviates from the lead conductance G_0 when backscattering is taken into account. In the lattice model (5) single-particle backscattering is due to the sharp change of the on-site potential at the boundaries between the wire and leads [$-V_W$ in the wire, $-V_L$ in the leads, and $-(V_W + V_L)/2$ on the boundary sites j_1 and j_2], which is required to maintain a constant density in equilibrium.

We have found that the calculation of the frequency-resolved correlation function (2) with dynamical DMRG is

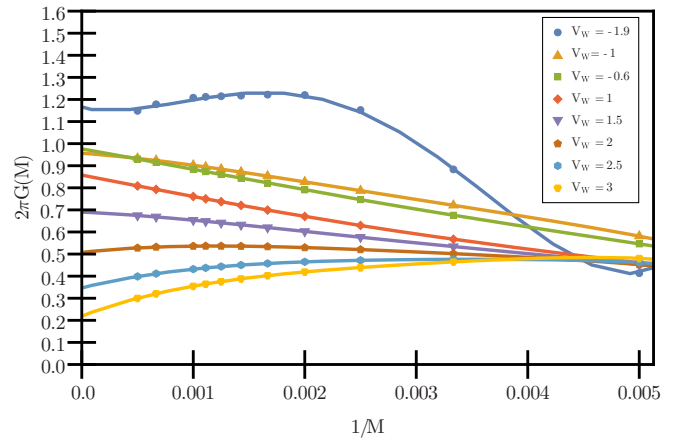


FIG. 2. Scaling of the finite-system conductance $G(M)$ with the inverse system length $1/M$ for spinless fermions in a short interacting wire ($M_W = 10$) between noninteracting leads ($V_L = 0$). The wire interaction strength is given in the inset. Lines are polynomial fits.

not more difficult for an inhomogeneous system ($V_W \neq V_L$) than for a homogeneous one ($V_W = V_L$). To investigate the conductance of a Luttinger liquid between leads, however, we would have to compute the conductance $G(M)$ in the limit of long wires $M_W \gg 1$ while maintaining much longer leads ($M \gg M_W$). In our study of homogeneous systems [12] we found that the conductance scales with M_W/M and thus we were able to determine its value in the thermodynamic limit using a fixed (and small) value of M_W . For the wire-lead system (5) with $V_W \neq V_L$ considered here, we have found that the scaling with M and M_W (up to $M_W = 82$) is much more complicated. As a consequence, it is not possible to compute the conductance of an infinitely long wire in most cases. Thus we discuss here the results obtained for short wires and present only results for $M_W = 10$.

In Fig. 2 we show the scaling of $G(M)$ with the system length M for noninteracting leads ($V_L = 0$) and various interaction strengths V_W in the wire. The extrapolated values $G = \lim_{M \rightarrow \infty} G(M)$ are shown in Fig. 3. For repulsive interactions ($V_W > 0$) we observe a progressive decrease of G with increasing coupling V_W . The conductance of the spinless fermion model connected to noninteracting leads was investigated previously for repulsive interactions using DMRG and

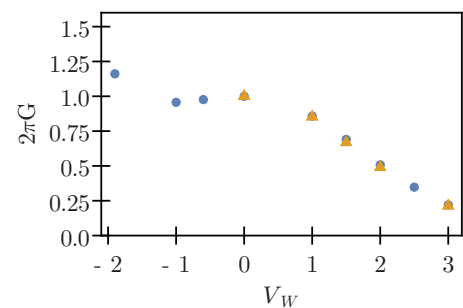


FIG. 3. Conductance of a short interacting wire connected to noninteracting leads as a function of the wire interaction V_W : Extrapolated values $G = \lim_{M \rightarrow \infty} G(M)$ of the data in Fig. 2 for $M_W = 10$ (circles) and DMRG data from Ref. [26] for 12-site wires (triangles).

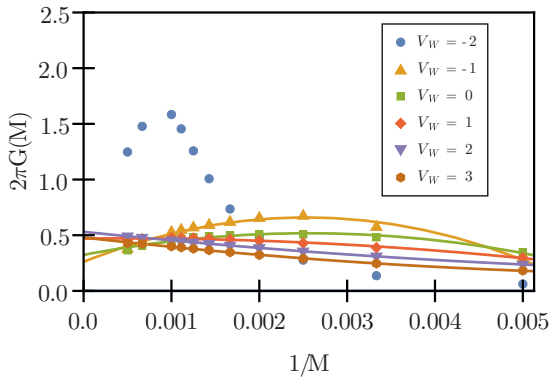


FIG. 4. Same as Fig. 2 but with a repulsive interaction $V_L = 2t$ in the leads.

the functional renormalization group method [26,27]. Our results for G agree quantitatively with the (DMRG) results presented in Ref. [26] for a slightly longer wire ($M_W = 12$), as shown in Fig. 3. In contrast, we observe in Fig. 2 that $G(M)$ tends to G_0 (i.e., the conductance of the noninteracting leads) for attractive interactions $0 > V_W > -2t$. The nonmonotonic behavior of $G(M)$ for $V_W = -1.9t$ in Fig. 2 and the resulting large deviation of the extrapolated value from G_0 in Fig. 3 illustrate the problems that one encounters when analyzing finite-size effects in the wire-lead system.

For an interaction $V_W > 2t$ the homogeneous half-filled spinless fermion model is in an insulating charge-density-wave (CDW) phase and thus we expect that G diminishes exponentially with increasing wire length M_W . In the Luttinger liquid phase with repulsive interactions ($2t \geq V_W > 0$) a power-law suppression of G with increasing wire length was observed previously [27]. This deviation from the field-theoretical predictions mentioned above is due to the single-particle backscattering caused by the sharp change of the interaction at the wire boundaries. The scaling of G with the wire length in the attractive Luttinger liquid phase ($-2t < V_W < 0$) is not known. As explained above, we cannot determine the conductance for an infinitely long wire ($M_W \rightarrow \infty$) with the present method. Nevertheless, our data suggest that for attractive wire interactions within the Luttinger liquid regime the noninteracting leads determine the conductance of the system in agreement with field theory. This is in stark contrast to repulsive wire interactions, for which even a small $V_W > 0$ results in a reduction of G from the noninteracting lead conductance G_0 , as already reported previously [26,27,38].

While there are numerous studies of the conductance of wires connected to noninteracting leads [14,26–28,30–39], there seem to be only a few field-theoretical results for interacting leads [33,36,38]. Figure 4 shows the scaling of $G(M)$ with the system size M for leads with a repulsive interaction $V_L = 2t$. From the Bethe ansatz solution of the homogeneous spinless fermion model we know that this corresponds to a Luttinger liquid parameter $K_L = 1/2$ [40] and thus to a conductance $G = G_0/2$ for perfect contacts according to field theory. Clearly, all our results for $G(M)$ with $V_W > 0$ converge toward this value and thus agree with the field-theoretical predictions. Surprisingly, this also holds for the wire with

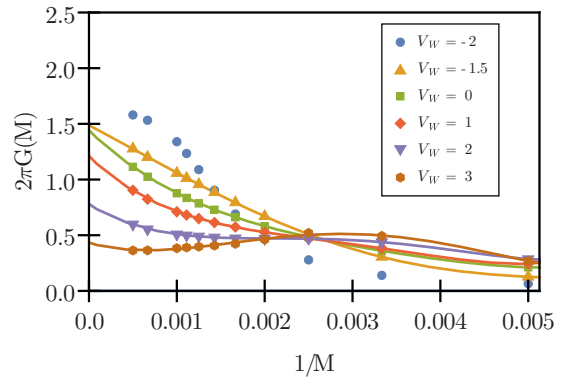


FIG. 5. Same as Fig. 2 but with an attractive interaction $V_L = -t$ in the leads.

$V_W = 3t$, which would correspond to a CDW insulator in the thermodynamic limit $M_W \rightarrow \infty$. Therefore, we expect that G will decrease with increasing M_W for $V_W = 3t$. For a noninteracting wire or an attractive interaction in the wire ($0 \geq V_W > -2t$), however, we observe in Fig. 4 a different, nonmonotonic behavior of $G(M)$, which hinders the extrapolation of $G(M)$ to the limit $M \rightarrow \infty$. Apparently, G is lower than the lead conductance $G_0/2$ for $V_W = 0$ and $-t$.

Figure 5 shows the scaling of $G(M)$ with system length M for leads with an attractive interaction $V_L = -t$. This corresponds to a Luttinger liquid parameter $K_L = 3/2$ [40] and thus to a conductance $G = (3/2)G_0$ for perfect contacts according to field theory. We see in Fig. 5 that $G(M)$ seems to converge to different values for different repulsive couplings in the wire ($V_W > 0$). Unfortunately, we cannot determine the limit $G = \lim_{M \rightarrow \infty} G(M)$ accurately even with system lengths up to $M = 2000$. The values of $G(M)$ for $M = 2000$ are above the conductance of a homogeneous Luttinger liquid with the corresponding interaction V_W . They seem to increase further with M but to converge to lower values than the lead conductance $G = (3/2)G_0$. Therefore, it appears that the conductance of the wire-lead system is lower than the lead conductance in that case, similarly to what is found for noninteracting leads due to single-particle backscattering. For $V_W = 3t$ the conductance seems again to converge to a finite value. As for noninteracting leads it should vanish in the limit $M_W \rightarrow \infty$ as this interaction strength leads to a CDW insulating state in the wire. For a noninteracting wire and for attractive interactions in the wire ($0 \geq V_W \geq -2t$), however, we find that $G \approx (3/2)G_0$ as predicted by field theory but it is difficult to extrapolate $G(M)$ reliably close to the Luttinger phase boundary $V_W = -2t$.

In summary, our results agree with the known results for the conductance of the spinless fermion wire-lead system and thus confirm the validity of our method. Moreover, they also reveal complex qualitative differences in the attractive and repulsive interaction regimes. The conductance seems to be given by (7) with the lead Luttinger parameter (as predicted by field theory) only when the interactions have the same sign in the wire and leads. The properties of short wires with attractive interactions connected to leads with repulsive interactions (or vice versa) seem to be more complex than

anticipated from the results reported so far (using field theory) and should be investigated further.

IV. HOLSTEIN CHAIN

The interaction between charge carriers and phonons plays an important role for transport properties [41–43], in particular for atomic or molecular wire junctions between leads [8–11]. Therefore, we have to generalize our method to models that include phonon degrees of freedom coupled to the charge carriers. It is relatively straightforward to extend a DMRG program to models with phonons if one uses a truncated eigenbasis of the boson number operator with at most N_b states to represent each phonon mode [44]. The only real challenge is the computational cost that increases as N_b^3 and thus limits most applications to small N_b . For Einstein phonons (i.e., dispersionless) and purely local couplings with the fermion degrees of freedom it is possible to speed up DMRG calculations using a pseudosite representation for bosons described in [45].

Therefore, we have tested our method on the simplest model with these properties, the spinless fermion Holstein model [46], which is defined by the Hamiltonian

$$\begin{aligned}
 H = & -t \sum_{j=2}^M (c_j^\dagger c_{j-1} + c_{j-1}^\dagger c_j) + \omega_b \sum_{j=1}^M b_j^\dagger b_j \\
 & - g \omega_b \sum_{j=1}^M (b_j^\dagger + b_j) n_j,
 \end{aligned} \quad (8)$$

where ω_b is the frequency of the Einstein phonons created (annihilated) by the boson operators b_j^\dagger (b_j) and g is the dimensionless coupling between spinless fermions and phonons. The spinless fermion operators c_j^\dagger , c_j , and n_j have the same meaning as in the previous section and the hopping term again sets the energy unit $t = 1$, while we consider a system with an even number of sites M filled with $M/2$ spinless fermions. This Hamiltonian is homogeneous and thus the wire and lead sections are defined by the potential profile (1) only. The current operator is again given by (6).

We have found that calculating the conductance with our method is more difficult for the Holstein model than for purely fermionic models such as (5). This is due not only to the increase of the computational cost with the phonon cutoff N_b but also to the fact that the dynamical DMRG algorithm [23,24] often fails to converge in a reasonable time for large M . Thus we can compute $G(M)$ systematically for smaller system sizes M than in fermionic systems and we show here results for M up to 800 sites only. (One calculation for this system size requires about 600 CPU hours and 4 GB of memory. Thus one could certainly treat larger systems using supercomputer facilities.) In contrast, the scaling of $G(M)$ with the system size is regular in the homogeneous Holstein wire as found previously for homogeneous fermionic systems [12]. Thus we can estimate the conductance G in the thermodynamic limit despite the short system lengths as illustrated in Fig. 6 for the adiabatic regime ($\omega_b = 0.1t$) and in Fig. 7 for the intermediate regime ($\omega_b = t$).

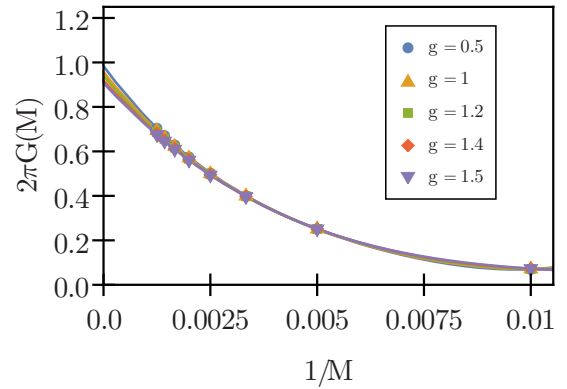


FIG. 6. Scaling of the finite-system conductance $G(M)$ with the inverse system length $1/M$ for the spinless fermion Holstein model in the adiabatic regime ($\omega_b = 0.1t$). The coupling g between fermions and phonons is given in the inset. Lines are polynomial fits.

The phase diagram of the half-filled spinless fermion Holstein model was determined previously with DMRG [47] and quantum Monte Carlo computations [48]. It exhibits a Luttinger liquid phase at weak coupling or high phonon frequency. The Luttinger liquid parameter K was calculated from the long-wavelength limit of the static structure factor [47,48]. This corresponds to the parameter K determining the exponents in the power-law correlation functions of the Luttinger liquid theory for purely fermionic systems [2].

As seen in Fig. 6, we have found that the conductance corresponds to $K = G/G_0 \approx 1$ in the adiabatic regime $\omega_b = 0.1t$ for a coupling up to at least $g = 1.5$ in agreement with the values determined from the structure factor [47,48]. In the intermediate regime $\omega_b = t$ shown in Fig. 7, the conductance $G(M)$ clearly decreases with increasing coupling g . The extrapolated values of G for $1/M \rightarrow 0$ yield parameters $K = G/G_0$ that agree well with the values determined from the structure factor in Ref. [47], as shown in Fig. 8. In particular, we do not observe any sign of superconducting fluctuations ($K > 1$ or $G > G_0$). Unfortunately, we are not able to determine the conductance close to the metal-insulator transition because this requires too many computational resources (the phonon cutoff N_b should be larger than the value $N_b = 4$ used here).

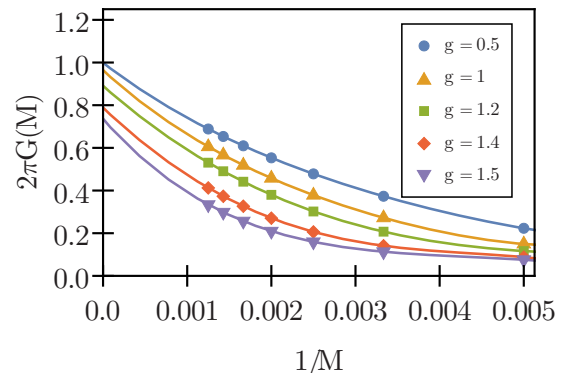


FIG. 7. Same as Fig. 6 but for an intermediate phonon frequency $\omega_b = t$.

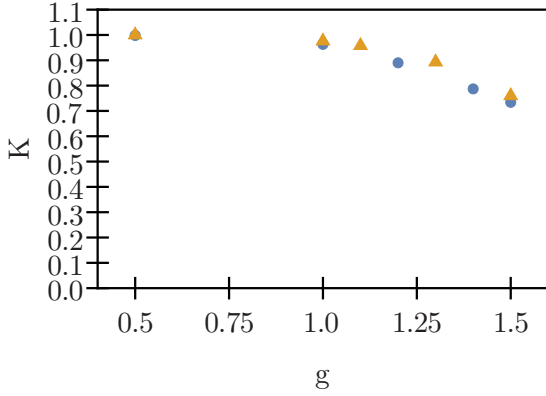


FIG. 8. Luttinger parameter K of the spinless fermion Holstein model with $\omega = t$ as a function of the coupling g . K was determined from the extrapolated value of the conductance G in Fig. 7 (circles) and from the charge structure factor in Ref. [47] (triangles).

In summary, our results for the conductance in the spinless fermion Holstein model agree with the Luttinger parameter K defined from the power-law decay of correlation functions (or equivalently from the static structure factor). This confirms the validity of our method for models with charge carriers coupled to phonon degrees of freedom. It also shows that the relation (7) for the conductance, which was derived for purely fermionic systems using field theory [2,20–22], remains valid for the Luttinger liquid phase of models including phonons.

V. HUBBARD CHAIN

A necessary but simple extension of our method is the generalization to electrons (i.e., fermions with spin $\frac{1}{2}$). To illustrate this extension we consider the one-dimensional homogeneous Hubbard chain with the Hamiltonian

$$H = -t \sum_{j=2}^M \sum_{\sigma} (c_{j,\sigma}^{\dagger} c_{j-1,\sigma} + \text{H.c.}) + U \sum_{j=1}^M n_{j,\uparrow} n_{j,\downarrow}, \quad (9)$$

where $c_{j,\sigma}^{\dagger}$ ($c_{j,\sigma}$) creates (annihilates) an electron with spin σ (\uparrow, \downarrow) on site j and $n_{j,\sigma} = c_{j,\sigma}^{\dagger} c_{j,\sigma}$ is the corresponding particle number operator. The strength of the on-site coupling between electrons is given by the Hubbard parameter U and the hopping term again sets the energy unit $t = 1$. We assume that the system length M is even and that the system contains $M/2$ electrons of each spin (half filling).

The current operator for the electrons with spin σ in the wire is a simple generalization of (6):

$$J_{\sigma} = \frac{1}{M_W - 1} \frac{it}{\hbar} \sum_{j=j_1+1}^{j_2} (c_{j,\sigma}^{\dagger} c_{j-1,\sigma} - c_{j-1,\sigma}^{\dagger} c_{j,\sigma}). \quad (10)$$

The current operator for the charge transport is then given by

$$J_C = J_{\uparrow} + J_{\downarrow}. \quad (11)$$

Using this definition in Eqs. (2) and (3) we obtain the (charge) conductance $G(M)$ of the electronic system. The current

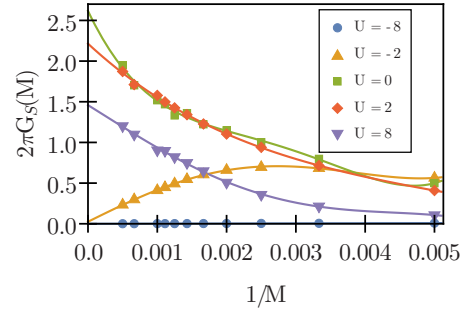


FIG. 9. Spin conductance $G_S(M)$ of the homogeneous Hubbard chain as a function of the inverse system length $1/M$. The Hubbard interaction U is given in the legend. Lines are polynomial fits.

operator for the spin transport is similarly given by

$$J_S = J_{\uparrow} - J_{\downarrow}. \quad (12)$$

Using this definition in Eqs. (2) and (3) we obtain the spin conductance $G_S(M)$ of the electronic system. This describes the linear response of the system to an external magnetic field with the profile (1).

The one-dimensional Hubbard model is exactly solvable using the Bethe ansatz method [49,50]. Its low-energy properties are characterized by a separation of charge and spin excitations and its gapless excitation modes are described by the Luttinger liquid theory. At half filling there is an exact symmetry between the charge (spin) properties for U and the spin (charge) properties for a coupling $-U$. In particular, the ground state is a Mott insulator with gapped charge excitations and gapless spin excitations for $U > 0$, while it is a Luther-Emery liquid [2] with gapless charge excitations and gapped spin excitations for $U < 0$.

We have found that calculating the (charge or spin) conductance with our method is only slightly more difficult for the homogeneous electronic model (9) with $U \neq 0$ than for the homogeneous spinless fermion model. This is understandable because in both cases there is only one gapless excitation mode in the system. As expected the charge conductance $G(M)$ for any U is equal within the numerical errors to the spin conductance $G_S(M)$ for an interaction $-U$. Thus we discuss only the latter case.

In Fig. 9 the scaling of $G_S(M)$ with M is plotted for several values of the interaction U . For noninteracting electrons $G_S(M)$ approaches G_0 as expected. [Note that the quantum of conductance (4) for electrons ($n = 2$) equals $2\pi G_0 = 2$ in our units.] The scattering of the $G_S(M)$ data and the resulting poor extrapolation are due to the lesser accuracy of DMRG for a chain with two gapless excitation modes (i.e., for $U = 0$) than for a single one (i.e., for $U \neq 0$). For $U < 0$, $G_S(M)$ vanishes in the thermodynamic limit as required for a phase with gapped spin excitations. The qualitatively different behaviors for weak and strong attractive interactions is probably due to the different correlation length, which is smaller than $M_W = 10$ for $U = -8t$ but larger for $U = -2t$. The Luttinger liquid parameter for the spinless fermion excitations is $K_S = 1$ in the Mott insulating phase at half filling for any $U > 0$. Concordantly, we observe in Fig. 9 that $G_S(M)$ approaches G_0 for a weak repulsive interaction ($U = 2t$). For stronger

interactions the convergence of $G_S(M)$ toward G_0 is less clear as shown by the results for $U = 8t$ in Fig. 9. This is due to the small bandwidth of the gapless spin excitations (on the order of $4t^2/U$ for large U) which requires a smaller broadening $\eta \sim 4t^2/U$ and thus a larger M to reach the same resolution for the dynamical correlation functions (2).

VI. CONCLUSION AND OUTLOOK

We have extended the DMRG method for the linear conductance of one-dimensional correlated lattice models to more complex systems including interacting leads, coupling to phonons, and the electron spin properties. The tests conducted in this work reveal intriguing differences when the sign of the interaction (attractive/repulsive) differs in the wire and leads and confirm that the renormalization of the conductance by the Luttinger parameter (7) remains valid for the Luttinger liquid phase of homogeneous models with coupling to phonons. Unfortunately, we have found that we cannot determine the conductance of a Luttinger liquid wire between leads with a different interaction but can only investigate short wires because of the complicated finite-size scaling. Moreover, for models with coupling to phonon degrees of freedom the high

computational cost of dynamical DMRG calculations limits the system sizes that can be used.

Nevertheless, the extensions presented in this work will certainly allow us to compute the conductance of short electron-phonon-coupled wires connected to interacting leads (without phonons). Therefore, we will be able to study more realistic models for realizations of quasi-one-dimensional electronic conductors such as atomic or molecular wire junctions [8–11]. Moreover, we point out that our approach is not limited to the charge and spin conductance but could be extended to other transport properties that are described by a local current operator, such as the energy current [51–54].

ACKNOWLEDGMENTS

J.B. would like to thank the Lower Saxony Ph.D. program *Contacts in Nanosystems* for financial support. We also acknowledge support from the DFG (Deutsche Forschungsgemeinschaft) through Grant No. JE 261/2-2 in the Research Unit *Advanced Computational Methods for Strongly Correlated Quantum Systems* (FOR 1807). The cluster system at the Leibniz Universität Hannover was used for the computations.

-
- [1] D. Baeriswyl and L. Degiorgi, *Strong Interactions in Low Dimensions* (Kluwer Academic Publishers, Dordrecht, 2004).
- [2] T. Giamarchi, *Quantum Physics in One Dimension*, International Series of Monographs on Physics (Clarendon Press, Oxford, 2003).
- [3] A. Kawabata, Electron conduction in one dimension, *Rep. Prog. Phys.* **70**, 219 (2007).
- [4] S. Tarucha, T. Honda, and T. Saku, Reduction of quantized conductance at low temperatures observed in 2 to 10 μm long quantum wires, *Solid State Commun.* **94**, 413 (1995).
- [5] C. Blumenstein, J. Schäfer, S. Mietke, S. Meyer, A. Dollinger, M. Lochner, X. Y. Cui, L. Patthey, R. Matzdorf, and R. Claessen, Atomically controlled quantum chains hosting a Tomonaga-Luttinger liquid, *Nat. Phys.* **7**, 776 (2011).
- [6] Y. Ohtsubo, J.-i. Kishi, K. Hagiwara, P. Le Fèvre, F. Bertran, A. Taleb-Ibrahimi, H. Yamane, S.-i. Ideta, M. Matsunami, K. Tanaka, and S.-i. Kimura, Surface Tomonaga-Luttinger-Liquid State on Bi/InSb(001), *Phys. Rev. Lett.* **115**, 256404 (2015).
- [7] M. Bockrath, D. H. Cobden, J. Lu, A. G. Rinzler, R. E. Smalley, L. Balents, and P. L. McEuen, Luttinger-liquid behaviour in carbon nanotubes, *Nature (London)* **397**, 598 (1999).
- [8] N. Agraït, C. Untiedt, G. Rubio-Bollinger, and S. Vieira, Onset of Energy Dissipation in Ballistic Atomic Wires, *Phys. Rev. Lett.* **88**, 216803 (2002).
- [9] N. Agraït, C. Untiedt, G. Rubio-Bollinger, and S. Vieira, Electron transport and phonons in atomic wires, *Chem. Phys.* **281**, 231 (2002).
- [10] H. Ness and A. Fisher, Coherent electron injection and transport in molecular wires: Inelastic tunneling and electron-phonon interactions, *Chem. Phys.* **281**, 279 (2002).
- [11] J. Hihath and N. Tao, Electron-phonon interactions in atomic and molecular devices, *Prog. Surf. Sci.* **87**, 189 (2012).
- [12] J.-M. Bischoff and E. Jeckelmann, Density-matrix renormalization group method for the conductance of one-dimensional correlated systems using the Kubo formula, *Phys. Rev. B* **96**, 195111 (2017).
- [13] R. Kubo, Statistical-mechanical theory of irreversible processes. I. General theory and simple applications to magnetic and conduction problems, *J. Phys. Soc. Jpn.* **12**, 570 (1957).
- [14] D. Bohr, P. Schmitteckert, and P. Wölfle, DMRG evaluation of the Kubo formula: Conductance of strongly interacting quantum systems, *Europhys. Lett.* **73**, 246 (2006).
- [15] J. Eisert, M. Cramer, and M. B. Plenio, *Colloquium: Area laws for the entanglement entropy*, *Rev. Mod. Phys.* **82**, 277 (2010).
- [16] S. R. White, Density Matrix Formulation for Quantum Renormalization Groups, *Phys. Rev. Lett.* **69**, 2863 (1992).
- [17] S. R. White, Density-matrix algorithms for quantum renormalization groups, *Phys. Rev. B* **48**, 10345 (1993).
- [18] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, *Ann. Phys.* **326**, 96 (2011).
- [19] E. Jeckelmann, Density-matrix renormalization group algorithms, in *Computational Many-Particle Physics*, edited by H. Fehske, R. Schneider, and A. Weiße, Vol. 739 of Lecture Notes in Physics (Springer, Berlin, 2008), Chap. 21, pp. 597–619.
- [20] W. Apel and T. M. Rice, Combined effect of disorder and interaction on the conductance of a one-dimensional fermion system, *Phys. Rev. B* **26**, 7063 (1982).
- [21] C. L. Kane and M. P. A. Fisher, Transport in a One-Channel Luttinger Liquid, *Phys. Rev. Lett.* **68**, 1220 (1992).
- [22] C. L. Kane and M. P. A. Fisher, Transmission through barriers and resonant tunneling in an interacting one-dimensional electron gas, *Phys. Rev. B* **46**, 15233 (1992).
- [23] E. Jeckelmann, Dynamical density-matrix renormalization-group method, *Phys. Rev. B* **66**, 045114 (2002).

- [24] E. Jeckelmann and H. Benthien, Dynamical density-matrix renormalization group, in *Computational Many-Particle Physics*, edited by H. Fehske, R. Schneider, and A. Weiße, Vol. 739 of Lecture Notes in Physics (Springer, Berlin, 2008), Chap. 22, pp. 621–635.
- [25] A. Rahmani, C.-Y. Hou, A. Feiguin, M. Oshikawa, C. Chamon, and I. Affleck, General method for calculating the universal conductance of strongly correlated junctions of multiple quantum wires, *Phys. Rev. B* **85**, 045120 (2012).
- [26] V. Meden and U. Schollwöck, Conductance of interacting nanowires, *Phys. Rev. B* **67**, 193303 (2003).
- [27] V. Meden, S. Andergassen, W. Metzner, U. Schollwöck, and K. Schönhammer, Scaling of the conductance in a quantum wire, *Europhys. Lett.* **64**, 769 (2003).
- [28] D. Bohr and P. Schmitteckert, Strong enhancement of transport by interaction on contact links, *Phys. Rev. B* **75**, 241103(R) (2007).
- [29] P. Schmitteckert and F. Evers, Exact Ground State Density-Functional Theory for Impurity Models Coupled to External Reservoirs and Transport Calculations, *Phys. Rev. Lett.* **100**, 086401 (2008).
- [30] A. Branschädel, G. Schneider, and P. Schmitteckert, Conductance of inhomogeneous systems: Real-time dynamics, *Ann. Phys. (Berlin)* **522**, 657 (2010).
- [31] F. Heidrich-Meisner, I. González, K. A. Al-Hassanieh, A. E. Feiguin, M. J. Rozenberg, and E. Dagotto, Nonequilibrium electronic transport in a one-dimensional Mott insulator, *Phys. Rev. B* **82**, 205110 (2010).
- [32] L. G. G. V. Dias da Silva, K. A. Al-Hassanieh, A. E. Feiguin, F. A. Reboredo, and E. Dagotto, Real-time dynamics of particle-hole excitations in Mott insulator-metal junctions, *Phys. Rev. B* **81**, 125113 (2010).
- [33] D. Morath, N. Sedlmayr, J. Sirker, and S. Eggert, Conductance in inhomogeneous quantum wires: Luttinger liquid predictions and quantum Monte Carlo results, *Phys. Rev. B* **94**, 115162 (2016).
- [34] F. Lange, S. Ejima, T. Shirakawa, S. Yunoki, and H. Fehske, Spin transport through a spin- $\frac{1}{2}$ XXZ chain contacted to fermionic leads, *Phys. Rev. B* **97**, 245124 (2018).
- [35] V. V. Ponomarenko, Renormalization of the one-dimensional conductance in the Luttinger-liquid model, *Phys. Rev. B* **52**, R8666 (1995).
- [36] I. Safi and H. J. Schulz, Transport in an inhomogeneous interacting one-dimensional system, *Phys. Rev. B* **52**, R17040 (1995).
- [37] D. L. Maslov and M. Stone, Landauer conductance of Luttinger liquids with leads, *Phys. Rev. B* **52**, R5539 (1995).
- [38] K. Janzen, V. Meden, and K. Schönhammer, Influence of the contacts on the conductance of interacting quantum wires, *Phys. Rev. B* **74**, 085301 (2006).
- [39] R. Thomale and A. Seidel, Minimal model of quantized conductance in interacting ballistic quantum wires, *Phys. Rev. B* **83**, 115330 (2011).
- [40] J. Sirker, The Luttinger liquid and integrable models, *Int. J. Mod. Phys. B* **26**, 1244009 (2012).
- [41] J. M. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids* (Clarendon Press, Oxford, 1960).
- [42] G. D. Mahan, *Many-Particle Physics* (Kluwer Academic Publishers, New York, 2000).
- [43] J. Sólyom, *Fundamentals of the Physics of Solids, Volume 2: Electronic Properties* (Springer, Berlin, 2009).
- [44] E. Jeckelmann and H. Fehske, Exact numerical methods for electron-phonon problems, *Riv. Nuovo Cimento* **30**, 259 (2007).
- [45] E. Jeckelmann and S. R. White, Density-matrix renormalization-group study of the polaron problem in the Holstein model, *Phys. Rev. B* **57**, 6376 (1998).
- [46] T. Holstein, Studies of polaron motion: Part I. The molecular-crystal model, *Ann. Phys.* **8**, 325 (1959).
- [47] S. Ejima and H. Fehske, Luttinger parameters and momentum distribution function for the half-filled spinless fermion Holstein model: A DMRG approach, *Europhys. Lett.* **87**, 27001 (2009).
- [48] J. Greitemann, S. Hesselmann, S. Wessel, F. F. Assaad, and M. Hohenadler, Finite-size effects in Luther-Emery phases of Holstein and Hubbard models, *Phys. Rev. B* **92**, 245132 (2015).
- [49] E. H. Lieb and F. Y. Wu, Absence of Mott Transition in an Exact Solution of the Short-Range, One-Band Model in One Dimension, *Phys. Rev. Lett.* **20**, 1445 (1968).
- [50] F. Essler, H. Frahm, F. Göhmann, A. Klümper, and V. Korepin, *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, 2005).
- [51] X. Zotos, F. Naef, and P. Prelovsek, Transport and conservation laws, *Phys. Rev. B* **55**, 11029 (1997).
- [52] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Thermal conductivity of anisotropic and frustrated spin- $\frac{1}{2}$ chains, *Phys. Rev. B* **66**, 140406(R) (2002).
- [53] R. Steinigeweg, J. Herbrych, X. Zotos, and W. Brenig, Heat Conductivity of the Heisenberg Spin-1/2 Ladder: From Weak to Strong Breaking of Integrability, *Phys. Rev. Lett.* **116**, 017202 (2016).
- [54] C. Karrasch, D. M. Kennes, and F. Heidrich-Meisner, Thermal Conductivity of the One-Dimensional Fermi-Hubbard Model, *Phys. Rev. Lett.* **117**, 116401 (2016).