The conductance of interacting nano-wires

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The conductance of one-dimensional nano-wires of interacting electrons connected to non-interacting leads is calculated in the linear response regime. Two different approaches are used: a many-body Green function technique and a relation to the persistent current recently proposed based on results of the non-interacting case. The conductance is evaluated using the functional renormalization group method and the density matrix renormalization group algorithm. Our results give a strong indication that the idea of obtaining the conductance from the persistent current holds for interacting systems.

The last few years brought fast progress in the experimental techniques to design and manipulate mesoscopic quasi-one-dimensional electron systems. Electron correlations play a crucial role in one spatial dimension leading to Luttinger liquid behavior in the infinite wire limit. [1] Furthermore the interplay of electron correlations and impurities leads to a drastic effect. Even in the presence of a single impurity in the infinite wire limit and at low energy scales physical observables behave as if the system is split in two chains with open boundary conditions at the end points. [2] A deeper theoretical understanding of the electron transport through interacting nano-wires is thus of great importance in connection with experiments and possible applications in nanotechnology. Additionally it will shed light on the question how electron correlations and the interplay of correlations and impurities influence the physical behavior of finite one-dimensional systems.

In a typical experimental setup the wire - or more general the nano-system - is connected to leads which act as reservoirs and the two-terminal conductance is measured. The leads are considered to be free of impurities and non-interacting. They have different chemical potentials $\mu_l$ and $\mu_r$ where $\mu_l - \mu_r$ is given by the applied voltage. The wire might contain impurities and the electrons in the wire will later be assumed to be strongly correlated. For non-interacting electrons, at temperature $T = 0$ and in linear response the two-terminal conductance is given by the Landauer formula $G = 2e^2 |T(k_F)|^2/h$ with the electron charge $e$ and the transmission probability $|T(k_F)|^2$ of the wire at the Fermi wave vector $k_F$. [3,4] The factor 2 is related to the two spin directions. In the following we consider spinless fermions and use the dimensionless conductance $g = G h/e^2$. The above expression was derived using scattering theory. For an interacting wire at $T = 0$ and in linear response $g$ can be expressed by the one-particle Green function of the wire taken at the chemical potential and calculated in the presence of the non-interacting semi-infinite leads. [5,6]

Unfortunately even this Green function cannot be calculated exactly in most cases of physical interest. Thus appropriate approximations are required. We use a functional renormalization group (RG) method [7,8] which we have applied successfully in the context of impurities in interacting one-dimensional systems. [9,10] We neglect the flow of the two-particle vertex which provides a good approximation to the exact result for interactions which are not too large (see below). [9,10] This establishes one way to approximately determine $g$.

Here we exclusively study the zero temperature and linear response regime. We focus on the case of an impurity free interacting wire. The generalization to the case including impurities is straightforward. The wire will be modeled by the lattice model of spinless fermions with nearest neighbor interaction $U$ and the leads by a spinless tight-binding Hamiltonian.

Within Luttinger liquid theory the conductance of an impurity free interacting wire has been determined using an effective field theory and bosonization. [11,12] Even though these works were clearly a step forward in clarifying the issue that for “perfectly connected” leads the conductance is independent of the electron-electron interaction and the length of the wire, i.e. $g = 1$, in connection with experimentally accessible wires the modeling has to be doubted. Within the effective field theory it is clear what “perfectly connected” means; a sharp jump of the Luttinger liquid parameter $K = 1$ in the leads to $K < 1$ in the interacting region. Assuming a spatially varying $K$ is an extension of standard Luttinger liquid theory and it is not clear how to describe such a situation starting from a microscopic model. As later discussed briefly we find $g = 1$ for a lattice model in which the interaction is turned on infinitely slowly (in space). [13,14] For the generic case relevant for experiments $g$ depends on the interaction and the length of the wire even if no additional one-particle scattering terms are considered at the contacts and in the wire.

Very recently Sushkov suggested to calculate $g$ from the persistent current $I(\phi)$ of a one-dimensional ring penetrated by a magnetic flux $\phi$. [15] The ring of $N$ lattice sites is build of two parts: the interacting wire with $N_W$ sites, and non-interacting “leads” with $N_L$ sites. The
We consider the Hamiltonian \( (N = N_W + N_L) \) \[ H = -\sum_{j=-N_L/2}^{N_W-1} \left( c_j^\dagger c_{j+1} e^{i\phi/N} + c_{j+1}^\dagger c_j e^{-i\phi/N} \right) + U \sum_{j=1}^{N_W} (n_j - 1/2)(n_{j+1} - 1/2) \] in standard second-quantized notation. The hopping matrix element and the lattice constant are set to one and the flux \( \phi \) is measured in units of the flux quantum. When calculating the persistent current periodic boundary conditions are used. When using the infinite leads method \( \phi \) is set to zero. The interaction in the wire (lattice sites 1 to \( N_W \)) has to be compensated by an external potential. Otherwise the fermions would depopulate the interacting region. We here exclusively consider the case of a half-filled system. The connection between the leads and the wire is considered to be perfect in the sense that no local scattering terms, as e.g. a smaller hopping matrix element between the sites 0 and 1 (and \( N_W \) and \( N_W + 1 \)) or site impurities on the sites 0 and \( N_W + 1 \), are included. Such terms can be added and the more complex Hamiltonian can still be treated by the methods applied in this work.

In the infinite leads limit and for the model discussed here \( g \) is given by \([5,6]\)
\[ g = 4 \left| G_{N_W,1}(0) \right|^2, \]
where \( G_{N_W,1} \) is the interacting one-particle Green function in the Wannier basis. In Refs. \([9,10]\) we describe how to determine Green functions using the functional RG method of a system with interaction on all sites. As in these investigations we neglect the flow of the two-particle vertex. In the above references it was demonstrated that this approximation is valid for interactions as large as \( U \approx 1 \). Later it will be shown that the same holds here. Crucially within the approximation physical observables still show typical Luttinger liquid behavior (for \( U \leq 2 \)) in the infinite wire limit. \([9,10]\) Thus the relevant correlations are included. This has to be contrasted to simple perturbative methods \([15,21]\) which do not include Luttinger liquid effects. In the present context the infinite non-interacting leads can be integrated out only leading to additional contributions on the lattice sites 1 and \( N_W \). The effective Hamiltonian can then be treated using the RG and \( G_{N_W,1}(\varepsilon) \) can be calculated numerically. The scattering properties can be understood in terms of an effective oscillating one-particle potential. This helps to obtain an intuitive understanding of the observed physics. \([9,10]\) Technical details about this method will be presented elsewhere. \([14]\)
In Ref. [10] we have investigated the persistent current of a ring with interaction on all \( N \) sites using RG and complex-valued DMRG. A generalization to the present situation is straightforward. Fig. 1 shows typical curves for \( NI(\phi) \) at even \( N_W \) obtained from DMRG and RG. The parameters are \( N = 64, N_W = 12, \) and \( U = 1 \). Both curves agree quantitatively. This holds for even larger \( N_W \) and \( N \) we have investigated. The current for this typical set of parameters is far from being sinusoidal. Thus the phase sensitivity \( \Delta E_0 \) can obviously not be used directly to determine \( I(\pi/2) \) and \( g \). Only in the limit of a strong effective impurity \( I(\phi) \) becomes proportional to \( \sin \phi \). [10] In the present context and for even \( N_W \) this limit is reached for very large \( U \) and \( N_W \). Increasing \( N \) for fixed \( N_W \) (even) the curves of Fig. 1 only change slightly and the infinite leads limit can reliably be extrapolated from \( N \approx 100 \). The \( NI(\phi) \) extrapolated to the infinite lead limit decreases if \( N_W \) (even) is increased. This is related to the Luttinger liquid scaling of \( I(\phi) \). [10,17] For odd \( N_W \) and all \( U \) we have studied the persistent current is of almost saw tooth like shape. Increasing \( N \) at fixed \( N_W \) the data seem to converge to the non-interacting and impurity free curve \( NI_0(\phi) = v_F(\phi - \pi)/\pi \), with \( 0 \leq \phi < 2\pi \) and the Fermi velocity \( v_F \), [10] which implies \( g = 1 \). To obtain the conductance following the suggestion of Sushkov we have determined \( E_0(\phi) \) (and the non-interacting groundstate energy \( E_0^0(\phi) \)) for a few fluxes around \( \pi/2 \) using DMRG and RG. From this \( I(\pi/2) \) and \( I_0(\pi/2) \) were obtained by numerical differentiation. Since around \( \phi = \pi/2 \), \( E_0(\phi) \) is a fairly smooth function (see also Fig. 1), this procedure leads to reliable results. For fixed \( N_W \) and \( U \) we have done this for \( N = 16, 32, 64, \) and \( 128 \). As an example in Fig. 2 we present DMRG data of \( NI(\pi/2) \) for \( N_W = 12 \) and \( N_W = 13 \) and different \( U \) as a function of \( \ln N \). To extrapolate we have fitted the data to a quadratic polynomial in \( 1/N \). For even \( N_W \) the \( N \rightarrow \infty \) limit of \( NI(\pi/2) \) can be obtained up to high precision. We have also tried different extrapolation schemes to ensure that the asymptotic current only very weakly depends on the details of the assumed scaling. For odd \( N_W \) and \( U \geq 3 \) the finite \( N_W \) data still change significantly even for \( N \) as large as 128 and the asymptotic limit obtained by extrapolation is clearly less reliable. The DMRG data strongly tend to \( NI(\pi/2) = 1 \) which corresponds to \( g = 1 \). The same behavior can be found for other odd \( N_W \). This suggests \( g = 1 \) for all odd \( N_W \) but a definite statement would require larger \( N \). The RG data for \( NI(\pi/2) \) show a quite similar behavior, with the difference that using this technique for odd \( N_W \) the large \( N \) data are closer to 1 and clearly extrapolate to \( g = 1 \). Additionally \( g \) was determined within the RG using Eq. (5) which already implies infinite leads.

**Fig. 1.** Persistent current \( NI(\phi) \) for \( N = 64, N_W = 12, \) and \( U = 1 \). The filled symbols are DMRG data and the open symbols RG data.

**Fig. 2.** \( NI(\pi/2) \) for \( N_W = 12 \) (open symbols), \( N_W = 13 \) (filled symbols), different \( N \), and \( U \) obtained from DMRG.

Fig. 3 summarizes our results for \( N_W = 12 \) and \( N_W = 13 \), which are typical also for other \( N_W \). Several conclusions can be drawn from this figure. Within the RG the two approaches to determine \( g \) lead to results which agree quite well. The small deviation between the two data sets has mainly two sources, both of them making the persistent current data [Eq. (1)] less precise than the infinite leads data [Eq. (5)]: (i) The numerical differentiation of \( E_0(\phi) \). (ii) The \( N_L \rightarrow \infty \) extrapolation. The estimated total error is smaller than the symbol size. Fig. 3 shows that Sushkov’s suggestion Eq. (1) indeed works for an interacting wire. For odd \( N_W \) in both approaches we find perfect conductance \( g = 1 \) for all \( U \). The infinite leads approach does not require an extrapolation and solving the flow equations within this approach is much faster compared to calculating the persistent current in a \( N \) lattice site system. Thus within the RG and also in perturbation theory [21] using Eq. (5) is clearly superior to the persistent current approach. The advantage of the persistent current method is that it enables us to determine \( g \) using DMRG. For up to \( U \approx 1 \) the RG and DMRG data agree quantitatively. For larger \( U \) the RG data still show the same qualitative behavior as the
DMRG results. As discussed in connection with Fig. 2 the $N \to \infty$ extrapolation for odd $N_W$ and large $U \geq 3$ leads to results which are less reliable. The surprising even-odd effect, observable also at other $N_W$, has been discussed earlier within the Hubbard model using perturbation theory. [21] Similar to perturbation theory within the RG the effect can be traced back to the combination of particle-hole and site inversion symmetry. [14] Using the RG the interaction generates a modulation of the hopping matrix element between the sites of the interacting wire. This acts as an effective impurity which for odd $N_W$ has a perfect resonance at $k_F$. For even $N_W$ and small $U$ the conductance goes like $g = 1 - c(N_W)U^2$ with a $c(N_W) > 0$ which increases with increasing $N_W$.

For fixed $U$, $g$ is a decreasing function of $N_W$ (even). In the limit of very large $N_W$ we find [14] a power-law suppression $g(U,N_W) \sim N_W^{2(1-1/K)}$ known from the problem of a single impurity in a Luttinger liquid. [2] Here the “switching on” of the interaction acts as an impurity. This behavior cannot be captured by simple perturbation theory [21] since it requires Luttinger liquid effects to be included. In the artificial limit of an interaction turned on infinitely slowly (in space) this suppression can be avoided leading to $g(U,N_W) = 1$ also for even $N_W$. [13,14]

In this work, we determine the conductance of an interacting nano-system (i) by a Green function technique and (ii) using the mapping on a persistent current problem suggested by Sushkov, [15,13] both at the level of a functional RG calculation. The resulting conductances are equal and show for interactions $U \leq 1$ (iii) excellent agreement with the conductance obtained following Sushkov’s idea and using essentially exact complex-valued DMRG calculations of the numerical key quantity, the persistent current $I(\pi/2)$. (i)-(iii) give a very strong indication that Sushkov’s suggestion, which analytically can only be justified for non-interacting nano-systems also holds for the interacting case. The conductance can be obtained for microscopic models avoiding the mapping to an effective field theory using bosonization. As an application we calculate the conductance of an interacting, impurity free nano-wire connected to infinite leads. The methods used can easily be generalized to (i) more complex nano-systems with different geometries, (ii) wires with interaction and impurities, (iii) more complex contacts, (iv) multi-channel leads, (v) models with spin, and (vi) other filling factors. We thus believe that combining the two approaches (infinite lead, persistent current) and the two methods (DMRG, RG) gives a very powerful tool to investigate transport properties of realistic models for complex interacting nano-systems.

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![Figure 3](image-url)

**FIG. 3.** Dimensionless conductance $g$ as a function of $U$ for $N_W = 12$ and $N_W = 13$.

For fixed $U$, $g$ is a decreasing function of $N_W$ (even). In the limit of very large $N_W$ we find [14] a power-law suppression $g(U,N_W) \sim N_W^{2(1-1/K)}$ known from the problem of a single impurity in a Luttinger liquid. [2] Here the “switching on” of the interaction acts as an impurity. This behavior cannot be captured by simple perturbation theory [21] since it requires Luttinger liquid effects to be included. In the artificial limit of an interaction turned on infinitely slowly (in space) this suppression can be avoided leading to $g(U,N_W) = 1$ also for even $N_W$. [13,14]

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[1] F.D.M. Haldane, J. Phys. C 14, 2585 (1981).
[2] C.L. Kane and M.P.A. Fisher, Phys. Rev. B 46, 15233 (1992).
[3] R. Landau, IBM J. Res. Dev. 1, 223 (1957).
[4] M. Büttiker, Phys. Rev. Lett. 57, 1761 (1986).
[5] J.S. Langer, Phys. Rev. 127, 5 (1962).
[6] A. Oguri, Phys. Rev. B 56, 13422 (1997).
[7] J. Polchinski, Nucl. Phys. B 231, 269 (1984).
[8] C. Wetterich, Phys. Lett. B 301, 90 (1993).
[9] V. Meden, W. Metzner, U. Schollwöck, and K. Schönhammer, to be published.
[10] V. Meden and U. Schollwöck, Phys. Rev. B 67, 035106 (2003).
[11] I. Safi and H.J. Schulz, Phys. Rev. B 52, R17040 (1995).
[12] D.L. Maslov and M. Stone, Phys. Rev. B 52, R5539 (1995).
[13] R.A. Molina et al., cond-mat/0209552.
[14] V. Meden, W. Metzner, U. Schollwöck, and K. Schönhammer, to be published.
[15] O.P. Sushkov, Phys. Rev. B 64, 155319 (2001).
[16] We here present a “derivation” different from Ref. [15].
[17] A.O. Gogolin and N.V. Prokof’ev, Phys. Rev. B 50, 4921 (1994).
[18] In contrast to a statement in Ref. [15] the current is maximal at $\phi = \pi/2$ only in the limit of a very strong impurity.
[19] S.R. White, Phys. Rev. Lett. 69, 2863 (1992).
[20] Without loss of generality we only consider even $N_I$.
[21] A. Oguri, Phys. Rev. B 59, 12240 (1999); ibid. 63, 115305 (2001).