Conductance through a One-Dimensional Correlated System: Relation to Persistent Currents and Role of the Contacts

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Based on a recent proposal (O.P. Sushkov, Phys. Rev. B 64, 155319 (2001)), we relate the quantum conductance through a sample in which electrons are strongly correlated to the persistent current of a large ring, composed of the sample and a non-interacting lead. A scaling law in the lead length allows to extrapolate to a well-defined value of the conductance, depending only on intrinsic properties of the sample and the nature of the contacts between the sample and the lead. For strongly disordered samples, the conductance is found to be enhanced by the interaction.

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Viewing quantum transport as a scattering problem1,2 generated a new understanding of the electronic conductance. This approach is able to explain a wealth of experimental results3 in mesoscopic systems when electron-electron (e-e) correlations are not important. To include these correlations is non-trivial and remains one of the major challenges in the field (see e.g.4). While none of the proposals to calculate the conductance for a correlated system is well suited for numerical calculations3,5 or free of certain assumptions7, such an issue becomes crucial in present day’s research exploring electronic transport through nanosystems (carbon nanotubes8, molecules9, and point contacts10), where the Coulomb repulsion leads to important correlations.

Reservoirs and leads are key elements in the scattering approach, and possess very clear physical meanings since the measurement is made with electrodes which behave as electron reservoirs. In a good electrode, the electron density $n_e$ is large, the ratio $r_s$ between Coulomb and Fermi energy is small, hence the e-e interaction is negligible. In contrast, $n_e$ in a nanosample can be very small, yielding a large ratio $r_s$ and important e-e correlations.

The dimensionless conductance $g$ does not only depend on the intrinsic properties of the sample, but also on the way it is connected to the electrodes. The quality of the contacts is particularly important for correlated electrons. For a clean Luttinger liquid attached to non-interacting leads through reflectionless contacts, it has been found11 that the interactions do not influence $g$. In the other extreme, if the contacts are tunnel barriers, the interactions lead to Coulomb blockade12, thereby dominating $g$. In carbon nanotubes, various transport regimes are observed depending on the nature of the contacts8.

As shown by Kohn13 and Thouless14, $g$ is also related to the sensitivity of the sample’s eigenstates to a change of the boundary conditions. This sensitivity can be tested by closing a system to a ring and measuring the persistent current as the response to an enclosed magnetic flux $\phi$. At zero temperature, the persistent current is given by $J = -\partial E/\partial \phi$, where $E$ is the ground state energy of the many-body system. Interactions play an important role for $J$, and it is generally accepted that they account for the large difference between experiments and one-particle calculations15. There have been various attempts16,10 to link $J$ and $g$ for an interacting ring. However, the ring built from the sample itself does not contain any reservoirs in which energy relaxation can take place. Negative zero-frequency conductivities occur17, unlike in the dissipative case in which we are interested here.

As pointed out in Refs.16,11, at zero temperature, not only for the non-interacting case, but also for correlated samples, $g$ is given by $|t(E_F)|^2$, the probability for an electron at the Fermi energy $E_F$ to be elastically transmitted through the sample. Moreover, if one replaces the massive electrodes (with negligible e-e correlations) used in a real measurement by very long non-interacting one-dimensional leads, one can expect that they have a similar effect16. Sushkov recently proposed10 that $|t(E_F)|^2$ can be extracted from the persistent current of a much larger ring, composed of the sample itself, together with a long lead closing the system. This has the considerable advantage that a ground state property ($J$) suffices to determine $g$. However, one needs the $J$ of the combined system (sample plus lead), and not the one of the system alone as in previous works13,12,11,14,16.

In the following, we adapt the approach of Ref.10 to calculate $g$ for one-dimensional interacting electrons using the Density Matrix Renormalization Group (DMRG) algorithm15,19. We check that a scaling law allows to extrapolate to an infinite lead, yielding $g$ as a property of the sample and the way it is connected to the lead. The nature of the contacts turns out to play a major role...
role. Then, we extend our analysis to disordered samples, where we find that, similarly to the case of persistent currents [20], repulsive interactions may increase \( g \) for strong disorder.

We first present an alternative derivation of Sushkov’s result [10], pointing out the main assumptions, for the non-interacting case. As depicted in the upper inset of Fig. 1, we consider a sample (S, hashed region) closed to a ring by a non-interacting and disorder-free lead (L), and threaded by a flux \( \phi \). The total length \( L = L_S + L_L \) consists of the sample length \( L_S \) and the lead length \( L_L \). The one-particle eigenstates of the total system satisfy

\[
\det(I - M_S M_L) = 0,
\]

with the transfer matrices of the sample and the lead

\[
M_S = \frac{1}{\sin \varphi} \begin{pmatrix}
\frac{e^{i\alpha}}{\sin \theta} & -i\cot \theta + \cos \varphi \\
i\cot \theta + \cos \varphi & \frac{e^{-i\alpha}}{\sin \theta}
\end{pmatrix},
\]

\[
M_L = e^{i\Phi} \begin{pmatrix}
e^{ik_{LL}} & 0
0 & e^{-ik_{LL}}
\end{pmatrix},
\]

respectively. Here, \( \Phi = 2\pi \phi/\phi_0 \) where \( \phi_0 \) is the flux quantum. The scattering is characterized by the angle \( \theta \), the phase-shift \( \alpha \), and the angle \( \varphi \) (equal to \( \pi/2 \) if right-left symmetry is respected). These angles are functions of \( k \), the wave-vector in the lead. The transmission amplitude is given by \( t = e^{i\alpha} \sin \theta \sin \varphi \). With (2), the quantizing condition \([1]\) can then be written as

\[
\cos \Phi = \frac{1}{|t|} \cos(kL + \delta \alpha),
\]

with the relative phase-shift \( \delta \alpha = \alpha - kl_S \). The persistent current carried by a one-particle state (with energy \( \epsilon \)) is \( j(\phi) = -(\partial \epsilon/\partial k)(\partial \phi/\partial k)^{-1} \). We work at \( \Phi = \pi/2 \) and establish two crucial assumptions: i) \( |\partial (\delta \alpha)/\partial k| \ll L \); ii) \( \partial \epsilon/\partial k \approx \hbar^2 k/m \). The first one states that the Wigner time associated with the scattering region is negligible compared with the time spent in the leads. Notice that we work with a relative Wigner time \( \tau_W = (m/\hbar^2 k)\partial (\delta \alpha)/\partial k \), that is, the difference between the delay time of the scattering region and that of a potential-free region having the same length. The second assumption implies that the dispersion relation is essentially unaffected by the scattering potential.

The persistent current of \( N \) non-interacting spinless fermions (for simplicity we take \( N \) even) is given by [21]

\[
J(\Phi = \pi/2) = \frac{e\hbar}{mL} k_F |t(k_F)|.
\]

Denoting by \( J_0 \) the persistent current of a clean ring of length \( L \), the conductance may be expressed as [10]

\[
g = \lim_{L_L \to \infty} \left( \frac{J(\pi/2)}{J_0(\pi/2)} \right)^2.
\]

With interaction [22], assumptions i) and ii) always hold in the large \( L \) limit. Moreover, the use of Eq. [3] implies that the one-particle states of the correlated system can still be indexed by the lead wave-vectors \( k \). That is, adding an infinite non-interacting lead to a finite non-Fermi-liquid sample restores the Fermi-liquid behavior. This assumption, which has been used in the perturbative calculation of transport through Hubbard chains connected to reservoirs [23], requires that the interactions are completely switched off in the one dimensional lead. Otherwise the Luttinger liquid behavior [24] sets in, and one cannot obtain a result which is independent of the length of the auxiliary lead. In this, our approach differs from Sushkov’s, where the interactions in the lead are kept (within the Hartree-Fock approximation).

Eq. (3) allows to calculate \( g \) from ground-state energies. We do this for spinless fermions (polarized electrons) in a ring described by the Hamiltonian

\[
H = -\sum_{i=1}^{L} (c_i^{\dagger} c_{i-1} + c_{i-1}^{\dagger} c_i) + \sum_{i=2}^{L_S} U n_i - \frac{1}{2} \sum_{n_i-1}^{n_i-1} \frac{1}{2},
\]

where \( c_i \) is the annihilation (creation) operator at site \( i \), \( n_i = c_i^{\dagger} c_i \) the number operator, and the flux-dependent boundary condition enters through \( c_0 = \exp(\Phi) c_L \). The interaction is restricted to nearest neighbors and effective in the sample, but vanishing in the lead. It is equilibrated by a compensating potential that prevents the particles from emptying the interacting region. The form of the Hamiltonian allows to have

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Scaling of \( \ln D \) with the total length \( L \) of the system, showing a linear increase of \( \ln D \) with \( 1/L \) for even \( L_S = 12 \) \(( U = 1 (\bullet), U = 2 (\square), U = 3 (\bigtriangleup), U = 4 (\bigcirc) \)), and a decrease for odd \( L_S = 13 \) \(( U = 1 (\circ) \) and \( U = 2 (\square) \)). Lower inset: scaling for unpolarized electrons within the Hubbard model \(( L_S = 2, U = 1 \)). Upper inset: sketch of a ring consisting of the sample (hashed region) and a non-interacting lead threaded by a flux \( \phi \).}
\end{figure}
asymptotic behavior, described by the scaling law

\[ L \]

the first numerical step is to compute

\[ J \]

is directly proportional to the maximum

\[ C \]

and \( \Phi = \pi \) and \( \Phi = \pi \) (which is simpler to calculate than \( J \)). When the flux-dependence of the ground-state energy is sinusoidal, which is the case in one-dimensional localized systems, \( D \) is directly proportional to the maximum \( J \). We will use such an identification to calculate \( g \) from Eq. (5), taking \( D \) instead of \( J \) [22].

An obvious requirement for Eq. (5) to be useful is that the sign of \( C \) depends on the parity of the number of sites \( S \) in the sample: \( C > 0 \) for even \( S \) and \( C < 0 \) for odd \( S \) (open symbols). Samples with odd \( S \) exhibit almost perfect transmission up to large values of \( U \), while an even \( S \) results in a decrease of \( g(U) \) already at weak interaction. For odd \( S \), particle hole symmetry leads to degenerate sample configurations with \( (S\pm1)/2 \) particles in the interacting region. This is similar to a Coulomb blockade resonance. The traveling particle can thus become trapped for a long time \( (\tau_U > 0) \), consistent with negative \( C \) [22]. Since the two configurations are coupled by processes which transfer particles through the interacting sample, one obtains perfect transmission, as in the perturbative treatment of Ref. [23].

On the other hand, an even number of sites implies that the transport of one particle through the sample takes place via a virtual state with an energy of order \( U \) above the ground-state. Thus, no resonance can be expected and the transmission, which is suppressed already by moderate \( U \), is a fast process with \( \tau_U < 0 \), consistent with \( C > 0 \). In addition, increasing \( S \) reduces \( g \) linearly for small \( U \), and exponentially for \( U > 2 \), consistent with the Mott-insulating behavior.

The even-odd asymmetry, and the perfect transmission for the odd case, point to the importance of the contacts. In order to investigate their role, we introduce a position dependent interaction strength \( U_i \) which increases linearly from 0 to its maximum value \( U \), inside the “contacts” of length \( L_A \) (see inset of Fig. 3). As shown in

\[ U \]

FIG. 2: Conductance \( g \) as a function of the interaction strength \( U \), for different values of the sample length \( L_S \).

FIG. 3: Conductance \( g \) as a function of the interaction strength \( U \), for a fixed \( L_S = 12 \), and increasing smoothing of the contacts, defined by the length \( L_A \) (see inset). Filled (open) symbols correspond to even (odd) \( L_S \); \( L_A = 1 \) (○), and \( L_A = 9 \) (□), \( L_A = 0 \) (■), \( L_A = 4 \) (●), and \( L_A = 10 \) (▲). Using the same smoothing length \( (L_A = 10) \) but improving in the shape (a tanh function (thick solid line) instead of a linear increase (▲)) helps \( g \) to approach the perfect value.
FIG. 4: Ensemble averages of \( \ln g \) as a function of the interaction at \( L_S = 8 \), in the presence of disorder \( W = 1 \) (▲), 5 (●) and 9 (▲). The statistical errors are smaller than the symbol size. The dash-dotted line represents the clean case, the dotted lines represent four individual samples at \( W = 9 \).

In conclusion, starting from a recent proposal, we have provided a well-defined procedure for calculating the conductance \( g \) of interacting one-dimensional wires, and used it to investigate correlation and disorder effects. While the interaction reduces \( g \) for spinless fermions in the presence of weak or moderate disorder, a moderate repulsive interaction increases \( g \) at strong disorder. We also determined the crucial role of the sample-to-lead contacts on the conductance.

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