Tunneling of interacting one-dimensional electrons through a single scatterer: Luttinger liquid behavior in the Hartree-Fock model

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Abstract

We study tunneling of weakly-interacting spinless electrons at zero temperature through a single $\delta$ barrier in one-dimensional wires and rings of finite lengths. Our numerical calculations are based on the self-consistent Hartree-Fock approximation, nevertheless, our results exhibit features known from correlated many-body models. In particular, the transmission in a wire of length $L$ at the Fermi level is proportional to $L^{-2\alpha}$ with the universal power $\alpha$ (depending on the electron-electron interaction only, not on the strength of the $\delta$ barrier). Similarly, the persistent current in a ring of the circumference $L$ obeys the rule $I \propto L^{-1-\alpha}$ known from the Luttinger liquid and Hubbard models. We show that the transmission at the Fermi level in the wire is related to the persistent current in the ring at the magnetic flux $h/4e$.

Key words: one-dimensional transport, mesoscopic wire and ring, electron-electron interaction, persistent current, Hartree-Fock approximation, Luttinger liquid

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It is known that a one-dimensional (1D) wire which is free of impurities and biased by macroscopic contacts yields the quantized conductance. This effect can be derived within a simple model of non-interacting electrons if we assume a negligible electron back-scattering. Placing a single impurity (scatterer) into the wire, the conductance is not quantized any more. It is because of the back-scattering of the electrons from the scatterer. The wire conductance (given by the Landauer formula) is proportional to the electron transmission at the Fermi level [1].

When the electron-electron (e-e) interaction is considered, the conductance of an infinitely long wire with a single scatterer decreases as $T^{-2\alpha}$ for ($T \rightarrow 0$). This behavior is known from the Luttinger liquid model [2] where the power $\alpha$ depends on the e-e interaction only. Assuming a repulsive interaction ($\alpha > 0$), the scatterer becomes impenetrable at zero temperature regardless the strength of the scatterer.

Matveev et al. [3] studied the Landauer conductance of the interacting 1D electrons through a $\delta$ barrier in a wire with contacts. They analyzed the effect of the Hartree-Fock potential on the tunneling transmission assuming a weak e-e interaction. They derived the transmission using the renormalization group (RG) approach and confirmed the universal power law $T^{-2\alpha}$. It is believed that this approach goes beyond the Hartree-Fock approximation.

In this paper we consider the non-Luttinger liquid model of the same type as analyzed by Matveev et al. [3]. However, we do not use the RG theory. We apply the self-consistent Hartree-Fock solution by means of
numerical calculations instead. We calculate the transmission probability at zero temperature which is related to the Landauer conductance. A good agreement with the theory of Matveev et al. is found. In particular, we simulate dependence of the conductance on the wire length \( L \) for various \( \delta \) barriers and we reproduce the universal power law \( L^{-2\nu} \) that becomes asymptotic for large wire lengths and/or strong \( \delta \) barriers.

We also consider a mesoscopic ring threaded by the magnetic flux. As a consequence, the persistent current \( I \) arises \[4\]. We study the persistent current of interacting spinless electrons with a single \( \delta \) barrier at zero temperature. We show how the transmission can be extracted from the persistent current in the 1D ring where \( I \propto L^{-\alpha-1} \) and compare it with the transmission obtained from the 1D wire.

First, consider 1D wire of length \( L \) with interacting spinless electrons. Both wire ends are connected to contacts and the single \( \delta \) barrier is localized in the center of the wire. The single-electron wave functions \( \psi_k(x) \), where \( k \) is the electron wave vector, are described by the Hartree-Fock equation \( H\psi_k(x) = \epsilon_k \psi_k(x) \). The Hamiltonian has the form

\[
H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \gamma \delta(x-L/2) + U_H(x) + U_F(k, x), \tag{1}
\]

where \( \gamma \delta(x-L/2) \) represents the localized scatterer. We apply the boundary conditions

\[
\begin{align*}
\psi_k(x=0) &= e^{ikx} + r_k e^{-ikx}, \\
\psi_k(x=L) &= t_k e^{ikx}, \\
\psi_{-k}(x=0) &= i_k e^{-ikx}, \\
\psi_{-k}(x=L) &= e^{-ikx} + r'_k e^{ikx}
\end{align*}
\tag{2}
\]

with \( r_k \) and \( t_k \) being the reflection and transmission amplitudes, respectively and \( k > 0 \). Knowing the transmission, we can easily evaluate the Landauer conductance \( (e^2/h) |t_{k_F}|^2 \).

The Hartree potential induced by the \( \delta \) barrier reads

\[
U_H(x) = \int_0^L dx' V(x-x')
\]

\[
\times \int \frac{dk'}{2\pi} \left[ |\psi_{k'}(x')|^2 - |\psi_{k'}^*(x')|^2 \right] \tag{3}
\]

and the Fock non-local exchange potential is written as

\[
U_F(k, x) = -\frac{1}{\psi_k(x)} \int_0^L dx' V(x-x')
\]

\[
\times \int \frac{dk'}{2\pi} \psi_k(x) \psi_{k'}^*(x') \psi_{k'}(x) \tag{4}
\]

with \( V(x-x') \) being the e-e interaction. Essentially the same one-dimensional model was considered by Matveev et al. \[3\].

The wire is connected to large contacts via adiabatically tapered non-reflecting connectors \[1\]. In the case of interacting electrons without presence of the scatterer \( (\gamma = 0) \), we assume that there is no backscattering at the wire ends due to the adiabatically tapered connectors. Then, the solution of Eq. \( (1) \) is described by the free wave, \( \psi_k^0(x) = e^{ikx} \), having the eigenenergy

\[
\epsilon_k = \hbar^2 k^2 / 2m + U_F^0(k) \tag{5}
\]

with \( U_F^0(k) \equiv U_F[\psi_k(x) = \psi_k^0(x)] \) being the nonzero Fock shift. Note that this solution is valid if we implicitly assume that the Fock interaction is present also in the contacts. If the energy in Eq. \( (5) \) holds inside the wire and we turn off the Fock shift to zero outside the wire, we obtain at each wire end the potential drop \( U_F^0(k) \). This would cause back-scattering at both wire ends and the solutions \( e^{ikx} \) and \( e^{-ikx} \) would be no longer valid (in contrast to the ballistic conductance of clean wires \[1\]).

If the barrier \( \gamma \delta(x-L/2) \) is positioned in the wire, this \( \delta \) barrier induces Friedel oscillations of the Hartree-Fock potential. The Friedel oscillations penetrate through the wire ends into the contacts, where they decay fast due to the higher dimensionality of the contacts and decoherence. To mimic this decay within our model, we sharply turn off the oscillations to zero at both wire ends keeping \( U_H = 0 \) and \( U_F = U_F^0(k) \) outside the wire. Such a constant potential emulates the non-reflecting connectors and justifies the above boundary conditions.

Our numerical results are carried out for the GaAs wire with the corresponding effective electron mass \( m = 0.067 \ m_0 \), the electron density \( n = 5 \times 10^7 \ \text{m}^{-1} \), and the short range e-e interaction

\[
V(x-x') = V_0 \ e^{-|x-x'|/\ell^2}. \tag{6}
\]

We use the short range e-e interaction \( (6) \) because of comparison with the RG theory \[3\] where the e-e in-
teraction is assumed to be finite. Physical meaning of the finite range is the screening.

The asymptotic formula for the transmission probability at the Fermi level derived for weak e-e interactions [3] reads

\[
|t_{kF}|^2 = \frac{|\tilde{t}_{kF}|^2 (d/L)^{2\alpha}}{|\tilde{r}_{kF}|^2 + |\tilde{t}_{kF}|^2 (d/L)^{2\alpha}} \approx \frac{|\tilde{t}_{kF}|^2}{|\tilde{r}_{kF}|^2} (d/L)^{2\alpha},
\]

where \( d \) is the range of the e-e interaction \( V(x-x') \) and \( \tilde{t}_k \) and \( \tilde{r}_k \) describes the transmission and the reflection amplitudes of the bare \( \delta \) barrier [3], respectively. The right hand side of Eq. (7) remains valid for small \( \tilde{t}_{kF} \) and/or large \( L \). For weak e-e interaction (\( \alpha \ll 1 \)), the power \( \alpha \) reads [3]

\[
\alpha = \frac{V(0) - V(2kF)}{2\pi \hbar v_F},
\]

where \( V(q) \) is the Fourier transform of the e-e interaction \( V(x-x') \). We evaluate \( \alpha \) for our e-e interaction (6), for which \( V(q) = 2V_0d/(1 + q^2d^2) \).

The bare amplitudes are \( \tilde{t}_k = k/(k + i\zeta) \) and \( \tilde{r}_k = -i\zeta/(k + i\zeta) \), where \( \zeta = \gamma m/h^2 \). As \( k_F \) and \( m \) remain fixed, we parametrize the bare \( \delta \) barrier by its transmission coefficient \( |\tilde{t}_{kF}|^2 \) in the following.

Second, consider a 1D wire for which the Hartree-Fock equation reads

\[
\left[ \frac{\hbar^2}{2m} \left( -i \frac{\partial}{\partial x} + \frac{2\pi e}{L \hbar} \phi \right)^2 + \gamma \delta(x - L/2) + U_H(x) + U_F(j, x) \right] \psi_j(x) = \varepsilon_j \psi_j(x) \quad (9)
\]

satisfying the boundary condition \( \psi_j(x + L) = \psi_j(x) \). The persistent current is given as

\[
I = \sum_j \left[ \varepsilon_j - \frac{1}{2} \langle \psi_j \left[ U_H(x) + U_F(j, x) \right] \psi_j \rangle \right].
\]

In case of the non-interacting electrons, the persistent current can be evaluated [5] as follows

\[
I = (e v_F/2L)|\tilde{t}_{\xi_F}| \sin(2\pi \phi/\hbar),
\]

with the transmission amplitude of the scatterer at the Fermi energy \( |\tilde{t}_{\xi_F}| \ll 1 \) and the Fermi velocity \( v_F \).

Assume \( L \to \infty \), the repulsive e-e interaction \( \alpha > 0 \), and \( \phi = \hbar/4e \). Then, replacing \( |\tilde{t}_{\xi_F}| \) by \( |t_{kF}| \) and inserting Eq. (7) into Eq. (11), we obtain [5]

\[
I = \frac{e v_F}{2L} |t_{kF}| = \frac{e v_F}{2L} |\tilde{t}_{kF}| \left( \frac{d}{L} \right)^{\alpha} \propto L^{-\alpha - 1}.
\]

![Fig. 1. Conductance in unit of the transmission probability at the Fermi level vs length for various \( \delta \) barriers \( |t_{kF}|^2 \) in a log-log scale. The dashed curves show the data corresponding to the formula (7). The filled circles connected by the full lines are our self-consistent Hartree-Fock data for the wire; the curves approach the same asymptotic power law as the dashed lines. The open circles are extracted from the persistent current using Eq. (12).](image)

We solve Eqs. (1) and (9) by means of the self-consistent iterative procedure and follow approximation in Ref. [6] in order to decrease computational time and memory. One can further simplify Eq. (4) to

\[
U_F(x) \approx - \int_0^L dx' V(x-x') \int_{-k_F}^{k_F} \frac{dk'}{2\pi} \text{Re}[\psi_k^*(x')\psi_k(x)]
\]

noticing that \( \int_{-k_F}^{k_F} dk' \psi_k^*(x') \psi_k(x) \approx 2\pi \delta(x-x') \). The Fock potential (13) becomes local and independent on \( k \). This allows us to simulate longer wires than in the case of the non-local Hartree-Fock model, cf. Eq. (4).

We also present the results without this simplification but for a substantially shorter wire lengths.

Figure 1 shows the transmission probability \( |t_{kF}|^2 \) for the wire and the ring versus the length \( L \) for various \( \delta \) barriers. The result of the RG (7) is presented by the dashed lines. For strong \( \delta \) barriers the dashed lines follow the asymptotic power law \( |t_{kF}|^2 \propto L^{-2\alpha} \) as manifested by the linear decay with slope \(-2\alpha\) in the log-log scale. Our Hartree-Fock curves (filled and open circles) show slightly higher transmission following the same slope \(-2\alpha\). Note that for \( |t_{kF}|^2 \) small enough and substantially longer wires and rings, all the Hartree-
and for the common range of e–e interactions

\[ \alpha \]

instead (in the case current). It is because the perfect reflection is resulted different results for the conductance (or the persistent imaginary part is omitted (stars). [6]

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