Correlated electron current and temperature dependence of the conductance of a quantum point contact

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We investigate finite temperature corrections to the Landauer formula due to electron-electron interaction within the quantum point contact. When the Fermi level is close to the barrier height, the interaction is strongly enhanced due to semiclassical slowing of the electrons. To describe electron transport we formulate and solve a nonlocal kinetic equation for the density matrix of electrons. The correction to the conductance $G$ is negative and strongly enhanced in the region $0.5 \frac{e^2}{h} \leq G \leq 1.0 \frac{e^2}{h}$. Our results for conductance agree with the so-called “0.7 structure” observed in experiments.

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Introduction. The conductance of a quantum point contact (QPC) - a 1D constriction in a 2D electron gas - has been known to be quantized in units of $G_0 = 2e^2/h$ since 1988 [1, 2]. The observed conductance plateaus can be easily understood in the single-electron picture [3, 4]. Below we write conductance in units of $G_0$.

The “0.7 structure” appears on the lowest conductance step as a narrow extra plateau at $G \approx 0.7$. The structure was first observed by Thomas et al. in 1996 [2] and has been the subject of numerous experiments since [2, 3, 4, 5, 6]. The position of the structure varies from 0.4 to 0.7 depending on the device, and the structure becomes more pronounced as the temperature is increased up to ~2K, where thermal smearing becomes significant. It is not clear from experiment whether the structure survives at $T = 0$. In a longitudinal magnetic field, which breaks the spin degeneracy, the structure evolves smoothly to the 0.5 plateau that is expected in the single-electron picture. This demonstrates that the effect is in some way related to electron spin.

Observations of the 0.7 structure have created much theoretical interest. There have been suggested explanations based on spontaneous magnetization within the contact [2, 3, 4, 5, 6, 11, 15, 17], charge density waves within the contact [18, 19], the Kondo effect [20, 21], and even on electron-phonon scattering in the contact [22]. The problem has also stimulated the development of general scattering theory in the presence of leads [23, 24].

In the present paper, using perturbation theory, we consider the finite temperature correction to the Landauer formula for the conductance of a QPC. Our results are very similar to experimental data on the 0.7 structure.

Model. Near the center of the QPC the single-particle dynamics are described by the parabolic saddle-point potential $U = U_0 - \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega_y^2y^2$, see, e.g., Ref. [4]. Here $m$ is the effective mass, $U_0$ is an energy that can be controlled in experiment using the gate voltage, and $\omega_y$ and $\omega$ are parameters with typical values in experiment of $\omega_y/\omega \sim 3$, $\omega_y \sim 4$meV. Throughout the paper we set $\hbar = k_B = 1$. The dynamics in the x-direction are described by different channels corresponding to quantization in the y-direction. The lowest, $n = 0$, channel has longitudinal potential $\frac{1}{2}m\omega^2x^2$, and hence the transmission probability is [27]

$$t_n = (1 + e^{-2\pi\epsilon})^{-1},$$

where $\epsilon = E/\omega$, $E$ is the energy. At $\epsilon = 0$ the turning point for the $n$th channel is $x_0 = \pm \sqrt{\frac{2\hbar}{m\omega^2}}$. So outside the barrier, from $x_{2D} \sim 2/\sqrt{m\omega}$, many transverse channels are occupied and hence the electron-electron Coulomb interaction is strongly screened. The interaction is un-screened only on the top of the barrier where the electron density is low. Therefore the effective electron-electron interaction in the $n = 0$ channel can be approximated as

$$\frac{e^2}{\kappa|x_1 - x_2|} \rightarrow H_{\text{int}} = \frac{e}{\pi \kappa \delta(x_1 - x_2)} \delta(y),$$

where $e$ is the electron charge, $\kappa$ is the dielectric constant, $\delta(x)$ is the dimensionless distance. In GaAs, $\kappa \approx 13$, $m \approx 0.07m_e$, and for $\omega \sim 1$meV the dimensionless coupling constant $g_e \approx \frac{e^2}{\pi \kappa \sqrt{m/\omega}}$ is about unity, $g_e \sim 1$. Another issue related to the many-body screening is the absence of pronounced structures in higher conductance steps. For higher steps there are always lower channels penetrating the QPC. This leads to high electron density in the contact and hence to screening of the effective interaction (2).

To represent single-particle wave functions in the $n = 0$ channel we consider a 1D wire of length $L$ with a potential barrier in the middle of the wire. The details of the potential shape are unimportant apart from the parabolic top, see, e.g., [25]. We need the “wire” to normalize wave functions according to $\int_0^L |\psi_k|^2 dx = 1$, since this normalization is convenient for discussion of the nonlocal kinetic equation, see below. The length $L$, which is
of the order of the ballistic mean free path, disappears from final answers. Away from the barrier the wave function \( \psi_k \) is the standard combination of incident, reflected and transmitted waves. Near the potential top the wave function is of the form, see, e. g., Ref. 22.

\[
\psi_k(x) \approx \frac{1}{\sqrt{L}} \left( \frac{mv_F^2}{2m} \right)^{1/4} \varphi_k(\xi),
\]

\[
\varphi_k(\xi) = \frac{e^{i \xi/2}}{\sqrt{2} \cosh(\pi \epsilon)} D_\nu(\sqrt{2} \xi e^{-i \pi/4}),
\]

where \( v_F \) is the Fermi velocity far from the barrier, \( D_\nu \) is the parabolic cylinder function, and \( \nu = i \epsilon - \frac{1}{2} \). Eq. 9 corresponds to the wave incident from the left, \( k \geq 0 \). Due to semiclassical slowing, the probability density at the top of the potential,

\[ \rho(\epsilon) = |\varphi_k(0)|^2 \]

is peaked at \( \epsilon \approx 0.2 \), see Fig. 1. This results in enhancement of the interaction 23, and in the end this leads to all effects considered in this paper.

![FIG. 1: The probability density at \( \xi = 0 \) versus the dimensionless energy \( \epsilon \).](image)

The current in state 11 is \( j_k = \frac{e}{\hbar} \frac{\partial}{\partial \epsilon} \varphi_k(\xi) \), and hence the total current obeys the Landauer formula

\[ J = 2e \int \frac{Ldk}{2\pi} j_k n_{0k} = \frac{2e^2}{\hbar} \mu V, \]

\[ n_{0k} = n_f + \frac{eV}{2\omega} n'_f. \]

Here \( n_{0k} \) is the non-equilibrium occupation number under a small applied voltage \( V \), \( n_f = n_f(\epsilon) \) is the equilibrium Fermi-Dirac distribution, \( s = k/k \) shows the direction of current flow in a particular state, and \( n'_f = -\frac{\partial n_f}{\partial \epsilon} \approx \delta(\epsilon - \mu) \); \( \mu \) is the chemical potential in units of \( \omega \).

The nonlocal kinetic equation. At zero temperature the interaction 12 in the leading order is described by the usual direct and exchange diagrams for the single-particle scattering amplitude. The corresponding corrections renormalize the frequency \( \omega \) in the single particle potential and even make the effective potential slightly nonparabolic (flattened). Nevertheless this does not materially change the profile of the transmission coefficient 11. We have checked numerically that the same is true with up to higher orders in perturbation theory. Thus the interaction 12 treated perturbatively does not influence the Landauer formula and does not materially change the shape of the transmission coefficient at zero temperature.

Nonzero temperature requires a consideration of the details of equilibration. Eq. 15 implies nonlocal equilibration, as the scattering states with \( s = +1 \) equilibrate due to collisions in the left lead and the states with \( s = -1 \) equilibrate due to collisions in the right lead. As a consequence, the many-body density matrix is diagonal not in the basis of plane waves or standing waves, but in the basis of the scattering states 13 (see also Ref. 29). Therefore, the occupation numbers \( n_k \), the diagonal matrix elements of the density matrix, obey the kinetic equation \[ \frac{\partial n_k}{\partial t} = -\frac{n_k - n_{0k}}{\tau} + \text{St}(n_k), \]

where \( \text{St}(n_k) \) is the collision term in the kinetic equation 27.

Here \( M_{k,1,2,3} \) is the matrix element of the interaction 12. This matrix element corresponds to the real transition between quantum states, \( |k, k_1 \rangle \rightarrow |k_2, k_3 \rangle \). Therefore in the matrix element the initial and final wave functions are given by 14. This differs from the rule for the scattering amplitude, where initial wave functions are given by 14, while final wave functions are \( \psi_k^{(\pm)}(x) = \psi_{\mp k}(x) \) (the Sommerfeld rule, see, e.g., Ref. 24).

Using occupation numbers from 15 and expanding the collision integral up to the first power in the bias \( V \), we find the integral at small temperature, \( T \ll \omega \),

\[ \text{St}(n_k) = \frac{2e^2 V L^3}{12v_F^3} \delta(E_k - \omega \mu) \times \sum_{s_1 s_2 s_3} |s + s_1 - s_2 - s_3| M_{k_1 k_2 k_3}^2. \]

All legs in the matrix element are taken at the Fermi surface, so we need only perform summations over the directions \( s_1, s_2, s_3 \). Calculating the matrix elements of...
interaction \( \mathcal{L} \) with the wave functions \( \psi \) we find

\[
\text{St}(n_k) = -\frac{T^2eV L^3}{3v_F^3} s\delta(E_k - \omega \mu) \\
\times \left( |M_{++-}|^2 + |M_{+++}|^2 \right) \\
= -seV \frac{\pi^4 g_e^2 v_F}{6} \left( \frac{T}{\omega} \right)^2 \rho^4(\mu) \delta(E_k - \omega \mu),
\]

where \( \rho(\mu) \) is given by \( \mathcal{L} \). Eq. \( \mathcal{L} \) leads to the following steady-state solution of the kinetic equation \( \mathcal{L} \)

\[
n_k = n_f + \frac{eV}{2} s\delta(E_k - \omega \mu) \\
\times \left\{ 1 - \frac{\pi^4 g_e^2 \tau v_F}{3} \left( \frac{T}{\omega} \right)^2 \rho^4(\mu) \right\}.
\]

Substitution of this expression into Eq. \( \mathcal{L} \), where \( n_{0k} \to n_k \), gives an altered conductance in units of \( G_0 \)

\[
t_\mu \to \tau_\mu = t_\mu \left\{ 1 - \frac{\pi^4 g_e^2 \tau v_F}{3} \left( \frac{T}{\omega} \right)^2 \rho^4(\mu) \right\}.
\]

Eq. \( \mathcal{L} \) is justified only if the temperature-dependent correction term is small compared to unity. The term is due to the current of correlated electrons. It will be most significant within the region \( 0.5 \leq G \leq 1.0 \) since above \( G = 0.5 \) electrons can flow without tunnelling. The length \( L \) is of the order of the mean free path in the leads, so it is most natural to assume that the factor \( \frac{\tau v}{2} \) in \( \mathcal{L} \) is of the order of unity, though we cannot exclude some dependence of the factor on temperature. In the latter case the \( T^2 \) dependence of the correlated current will be modified.

Note that the correction we have discussed is due to the interaction between electrons with opposite spins. The interaction between electrons with parallel spins vanishes because the exchange diagram exactly cancels out the direct one for the contact Hamiltonian \( \mathcal{L} \). Therefore under an applied longitudinal magnetic field \( B \) we should take \( \rho^4(\mu) \to \rho^2(\mu)\rho^2(\mu') \). Here \( \mu' = \mu - (2g_e \mu_B) B/\omega \), where \( g_e \) is the gyromagnetic ratio and \( \mu_B \) is the Bohr magneton. Since \( \rho(\mu) \) is a peaked function, see Fig. \( \mathcal{L} \) a magnetic field \( B \approx \omega/(2g_e \mu_B) \approx 5T \) effectively switches off the interaction. This gives an explanation for the smooth evolution of the 0.7 structure to the 0.5 plateau of non-interacting electrons under a magnetic field.

A set of plots of \( \tau_\mu \) for different temperatures is shown in Fig. \( \mathcal{L} \). Though the result looks quite sensible it is obtained for \( g_e \ll 1 \). However, according to our estimate \( \mathcal{L} \), the constant is not small, \( g_e \sim 1 \), and hence virtual rescattering must be taken into account.

Renormalization of the coupling constant. The leading correction to the Born scattering amplitude is given by the diagrams shown in Fig. \( \mathcal{L} \). This correction is equivalent to renormalization of the coupling constant, \( g_e \to g_e + \delta g_e \), where \( \delta g_e(\mu) = 2g_e^2 K(\mu) \) and

\[
K(\mu) = \frac{1}{4} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(\epsilon_1) \rho(\epsilon_2) \left\{ \frac{\theta(\epsilon_1 - \mu)\theta(\epsilon_2 - \mu)}{2\mu - \epsilon_1 - \epsilon_2} + \frac{\theta(\mu - \epsilon_1)\theta(\epsilon_2 - \mu)}{\epsilon_1 + \epsilon_2 - 2\mu} - \frac{2\theta(\mu - \epsilon_1)\theta(\epsilon_2 - \mu)}{\epsilon_1 - \epsilon_2} \right\} \, d\epsilon_1 \, d\epsilon_2.
\]

Here \( \theta(y) \) is the step function. The first term in \( K(\mu) \) (diagram Fig. \( \mathcal{L} \)) is logarithmically divergent at \( \epsilon_1, \epsilon_2 \to +\infty \). The divergence is a result of the contact approximation \( \mathcal{L} \). When the energy is large, \( \epsilon \gg 1 \), the wave length is smaller than the size of the barrier, \( \lambda \ll 1/\sqrt{\omega} \), and the contact approximation fails. To fix the problem, we introduce an ultraviolet cutoff \( \Lambda \), \( \epsilon_1 + \epsilon_2 \leq \Lambda \). Dependence on the cutoff is weak and we will present all results for \( \Lambda = 2 \). The integrals in \( \mathcal{L} \) cannot be calculated analytically. However numerical integration is very simple and we present a plot of \( K(\mu) \) in Fig. \( \mathcal{L} \).

Since the coupling constant \( g_e \sim 1 \), the second order correction alone is not sufficient. However in this regime the Brueckner approximation \( \mathcal{L} \) usually works well. Since the kernel \( K(\mu) \) is independent of external momenta, the Brueckner approximation is equivalent to the summation of a geometrical progression, and hence the renormalized coupling constant \( g_R \) is

\[
g_R^2 = g_e^2 R(\mu), \quad R(\mu) = \frac{1}{[1 - 2g_e K(\mu)]^2}.
\]

Plots of \( R(\mu) \) for \( g_e = 1 \) and \( g_e = 2 \) are presented in Fig. \( \mathcal{L} \). Fig. \( \mathcal{L} \) shows a set of plots of conductance \( \tau_\mu \) for different temperatures, using Eq. \( \mathcal{L} \) with \( g_e \to g_R(g_e) \) for \( g_e = 1 \).
in the present paper have a very simple physical origin: the electron wave function at the barrier and hence the electron-electron interaction is strongly peaked when the transmission coefficient is slightly higher than 0.5.

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FIG. 4: Dashed line: the function \( K(\mu) \) for the second order correction. Solid line: Brueckner correction factor \( R(\mu) \) for \( g_e = 1 \). Long dashed line: Brueckner correction factor \( R(\mu) \) for \( g_e = 2 \).

FIG. 5: Conductance in units of \( 2e^2/h \) versus \( \mu \) (chemical potential in units of \( \omega \)) for different temperatures: the intermediate coupling limit, \( g_e = 1 \). The uppermost curve corresponds to \( T = 0 \), while the lowest is \( T \approx 0.3K \), assuming \( \frac{\tau v_e}{K} \approx 1 \).

The results presented in Figs. 2 and 5 are very similar to the experimental data on the 0.7 structure. According to our calculation the exact position of the structure depends on the coupling constant \( g_e \): for small \( g_e \) it is more like a “0.5 structure” and for \( g_e \sim 1 \) it is a “0.6–0.7 structure”.

In conclusion. Within perturbation theory, we have considered transport of correlated electrons through a quantum point contact. At zero temperature, the approach results in the usual Landauer formula and the conductance does not show any structures. To describe the current at nonzero temperature we have formulated a nonlocal kinetic equation for the occupation numbers. A current of correlated electrons scales as temperature squared at very low temperatures. The corresponding correction to conductance is negative and strongly enhanced in the region \( 0.5 \leq G \leq 1.0 \). We believe that these results are directly relevant to the 0.7 conductance structure. For the case of weak coupling, the set of plots of the conductance for different temperatures is shown in Fig. 4. The corresponding plots for intermediate coupling, which is probably the regime most relevant to experiment, is shown in Fig. 5. Our model is consistent with the experimental behavior of the 0.7 structure under a magnetic field: a field smoothly “switches off” the effective interaction between electrons. Effects considered...