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Coherent transport in disordered metals: zero dimensional limit

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Abstract. We consider non-equilibrium transport in disordered conductors. We calculate the interaction correction to the current for a short wire connected to electron reservoirs by resistive interfaces. In the absence of charging effects we find a universal current-voltage-characteristics. The relevance of our calculation for existing experiments is discussed as well as the connection with alternative theoretical approaches.

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Rapid Note

In recent years considerable attention has been devoted to the effects of the Coulomb interaction on the transport properties of small structures, like thin diffusive films and wires [1–4], tunnel junctions [5–7], and quantum dots [8]. One interesting issue concerns the way an applied bias voltage affects the interaction corrections to the electrical conductivity. In diffusive metals these corrections arise from the combination of the electron-electron and impurity scattering and yield well known singularities at low temperature [9]. It has been shown that a finite voltage or, more in general, a non-equilibrium situation leads to a suppression of these singularities [10–14]. In particular, in [10,14] non-equilibrium transport in a short wire connected to electrical reservoirs by ideal interfaces has been considered. However, in actual experiments the interfaces need not be ideal. Recently Weber *et al.* [15] investigated experimentally the non-equilibrium transport through a metallic nano-scale bridge. Both in [15] and in [16] it has been suggested that the Coulomb interaction effects are responsible for the observed temperature dependence of the conductance and the current-voltage-characteristics. Whereas [15] found an agreement between theory and experiment starting from a tunneling Hamiltonian, [16] pointed out that the experimental data agree with what they expect for a diffusive conductor. In this paper we develop a formalism in which both the resistive behavior due to the interfaces and due to the diffusive wire region are treated on the same footing. From our results we conclude that the main resistive behavior in [15] occurs at the interfaces.

To begin with we recall the classical description of electrical transport through structures consisting of both interface barriers and diffusive regions. To be definite we consider a system made by a diffusive wire of length L which is attached to the reservoirs by two interface barriers. We study the system in a non-equilibrium situation with an applied voltage $V_l - V_r = V$ where the subscripts l and r indicate the left and right reservoirs, respectively. The classical resistance of the structure is the sum of the wire resistance and the interface resistances $R_{\rm tot} = R_{\rm wire} + R_l + R_r$, so that the current as a function of voltage is $I = V/R_{\rm tot}$. The microscopic calculations are conveniently carried out by using the Keldysh formalism [17]. In a disordered system the Keldysh component of the Green function reads as

$$G^K_\epsilon(\mathbf{x},\mathbf{x}) = F_\epsilon(\mathbf{x})[G^R_\epsilon(\mathbf{x},\mathbf{x}) - G^A_\epsilon(\mathbf{x},\mathbf{x})] \quad (1)$$
$$\approx -2\pi \mathrm{i} N_0 F_\epsilon(\mathbf{x}). \quad (2)$$

The first line is an exact relation and defines the distribution function F. In the second line it is assumed that the density of states is a position independent constant. The current flowing in the wire or through the boundaries is then given by

$$I_{\rm wire} = eDN_0\mathcal{A}\int \mathrm{d}\epsilon \partial_x F_\epsilon(x) \quad (3)$$

$$I_l = e\Gamma_l \mathcal{A} N_0 \int \mathrm{d}\epsilon [F_\epsilon(0) - F^l_\epsilon] \quad (4)$$

$$I_r = e\Gamma_r \mathcal{A} N_0 \int \mathrm{d}\epsilon [F^r_\epsilon - F_\epsilon(L)], \quad (5)$$

where D is the diffusion constant, $\mathcal{A}$ the cross section, $\Gamma_{l,r}$ are the interface transparencies, $x = 0 \ldots L$ is the position along the wire. The reservoirs are assumed to be in thermal equilibrium, with the distribution function given by $F^{l,r}_\epsilon = \tanh[(\epsilon - eV_{l,r})/2T]$. The boundary conditions

$$D\partial_x F|_{x=0} = -\Gamma_l[F^l - F(0)] \quad (6)$$
$$D\partial_x F|_{x=L} = -\Gamma_r[F(L) - F^r] \quad (7)$$

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guarantee current conservation at the interfaces. Furthermore we assume that the wire is so short that we can neglect inelastic scattering. In this case the kinetic equation for the distribution function inside the wire becomes $-D\partial_x^2 F = 0$. After solving this equation with the appropriate boundary conditions one finally finds the current as $I = V/(R_l + R_{\rm wire} + R_r)$ with

$$R_r = 1/(2e^2\mathcal{A}N_0\Gamma_l) \quad (8)$$

$$R_{\rm wire} = L/(2e^2\mathcal{A}N_0 D) \quad (9)$$

$$R_l = 1/(2e^2\mathcal{A}N_0\Gamma_r) \quad (10)$$

as one expects for three resistors in series.

We now discuss the quantum correction to the current. Following [14] we divide the quantum correction to the current in two contributions: The first contribution has the meaning of a correction to the conductance, $\delta I^{(1)} = V\delta G$. The second one is due to the quantum correction of the distribution function and can be interpreted as the redistribution of the voltage along the interfaces and the wire, $\delta I^{(2)} = G\delta V$. Both terms are necessary in order to ensure current conservation. By exploiting current conservation in the structure, $\delta I_l = \delta I_{\rm wire} = \delta I_r$, and fixing the voltage drop over the whole system to V, so that the sum $\delta V_l + \delta V_r + \delta V_{\rm wire}$ is zero, it is possible to eliminate $\delta I^{(2)}$ from the above equations to get for the correction to the current:

$$\delta I = \frac{R_l\delta I_l^{(1)} + R_r\delta I_r^{(1)} + R_{\rm wire}\delta I_{\rm wire}^{(1)}}{R_l + R_r + R_{\rm wire}}\,. \quad (11)$$

To proceed further we need the explicit form of $\delta I_{l,r,{\rm wire}}^{(1)}$. For an interface attached to an ideal lead on one side the quantum correction to the current is controlled by the correction to the density of states on the other side,

$$\delta I_l^{(1)} = e\mathcal{A}\Gamma_l \int {\rm d}\epsilon \delta N(\epsilon, 0)[F_\epsilon(0) - F_\epsilon^l] \quad (12)$$

$$\delta I_r^{(1)} = e\mathcal{A}\Gamma_r \int {\rm d}\epsilon \delta N(\epsilon, L)[F_\epsilon^r - F_\epsilon(L)]. \quad (13)$$

The limit where both sides of the interface are in thermal equilibrium has been studied many times in the literature [5,18]. Out of equilibrium we obtain the density of states correction as

$$\delta N(\epsilon, x) = -N_0 \int \frac{{\rm d}\omega}{2\pi} S(x, x) \quad (14)$$

$$S(x, x) = \Im \int {\rm d}x_1 \times F_{\epsilon-\omega}(x_1)\rho_\omega(x, x_1)\Phi_\omega(x_1, x), \quad (15)$$

where $\rho_\omega(x, x_1)$ describes the spreading of a charge injected into the system at x_1; it satisfies the equation

$$(-{\rm i}\omega - D\partial_x^2)\rho_\omega(x, x') = e\delta(x - x'). \quad (16)$$

The quantity $\Phi_\omega(x_1, x)$ is the electrical potential at x_1 of a charge that has been injected at x. It is given by the product of the dynamically screened Coulomb interaction with the diffusion propagator

$$e^2\Phi_\omega(x, x') = \int {\rm d}x_1 V_\omega(x, x_1)\rho_\omega(x_1, x'). \quad (17)$$

ρ and Φ depend on the details of the device under consideration and we will come back to them below.

The expression for the correction to the current in the wire has been obtained diagrammatically in [14] and is given by

$$\delta I_{\rm wire}^{(1)}(x) = -eDN_0\mathcal{A}\int {\rm d}\epsilon \int \frac{{\rm d}\omega}{2\pi}\partial_x[F_\epsilon(x)S(x, x)] + 2eDN_0\mathcal{A}\int {\rm d}\epsilon \int \frac{{\rm d}\omega}{2\pi} F_\epsilon(x)\partial_{x_1} S(x, x_1)|_{x_1=x}. \quad (18)$$

In general $\delta I_{\rm wire}^{(1)}(x)$ depends on the position x. Equation (11) however is constructed in such a way that the spacial average $\delta I_{\rm wire}^{(1)} = L^{-1}\int {\rm d}x \delta I_{\rm wire}^{(1)}(x)$ has to be inserted. Equations (12, 13, 18) allow to calculate the quantum corrections far from thermal equilibrium for an arbitrary geometry. One observes that the only ingredients are the position dependent distribution function F, the charge density ρ, and the field Φ. We have already discussed the distribution function F including the relevant boundary conditions in equations (6, 7) and below. Inside a diffusive wire the charge density ρ satisfies equation (16). At the boundaries with the left and right reservoir one may derive the matching conditions

$$\begin{aligned} D\partial_x\rho_\omega(x, x')|_{x=0} &= \Gamma_l\rho_\omega(0, x') \\ D\partial_x\rho_\omega(x, x')|_{x=L} &= -\Gamma_r\rho_\omega(L, x'), \end{aligned} \quad (19)$$

to be compared with equations (6) and (7). A careful analysis is also required for the field $\Phi_\omega(x, x')$. In the case of good metallic screening an injected charge is almost instantly screened so that the wire will be electrically neutral with the exception of a thin surface layer. In this case one has inside the wire

$$-\sigma\partial_x^2\Phi_\omega(x, x') = e\delta(x - x'), \quad (20)$$

where $\sigma = 2e^2DN_0\mathcal{A}$ is the conductivity. In the absence of surface charges the boundary conditions for Φ and ρ are identical. In the presence of these charges, however, this is not the case.

Many special cases where the general formalism discussed above applies have been discussed in the literature. For example standard Coulomb blockade physics is found when the resistance of the system is dominated by one of the interfaces [18,19]. In this limit a non-equilibrium analysis is not necessary since the distribution function has the equilibrium form on both sides of the interface. The limit of two highly resistive interfaces has been studied in [20,15] and the opposite limit of a resistive wire and no interface barriers has been discussed in [10,14]. In the following we concentrate on a short resistive wire with interfaces assuming temperatures of the order of and lower than the Thouless energy, $\hbar D/L^2$.

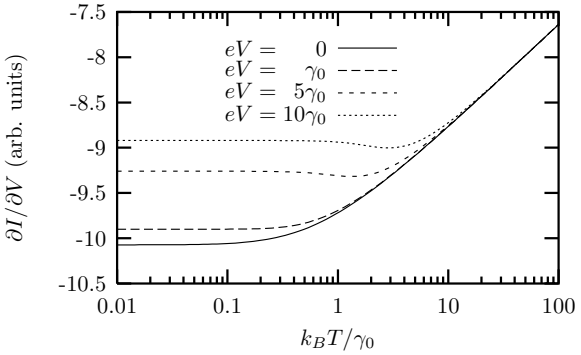

Fig. 1. Temperature dependence of the conductance for different values of the bias voltage. $\partial I/\partial V$ is in units of e^2/h and must be multiplied with the non-universal number A defined in the equation (23). γ_0 is the energy of the lowest diffusive mode; in the absence of interface barriers $\gamma_0 = \pi^2\hbar D/L^2$, for strongly resistive interfaces $\gamma_0 \to 0$.

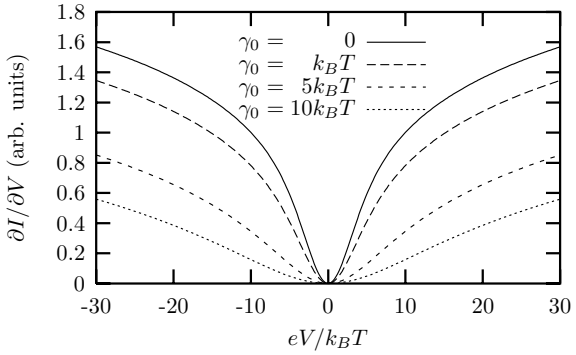

Fig. 2. Voltage dependence of the conductance. In all curves the linear conductance has been subtracted.

We start by expanding the charge density ρ in diffusive modes,

$$\rho_\omega(x,x') = e\sum_n \frac{f_n(x)f_n(x')}{-\mathrm{i}\omega+\gamma_n}, \tag{21}$$

where the (normalized) functions $f_n(x)$ are obtained by the eigenvalue equation

$$-D\partial_x^2 f_n(x) = \gamma_n f_n(x). \tag{22}$$

In the zero dimensional limit we approximate the sum in equation (21) by retaining only the eigenmode with the lowest energy, *i.e.* $\rho_\omega(x,x') \to ef_0(x)f_0(x')/(-\mathrm{i}\omega+\gamma_0)$. This approximation is justified when the energy scales related to the temperature and to the voltage remain below the energy of the second lowest diffusive mode. Let us for the moment ignore charging effects. Then the field $\Phi_\omega(x,x')$ is frequency independent and one observes that the frequency dependent factors in all the contributions to the current are identical, $\delta I(T,V) \sim F^l_{\epsilon-\omega}F^r_\epsilon/(-\mathrm{i}\omega+\gamma_0)$. The explicit result reads

$$\delta I = -A\frac{e}{2\pi}\int_0^\infty \mathrm{d}\eta \mathrm{e}^{-\gamma_0\eta}\left[\frac{\pi T}{\sinh(\pi T\eta)}\right]^2 \sin(eV\eta) \tag{23}$$

where only the dimensionless number A and the quantity γ_0 depend on the details of the system under consideration. Notice that the integral has to be cut off at short times in order to avoid a logarithmic divergence. Let us first discuss the temperature and voltage dependence of δI, before determining A and γ_0 explicitly in the two limits of perfectly transparent interfaces and for interfaces with low transparency. Figure 1 shows $\partial I/\partial V/(Ae^2/2\pi)$ as a function of temperature, the classical conductance has been subtracted. At high temperature there is a logarithmic behavior, which saturates below $T_{\mathrm{sat}} \sim \max(\gamma_0, eV)$. Figure 2 shows the voltage dependence of the conductance. Note that the linear conductance has been subtracted. For $\gamma_0 \ll T$ the conductance scales with voltage over temperature, while when γ_0 is large the relevant scale for conductance variations is γ_0.

How large are the amplitude A and the energy of the lowest diffusion mode γ_0? In the case of two well transmitting interfaces, $G_{\mathrm{wire}} \ll G_l, G_r$, the eigenfunction of equation (22) with the lowest eigenvalue is

$$f_0(x) = \sqrt{\frac{2}{L}}\sin(\pi x/L), \gamma_0 = \pi^2 D/L^2. \tag{24}$$

The distribution function and the potential Φ are determined as

$$F(x) = [(L-x)F_l + xF_r]/L \tag{25}$$

$$\Phi_\omega(x,x') = \frac{e}{G_{\mathrm{wire}}}\begin{cases}(L-x')x/L^2 & x<x'\\ (L-x)x'/L^2 & x>x'\end{cases} \tag{26}$$

and the amplitude of the correction to the current is found to be $A = 64/\pi^4 - 4/\pi^2 \approx 0.25$. In the opposite limit, $G_{\mathrm{wire}} \gg G_l, G_r$ the eigenvalue equation (22) may be solved perturbatively in the barrier transparency and one obtains

$$f_0(x) = 1/\sqrt{L}, \gamma_0 = (\Gamma_l+\Gamma_r)/L \tag{27}$$

$$F(x) = (\Gamma_l F_l + \Gamma_r F_r)/(\Gamma_l+\Gamma_r) \tag{28}$$

$$\Phi_\omega(x,x') = e/(G_l+G_r), \tag{29}$$

which leads to $A = 2\Gamma_l\Gamma_r/(\Gamma_l+\Gamma_r)^2$.

It is useful at this point to briefly discuss how the charging effects modify the above results. In the case of highly transmitting interfaces, we assume that the accumulated charge is proportional to the field as $\rho(x) = C\Phi(x)$, where C is a capacitance per unit length. This leads to a diffusion equation for the field

$$-\mathrm{i}\omega C\Phi_\omega(x,x') - \sigma\partial_x^2\Phi_\omega(x,x') = e\delta(x-x') \tag{30}$$

with the solution

$$\Phi_\omega(x,x') = 2e\sum_n \frac{\sin(n\pi x/L)\sin(n\pi x'/L)}{-\mathrm{i}\omega(CL)+(\pi n)^2 G_{\mathrm{wire}}}, \tag{31}$$

and the correction to the current is modified according to

$$\delta I = -\frac{e}{2\pi}\int_0^\infty \mathrm{d}\eta \mathrm{e}^{-\eta\gamma_0}\left[\frac{\pi T}{\sinh(\pi T\eta)}\right]^2 \sin(eV\eta) \times \sum_n A_n\{1-\exp[-\eta(\pi n)^2/R(CL)]\}. \tag{32}$$

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The numbers A_n depend on the wave-function of the diffusive mode n and $R = G_{\rm wire}^{-1}$. Notice that although the charge density $\rho_\omega(x,x')$ is zero dimensional many diffusive modes have to be taken into account in the field $\phi_\omega(x,x')$. For a small capacitance C the charging simply cures the short time divergence in the integral in equation (23). For a larger capacitance the I-V-characteristics is no longer a universal function. For the system with poorly transmitting interfaces, the field in equation (29) has to be replaced by $\Phi_\omega(x,x') = e/(-{\rm i}\omega\tilde{C} + G_l + G_r)$, where we denoted the capacitance of the system by $\tilde{C}$. The modification to the current is analogous to equation (32).

In several respects our results agree with [15] and [16]. We find, in the case of charge neutrality, a universal I-V-characteristics and, over a certain range of temperature, a logarithmic correction to the conductance. In some points, however, our results are remarkably different from [15,16]. For the closed system our improved treatment of the "zero mode" allows a more precise calculation of the amplitude of the $\ln T$ behaviour in the conductance than [15]. The major difference however concerns the low temperature saturation of $\partial I/\partial V$. We find that the scale for this saturation is set by the energy of the lowest diffusive mode in the system. This scale seems to be absent in [16], and the origin of this discrepancy is not clear to us.

Finally, as far as the experiments are concerned, a $\ln T$ behavior in the linear resistivity of a short metallic bridge together with an I-V-characteristics which agrees well with the universal function (23) has been observed in [15]. In [16] it has been suggested that the effect might be due to the Coulomb effects in a diffusive wire, whereas in [15] the Coulomb correction to the tunneling conductance has been suggested as the explanation. Our work shows that also in the intermediate regime with both diffusive and interface resistivity the predicted I-V-characteristics does not change and thus agrees with the experimentally observed one. Furthermore we can rule out a purely diffusive conductor: In [15] the Thouless energy, which sets the scale for the lowest diffusive mode in an open system and therefore the low temperature saturation of the conductance, has been estimated to be of the order of several Kelvin, whereas the $\ln T$ is observed down to 100 mK. In the case with resistive interfaces on the other hand the energy of the lowest diffusive mode is reduced, $\gamma_0 \sim \hbar D/L^2(R_{\rm wire}/R) \ll \hbar D/L^2$. From this consideration we conclude that in the experiment the diffusive resistance is considerably smaller than the interface resistance. A further hint for the importance of interfaces is found from the prefactor A: For the open system we found $A \approx 0.25$ and $A = 2G_lG_r/(G_r+G_r)^2$ in the tunnel limit. The experimental values [15] are between $A \approx 0.43 \ldots 0.7$, *i.e.* closer to the the tunnel limit than to the open system. In order to check these ideas it would be of interest to modify experimentally the resistance of the interface relative to the short bridge and observe both a change of the prefactor of the $\ln T$ behavior and of the saturation temperature.

In conclusion, we calculated the Coulomb interaction contribution to the current through structures which are composed of diffusive pieces and resistive interfaces. Our general formalism agrees with earlier studies on the Coulomb correction to the tunneling conductance [5,18,19] and on the Coulomb correction in diffusive conductors [1,9]. In contrast to those earlier studies our formalism treats both effects on equal footing and is valid even far from thermal equilibrium. We concentrated on the zero dimensional limit valid for temperatures below the Thouless energy and have shown that our theoretical results provide an explanation of the experimental findings of [15].

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