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Chemical potential oscillations near a barrier in the presence of transport

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The electrochemical potential drop across a single scatterer in an otherwise perfect conductor measured by weakly coupled probes is investigated. Phase sensitive probes yield a spatially oscillating voltage over distances of a phase-randomization length away from a scatterer. In a single-channel conductor these oscillations have a period $\lambda_F/2$ similar to the Friedel oscillations. The amplitude of the oscillations is the same on either side of the scatterer. The potential drop across the obstacle also oscillates and is, in general, not positive. Averaging the chemical potential over these oscillations yields a potential drop which is positive but smaller than the potential drop predicted by neglecting these oscillations altogether. In a multichannel system the chemical potential fluctuations are more complex with oscillatory components of a much longer period than λ_F.

In this paper, we discuss the chemical potential near a scattering center in an otherwise perfect conductor subject to current transport. The electrostatic potential near such a barrier was investigated by Landauer[1] many years ago and continues to be a subject of interest.[2] In this paper we focus on the chemical potential as measured by weakly coupled probes (see Fig. 1). It has been understood before, that there are Friedel-like oscillations[3] in the electric potentials near the barrier. In particular, we are concerned with the effect of these oscillations on the measured chemical potential difference across a scatterer. In small conductors on a length scale short compared to the phase-breaking length, these oscillations have a profound effect if the measurement is made with weakly coupled probes[4-7] (characterized by a conductance much less than e^2/h). A possible realization of weakly coupled probes is provided by a tunneling microscope[8] or by split gates operated near pinchoff.[9,10] We make no attempt to describe weak coupling probes in a realistic way,[11] but instead expand on the approach by Engquist and Anderson.[4] This leads to a discussion which is free of mathematical complexities but points to the effects of interest.

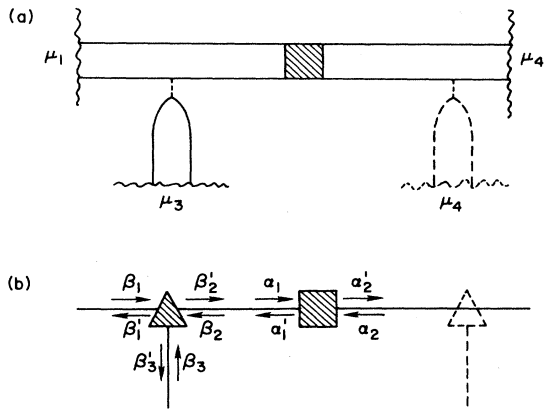

FIG. 1. (a) Multiprobe conductor with one or more weakly coupled probes. Aside from the probes, the only scattering process considered is that due to a barrier. (b) Schematic representation of the conductor depicted in (a). α and β are the current amplitudes which need to be calculated to determine the overall transmission probabilities.

The chemical potential measured with probe 3 in the presence of transport from probe 1 to probe 2 is[5,6]

$$\mu_3 = \frac{T_{31}\mu_1 + T_{32}\mu_2}{T_{31} + T_{32}}. \tag{1}$$

Here, T_{ij} is the probability for transmission from the reservoir with chemical potential μ_j to the reservoir with chemical potential μ_i. Since both the denominator and the numerator oscillate on a length scale of λ_F as the probe is moved along the conductor, the averaged chemical potential differs from a chemical potential calculated by using only averaged transmission probabilities.[6]

We study the simple geometry of Fig. 1 for the case of an effectively single-channel transmission problem. In the setup of Fig. 1 oscillations in the chemical potential are a consequence of the interference of the reflected wave with itself. A wave incident from terminal 1 gives two contributions to the current in probe 3. First, there is direct transmission into the probe and second, a portion of the carriers which are transmitted past the probe are scattered back at the barrier and enter the probe on their return trip. It is the superposition of these two amplitudes which determines the transmission into probe 3. Thus, the transmission probability T_{31} contains a quantum interference term. We term a voltage measurement which is sensitive to interference effects at the probe, *phase sensitive*. An averaged chemical potential can be determined by imagining that we move the probe along the conductor and take the average of these measurements. A potential obtained in this manner is termed a *phase-averaged* voltage measurement. We can compare a phase-sensitive or phase-averaged voltage to the result which is obtained by neglecting interference terms altogether. Physically, this requires a process which acts on the carriers between the barrier and the measurement probe in such a way that it destroys the phase memory of the carriers but does not affect their momentum. Alternatively, there might exist more complicated measurement probes which exclude the

interference described above by construction. We term the result of such a measurement *phase insensitive*. That voltage measurements can be sensitive to phase[5] has become well appreciated with a series of papers on voltage fluctuations[12,13] in microelectronic conductors and has been highlighted in electron focusing experiments.[9]

Oscillations of short wavelength would not be of great importance if it turned out that averaging over the oscillations leads to a result which could be obtained by neglecting these oscillations altogether. Our example demonstrates that situations exist where the phase-averaged and the phase-insensitive voltage measurement lead to very different answers. For a barrier (or sequence of obstacles) with transmission probability T, a phase-insensitive measurement yields the resistance found by Landauer,[1]

$$\mathcal{R}=\frac{h}{e^2}\frac{1-T}{T}. \tag{2}$$

Below we show that the same assumptions as made by Engquist and Anderson[4] in deriving Eq. (2), but viewing the sample and the probes as a coherent entity,[5] yields a phase-averaged resistance,

$$\langle\mathcal{R}\rangle=\frac{h}{e^2}\frac{1-\sqrt{T}}{T}. \tag{3}$$

The dependence on $\sqrt{T}$ rather than T alone is a consequence of interference effects.

To calculate the transmission probabilities in Eq. (1), we need first to specify the conductor and the coupling of the probes in more detail. As in Ref. 4 we proceed by specifying the elastic scattering properties in terms of scattering matrices s_{ij}. The scattering obstacle in the conductor is characterized by transmission amplitudes r and t for carriers incident from the left-hand side and r' and t' for carriers incident from the right-hand side [see Fig. 1(b)]. The junction of the conductor and the probe is determined in the following way:[4,14] The coupling parameter is ϵ and is assumed to be small. A version of the coupling matrix with real coefficients is given by $s_{31}=s_{32}=\sqrt{\epsilon}$. Transmission for carriers from branch 1 to branch 2 is almost unity and is given by $s_{21}=1-\epsilon/2+O(\epsilon^2)$. Carriers incident from branches 1 or 2 suffer very little reflection back into these branches, $s_{11}=s_{22}=-[\epsilon/2+O(\epsilon^2)]$. Most carriers incident from probe 3 are reflected back into probe 3, $s_{33}=-[1-\epsilon+O(\epsilon^2)]$. These elements of the matrix together with the requirement that s is symmetric in the absence of a magnetic field completely specify the matrix. (A more general coupling matrix which breaks the symmetry $|s_{31}|^2=|s_{32}|^2$ is discussed in Ref. 15.) Since we deal with phase-coherent voltage measurements we want to take into account that the scattering matrix is, in general, not real. We multiply the element s_{ij} of the matrix given above with a factor $\exp i(\delta_i+\delta_j)$, where the δ_i are arbitrary phase shifts. Such a choice preserves the symmetry and unitary property of the scattering matrix. We can now evaluate the transmission probabilities. Consider a unit current incident from probe 1 specified by $\beta_1=1$. The amplitudes β_3 and α_2 are zero. We want to calculate the amplitude $\beta_3'=s_{31}\beta_1+s_{32}\beta_2$. Carriers which directly pass the junction from branch 1 to branch 2 acquire a phase, $\beta_2'=s_{21}\cong\exp i(\delta_2+\delta_1)$. A portion of these carriers is reflected with probability amplitude r at the barrier and gives rise to a wave $\beta_2=\exp i(\delta_2+\delta_1+2\phi)r$ incident from the right-hand side. Here, $\phi=k_F d_L$ is the phase accumulated between the probe and the barrier separated a distance d_L. Thus we find, $\beta_3'=s_{31}+s_{32}\exp i(\delta_2+\delta_1+2\phi)r$. The total amplitude is thus $\beta_3'=\sqrt{\epsilon}\exp i(\delta_1+\delta_3)\times[1+\exp i(2\delta_2+2\phi)r]$. Therefore, we obtain a transmission probability $T_{31}=|\beta_3'|^2=\epsilon(1+R+2R^{1/2}\cos\chi_3)$. Here we have expressed the reflection amplitude in terms of the reflection probability R and the phase $\Delta\phi$ associated with reflection, $r=R^{1/2}\exp(i\Delta\phi)$. We have also introduced the abbreviation $\chi_3=2\delta_2+2\phi+\Delta\phi$ for the overall phase of carriers transmitted into probe 3. The transmission probability T_{32}, in contrast, does not contain an interference term. It is simply $T_{32}=|s_{32}t'|^2=\epsilon T$. Using these results and Eq. (1), we obtain the chemical potential measured at probe 3,

$$\mu_3=\frac{\mu_1+\mu_2}{2}+\frac{R+R^{1/2}\cos\chi_3}{1+R^{1/2}\cos\chi_3}\frac{\mu_1-\mu_2}{2}. \tag{4}$$

If the probe is to the right-hand side of the barrier, a repetition of the steps that led to Eq. (4) gives

$$\mu_4=\frac{\mu_1+\mu_2}{2}-\frac{R+R^{1/2}\cos\chi_4}{1+R^{1/2}\cos\chi_4}\frac{\mu_1-\mu_2}{2}. \tag{5}$$

The overall phase is given by $\chi_4=2\delta_1+2\phi'+\Delta\phi'$, where $\phi'=k_F d_R$ is the phase accumulated between the barrier and the probe to the right-hand side and $\Delta\phi'$ is the phase change associated with reflection of carriers incident from the right-hand side, $r'=R^{1/2}\exp i\Delta\phi'$. The chemical potentials are oscillatory functions of the distance of the probes d_L and d_R from the barrier (see Fig. 2). It is very remarkable that the amplitude multiplying $(\mu_1-\mu_2)/2$ is the same for both μ_3 and μ_4. The amplitude of the oscillations is proportional to $R^{1/2}$ and proportional to the chemical potential difference between reservoirs 1 and 2, $\Delta\mu=R^{1/2}(\mu_1-\mu_2)$. The amplitude, therefore, gives also the upper and lower bounds of the chemical potential

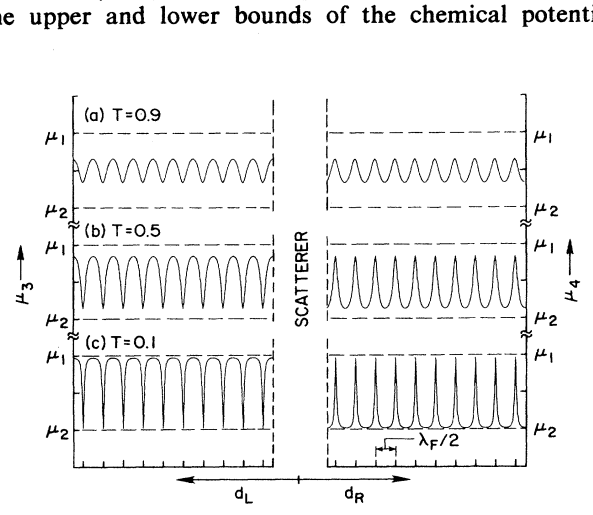

FIG. 2. Chemical potential oscillations as a function of the distance d_L and d_R of the probes away from the scatterer for the transmission probabilities, $T=0.9$, 0.5, and 0.1.

difference measured across the scatterer,

$$-R^{1/2}(\mu_1-\mu_2)\leq(\mu_3-\mu_4)\leq R^{1/2}(\mu_1-\mu_2)\,. \quad (6)$$

In Fig. 2 the chemical potentials μ_3 to the left-hand side of the barrier and μ_4 to the right-hand side of the barrier are plotted as a function of the distance from the barrier. In Fig. 2(a) the potentials are shown for a very transparent barrier $T=0.9$. For the transparent barrier the oscillations are nearly harmonic and the only effect of the barrier is a phase shift $\delta_2-\delta_1+\Delta\phi-\Delta\phi'+\pi$ across the barrier. In Fig. 2 the phase shift is taken to be π. As the barrier becomes more opaque the amplitude of the oscillations increases and so does the anharmonic content of the oscillations. Figure 2(b) shows the oscillations for a barrier with transmission probability $T=0.5$. For a very opaque scatterer, $T=0.01$, Fig. 2(c) shows that the oscillations are strongly anharmonic. μ_3 reaches its minimum value in sharp troughs and μ_4 reaches its maximum in sharp spikes. The spikes (and troughs) are Lorentzian with a height $\frac{1}{2}(1+\sqrt{R})$ and a width $2\sqrt{2}[(1-R^{1/2})]^{1/2}$.

The current from reservoir 1 to reservoir 2 is $I=(e/h)T(\mu_1-\mu_2)$ up to corrections of order ϵ. The four-probe resistance $\mathcal{R}_{12,43}=(\mu_1-\mu_2)/eI$, where the first two pairs of indices indicate current source and current drain and the second pair of indices indicates the probes used to measure the voltage,[16] will for simplicity be denoted by $\mathcal{R}$. Using Eqs. (4) and (5) yields

$$\mathcal{R}=\left(\frac{h}{e^2}\right)\left(\frac{1}{2}\right)\frac{2R+(1+R)R^{1/2}(\cos\chi_3+\cos\chi_4)+2R\cos\chi_3\cos\chi_4}{(1+R^{1/2}\cos\chi_3)(1+R^{1/2}\cos\chi_4)}\,. \quad (7)$$

This resistance is maximal for $\cos\chi_3=\cos\chi_4=1$ and given by $\mathcal{R}=(h/e^2)R^{1/2}/T$, and for $\cos\chi_3=\cos\chi_4=-1$ this resistance is minimal and given by $\mathcal{R}=-(h/e^2)R^{1/2}/T$, consistent with the bounds given in Eq. (6). Due to the oscillatory nature of the chemical potential the four-terminal resistance can be negative as has been demonstrated in a number of experiments (see Refs. 6 and 9). The negative four-terminal resistance does not violate any fundamental principle. The overall dissipation (to lowest order in ϵ) is given by the two-terminal resistance and is equal to $W=(1/h)T(\mu_1-\mu_2)^2$.

Suppose we move probe 3 along the conductor over a distance much larger than $\lambda_F/2$, record these measurements and calculate the average chemical potential. From Eq. (4) we find

$$\langle\mu_{3,4}\rangle=\frac{\mu_1+\mu_2}{2}\pm\tfrac{1}{2}(1-\sqrt{T})(\mu_1-\mu_2)\,, \quad (8)$$

where $\langle\,\rangle$ denotes an average over χ_i. In Eq. (8) the plus sign applies for μ_3 and the minus sign applies for μ_4. The phase-averaged resistance obtained from these potentials is given by Eq. (3). Note that after phase averaging we obtain a resistance which is positive.

If the oscillations are neglected altogether, we find $\mu_3=\mu_2+\frac{1}{2}(1+R)(\mu_1-\mu_2)$ and $\mu_4=\mu_2+\frac{1}{2}(1-R)\times(\mu_1-\mu_2)$. This leads to the resistance given by Eq. (2). In Fig. 3 we compare $\mu_3-\mu_4$ normalized by $\mu_1-\mu_2$ for the different voltage measurements. The dashed line gives the upper and lower bounds of the phase-sensitive voltage measurement and is obtained using Eq. (6). The solid line is the phase-averaged voltage difference [giving rise to the resistance Eq. (3)] and is obtained from Eq. (8). The dash-dotted line depicts the chemical potential difference for the phase insensitive voltage measurement [leading to the resistance given by Eq. (2)]. Figure 3 also shows the root mean square of the voltage fluctuations which we calculate below.

An additional measure of the significance of the oscillations discussed here is the root-mean-square deviations of the phase-sensitive voltage difference away from the phase-averaged voltage. (The mean-square deviations would be a complete characterization of these fluctuations only if their distribution were Gaussian.) We introduce $eV\equiv\mu_3-\mu_4$, and using Eqs. (4), (5), and (8), we find after performing the integrals,

$$\langle(eV-\langle eV\rangle)^2\rangle=\tfrac{1}{2}\sqrt{T}(1-\sqrt{T})(\mu_1-\mu_2)^2\,. \quad (9)$$

The resistance fluctuations are defined by $\Delta\mathcal{R}=\mathcal{R}-\langle\mathcal{R}\rangle=(V-\langle V\rangle)/I$. With the help of Eq. (9) we find

$$\langle(\Delta\mathcal{R})^2\rangle=\left(\frac{h}{e^2}\right)^2\frac{1}{2}\frac{1-\sqrt{T}}{T^{3/2}}\,. \quad (10)$$

Equations (9) and (10) show that the fluctuations in the measured resistance due to the self-interference of electron waves in the measurement probes are substantial. While these resistance fluctuations tend to zero for a completely transparent scatterer, they increase and grow over

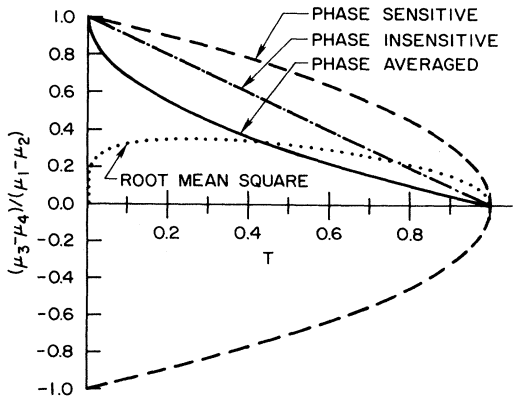

FIG. 3. Potential drop as a function of transmission probability for the phase-averaged measurement (solid line), the phase-insensitive measurement (dash-dotted line). A phase-sensitive measurement is bounded by the dashed line. Also shown (dotted) are the root-mean-square voltage fluctuations for the phase-sensitive voltage measurement.

every bound as the scatterer becomes opaque. We stress that Eqs. (9) and (10) have been obtained by considering a very special ensemble: We move probes along a specific conductor and do not, as typical in fluctuation theory, consider an ensemble of different conductors coupled to different probes.

We have illustrated the difference between phase-sensitive, phase-averaged, and phase-insensitive voltage measurements by discussing a very simple example. The differences between these measurements are very severe for an effectively single-channel transmission problem. In a multichannel channel conductor the effect depends sensitively on the particular way the probes couple to the conductor. There are many-channel probes which by construction avoid, at least in the geometry of Fig. 1, the interference of the incident wave with the reflected wave, and in our terminology are, therefore, phase insensitive.[5] In a many-mode conductor each channel contributes phase-sensitive terms which depend on the longitudinal momentum k_n of the nth transverse channel and, in general, the sum and differences between these.[6] Consequently, the oscillations do not only contain components with wavelength $\lambda_F/2$ only but contain much longer periods of the order of the width of the wire. Since the accumulated phases are different for each mode the chemical potential is not periodic but fluctuates in a complicated manner, similar to voltage fluctuations, but caused only by the interference of the incident wave and the reflected wave.

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