Nanoscale quantum transport - homework problems

Problem 1.

(a) The Fermi-Dirac distribution function is defined as

$$f = \frac{1}{1 + \exp\left[\frac{\varepsilon - \mu)}{k_B T}\right]}$$

where ε is the energy variable, μ is the chemical potential, k_B is the Boltzmann constant, and T is the temperature. Sketch (or plot in matlab or mathematica) the Fermi-Dirac distribution function for room temperature when the chemical potential is 1 eV.

(b) Study the window in energy within which the Fermi function changes from 1 to 0. Make a rough estimate of the window width by considering the energy range within which the exponential changes from e^{-2} to e^2 (for which f varies from ~0.9 to ~0.1); show that this window is of order $4k_BT$ wide.

(c) In the lecture on quantum transport we encountered the difference between two Fermi functions (of the two reservoirs) with chemical potentials shifted by a voltage eV relative to each other. Taylor expand for linear order in voltage and show that

$$\frac{1}{1 + \exp\left[\frac{\varepsilon - \mu - \frac{eV}{2})}{k_B T}\right]} - \frac{1}{1 + \exp\left[\frac{\varepsilon - \mu + \frac{eV}{2})}{k_B T}\right]} \approx eV \times \frac{\partial f}{\partial \mu} = eV \times \frac{1}{k_B T} \frac{1}{4\cosh\left[\frac{\varepsilon - \mu}{k_B T}\right]}$$

Now sketch (or plot in matlab or mathematica) the function $\frac{\partial f}{\partial \mu}$

Problem 2.

In the lecture we went throught the calculation of the conductance of a single-mode channel with the result $G=2e^2/h$. Then we studied the case of a barrier in the channel, with a transmission coefficient $t(\varepsilon)$. It was stated that the conductance at low temperature in this case is $G=(2e^2/h)|t(\varepsilon_f)|^2$, where ε_f is the Fermi energy. Show it by Taylor expansion of the Fermi functions in the Landauer formula:

$$I = \frac{2e}{h} \int_0^\infty |t(\varepsilon)|^2 \left[f\left(\varepsilon - \frac{eV}{2}\right) - f\left(\varepsilon + \frac{eV}{2}\right)\right] d\varepsilon$$

Hint: use that the function $df/d\mu$ [also studied in problem 1(c) above] is approaching a delta-function at low temperature.

Problem 3.

Repeat the calculation of the Sharvin resistance in the lecture for the case of three dimensions. This case describes a pinhole of area A in an otherwize inpenetrable barrier separating two contacts. Show that the conductance in this case is of the form

$$G^{3D} \propto e^2 \mathcal{A} \mathcal{N}^{3D}(\varepsilon_f)\, v_f$$

Show that this can be rewritten into the form

$$G^{3D} \propto \frac{2e^2}{h} \frac{\mathcal{A}}{\lambda_f^2}$$

Explain how the “number of conducting channels” is counted in this case.

Problem 4.

The two-dimensional electron gas (2DEG) is found at the interface between differently doped semiconductors, as shown in Fig. 1. The size quantization occurs in the z-direction and electrons are free to move in the xy-plane. Consider the case when only the lowest energy level ε_1 in the well is occupied. The wave function and the energy of an electron with 2-D wave vector $\boldsymbol{k}=(k_x,k_y)$ are

$$\begin{aligned} \Psi &= \phi_1(z)e^{ik_x x}e^{ik_y y} \\ E &= E_c + \varepsilon_1 + \frac{\hbar^2}{2m^*}(k_x^2+k_y^2) \end{aligned}$$

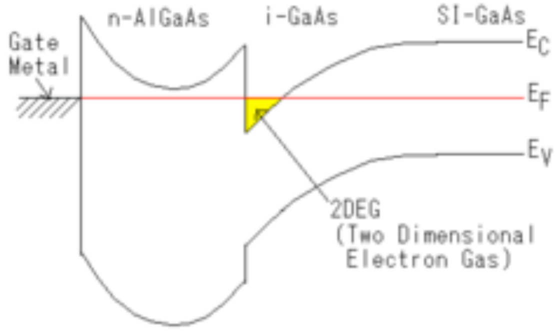

Fig. 1. The two-dimensional electron gas.

Thus, the band bottom in the 2DEG is $E_s=E_c+\varepsilon_1$. The density of states per unit area of the 2DEG is

$$\mathcal{N}(E) = \frac{m^*}{\pi\hbar^2}\Theta(E-E_s)$$

and the electron density (the number of electrons per unit area of the 2DEG) is

$$n_s = \frac{m^*}{\pi\hbar^2}(E_f - E_s)$$

where E_f is the Fermi energy.

(a) The effective mass of the 2DEG is $m^*=0.07m_0$, where m_0 is the free electron mass, while the electron density is $5\cdot10^{11}/\text{cm}^2$. Compute the Fermi energy relative to the bottom of the band in the 2DEG.

(b) Consider a narrow conductor etched out of a wide 2DEG conductor, as shown in Fig. 2.

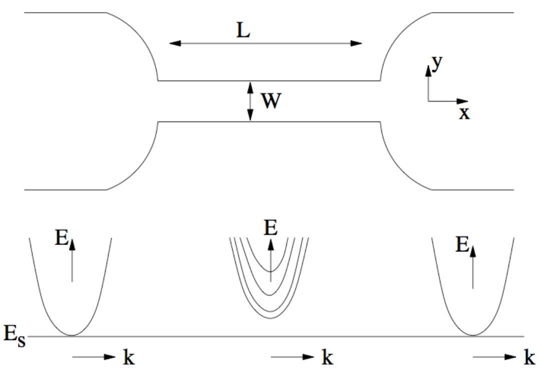

Fig. 2. Narrow conductor etched out of a wide conductor. In the wide regions the transverse modes are essentially continuous, but in the narrow region the modes are well-separated in energy.

In the narrow region we cannot use the 2-D density of states if the width W is small enough; it is necessary to take into account the discreteness of the transverse modes. Plot/sketch the electron density versus Fermi energy for W=1000 Å, assuming for the confining potential a hard-wall potential model.

(c) How many modes are open for the value of the Fermi energy that you computed in (a)?

(d) What is the conductance of the narrow conductor?

Problem 5.

The transmission probability of a double barrier structure was discussed in the lecture. Consider a symmetric structure, such that the transmission probability (near resonance) is

$$T_{12}(E) = \frac{(\Gamma/2)^2}{(E-E_r)^2 + (\Gamma/2)^2}$$

where the width of the Lorenzian is Γ and the level energy is E_r. Use the scattering approach (Landauer approach) to compute and plot/sketch the current-voltage characteristics *I(V)* and the conductance *dI(V)/dV* of the double barrier structure. Consider and discuss both the high temperature $T >> \Gamma$ and the low temperature $T << \Gamma$ limits. Hint: Use the 1-D set-up shown in Fig. 3 and consider that half of the voltage drops over each of the two barriers and that the electrons impinging on the scattering region (the double barrier structure) from the two reservoars (the left and the right) are distributed according to the Fermi-Dirac distribution function.

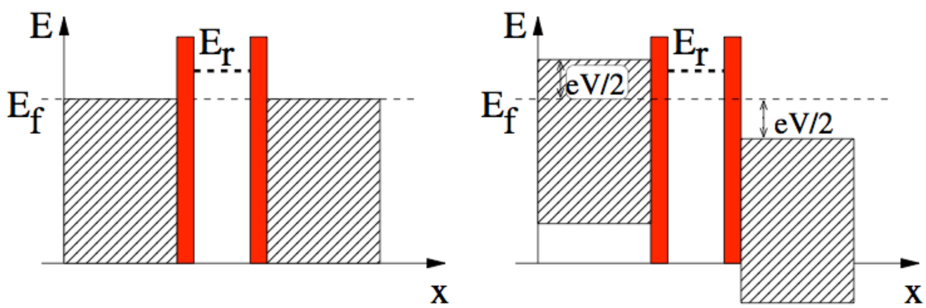

Fig 3. In the two reservoirs the electrons occupy states up to the Fermi energy (here illustrated for zero temperature). Under an applied voltage, half of the voltage drops at each barrier, which results in shifted chemical potentials in the two reservoirs as illustrated in the right figure.

Problem 6.

(a) Use the Master equation approach to derive the expression for the current through a one-level quantum dot (level energy ε) neglecting electron spin and excluding Coulomb interactions. In the multi-electron picture we here simply have two levels "0" and "1" corresponding to the level being empty of occupied, respectively. Denote the probabilities for these two "states" P_0 and P_1. Write down the appropriate rate equations and Master equation and use them to derive the following expressions for the current *I* throught the dot and the occupation of the dot level $f_r(\varepsilon)$:

$$I = \frac{e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[f_1(\varepsilon) - f_2(\varepsilon)\right]$$

$$f_r = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1+\gamma_2}$$

(b) Sketch (or plot in matlab or mathematica) the I-V characteristics, for an energy level ε, i) above and ii) below the Fermi energy. Sketch the I-V characteristics both for zero temperature and finite temperature.

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