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Transport in Mesoscopic Systems — WS 10 / 11

Exercise 1

1.1. Basic Notions of Mesoscopic Systems (3 + 3 points)

(For In-Class Presentation)

Let us consider a system of noninteracting fermions at low temperature T. The transport properties of the system are mainly determined by single-particle energy states in the interval $E_F - k_B T < E < E_F + k_B T$, where E_F is the Fermi energy. In the mesoscopic regime the following inequality should be satisfied:

$$\Delta(E_F) \ll k_B T \ll E_{cl}(E_F) \tag{1}$$

where $\Delta(E)$ denotes the average distance between individual energy levels in the neighbourhood of energy E (microscopic energy scale), while $E_{cl}(E) \sim \frac{\hbar}{\tau_{\text{fl}}(E)}$ is determined by the classical time of flight through the system $\tau_{\text{fl}}(E)$, i.e., a macroscopic energy scale.

a) We first look at a system in two dimensions, namely, an infinite square potential well with the potential

$$V(x,y) = \begin{cases} 0 & 0 \le x \le L, 0 \le y \le L \\ \infty & \text{otherwise} \end{cases} \tag{2}$$

Let $N(E)$ be a number of single-particle states with energies $E_{mn} < E$ (E_{mn} are eigenenergies of the Schrödinger equation with quantum numbers $m, n = 1, 2, \ldots$). Using (1), show that, in the mesoscopic regime,

$$N(E_F) \gg 1 \tag{3}$$

(*Hint:* $\frac{dN(E)}{dE} \simeq \frac{1}{\Delta(E)}$). When calculating $\Delta(E)$, $E_{cl}(E)$ and $N(E)$ use simple estimates; neglect proportionality constants like π, $\frac{1}{2}$, *etc.*

b) We can extend our estimates in Exercise (a) to a system of arbitrary dimension d. Derive a requirement for $N(E_F)$ similar to what you obtained in Exercise (a), and show that the mesoscopic regime is not reachable in dimension $d = 1$

1.2. Schrödinger Equation in an Infinite Lead (2 + 2 + 3 points)

(For Hand-In Homework)

We consider an infinitely long, two-dimensional lead. There is free propagation of waves in the interior of the lead, and infinitely high potential walls at the sides. This can be mathematically described in the following way:

$$V(x,y) = \begin{cases} 0 & \text{for } -\infty < x < \infty, |y| \le \frac{W}{2} \\ \infty & \text{otherwise} \end{cases} \tag{4}$$

where $V(x, y)$ is the potential at point (x, y) inside the lead. Let $\Psi(x, y)$ satisfy the Schrödinger equation in the form

$$\mathcal{H}\Psi(x, y) = E\Psi(x, y)$$

a) Show that inside the lead the wavefunction $\Psi(x, y)$ can be written in the general form

$$\Psi(x, y) = \sum_{m=1}^{N(E)} \left(A_m e^{ik_m(E)x} + B_m e^{-ik_m(E)x}\right) \varphi_m(y) \tag{5}$$

where $A_m(E)$ and $B_m(E)$ are unknown complex amplitudes, m label the "channels", $N(E)$ is the total number of channels in the lead, and $k_m(E)$ is the energy-dependent wavenumber. Solve this problem in two steps:

i) Find $k_m(E)$ and $\varphi_m(y)$. Use a usual separation of variable *Ansatz* $\Psi(x, y) = e^{\pm ikx}\varphi_m(y)$. Take care to normalize $\varphi_m(y)$, taking into account the lead width W.

ii) Obtain the total channel number $N(E)$, which corresponds to the maximum value of the quantum number m for a given energy E. Assume $k_m(E)$ to be real.

b) Calculate the probability current in the x-direction I_x by integrating the current density $j_x(y)$ over the total width of the lead $[-\frac{W}{2}, \frac{W}{2}]$, where

$$j_x(y) = \frac{\hbar}{M}\text{Im}\left[\Psi^*(x, y)\frac{\partial}{\partial x}\Psi(x, y)\right]$$

where M is the mass.

1.3. Properties of Scattering Matrices (2 + 2 points)

(For In-Class Presentation)

We have already seen from the lecture that an arbitrary wavefunction $\Psi(\vec{r})$ of a two dimensional mesoscopic system has the following asymptotic form in the leads:

$$\Psi(x_i, y_i) = \sum_{m=1}^{N_i}\left[\frac{a_m^{(i)}}{\sqrt{v_m^{(i)}}}e^{ik_m^{(i)}x_i} + \frac{b_m^{(i)}}{\sqrt{v_m^{(i)}}}e^{-ik_m^{(i)}x_i}\right]\varphi_m^{(i)}(y_i) \tag{6}$$

as $x_i \to \infty$ (See Figure 1 for explanation of indices). The complex coefficients $a_m^{(i)}$ ($b_m^{(i)}$) denote the outgoing (incoming) scattering amplitudes in channel m of lead i, $i = 1, 2$. From this expression we can then define a scattering matrix

$$\mathbf{a} = \mathbf{S}\mathbf{b} \tag{7}$$

where

$$\mathbf{a} \equiv (a_1^{(1)}, \ldots, a_m^{(1)}, \ldots, a_{N_1}^{(1)}, a_1^{(2)}, \ldots, a_m^{(2)}, \ldots, a_{N_2}^{(2)})^T$$
$$\mathbf{b} \equiv (b_1^{(1)}, \ldots, b_m^{(1)}, \ldots, b_{N_1}^{(1)}, b_1^{(2)}, \ldots, b_m^{(2)}, \ldots, b_{N_2}^{(N)})^T$$

and the scattering matrix has the general form

$$S = \left(\begin{array}{c|c} \mathbf{r}_{11} & \mathbf{t}_{12} \\ \hline \mathbf{t}_{21} & \mathbf{r}_{22} \end{array}\right) \tag{8}$$

where $\mathbf{r}_{ii}$ and $\mathbf{t}_{ji}$ are the reflection and transmission matrices (of dimensions $N_i \times N_i$ and $N_j \times N_i$ respectively). From the previously defined quantities we can obtain some physical quantities, which we recapitulate below (previously seen in the lecture):

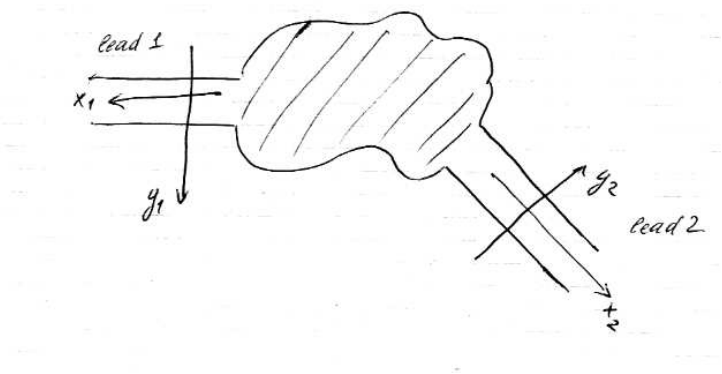

Figure 1: A sketch of a a two-dimensional sample with two leads.

- Currents in channel m of lead i

$$
\begin{aligned}
I^{(i)}_{m,\mathrm{out}} &= \mid a^{(i)}_m \mid^2 \\
I^{(i)}_{m,\mathrm{in}} &= \mid b^{(i)}_m \mid^2
\end{aligned}
$$

- Total transmission and reflection coefficients:

$$
\begin{aligned}
T_i \equiv \mathrm{Tr}(t^\dagger_{ji} t_{ji}) = \mathrm{Tr}(t_{ji} t^\dagger_{ji}) &= \sum_{m=1}^{N_i} \sum_{n=1}^{N_j} \mid t_{ji,nm} \mid^2 \\
R_i \equiv \mathrm{Tr}(r^\dagger_{ii} r_{ii}) = \mathrm{Tr}(r_{ii} r^\dagger_{ii}) &= \sum_{m,n=1}^{N_i} \mid r_{ii,nm} \mid^2
\end{aligned}
$$

where $i \neq j$.

a) From conservation of total current

$$I_{out} = I_{in}$$

where $I_{in} = \sum_{i,m} I^{(i)}_{m,in}$, $I_{out} = \sum_{i,m} I^{(i)}_{m,out}$ show the unitarity relation

$$S^{-1} = S^\dagger$$

b) Using the result in (a), namely, that $SS^\dagger = S^\dagger S = \mathbb{1}$, where $\mathbb{1}$ is the $(N_1 + N_2) \times (N_1 + N_2)$ unit matrix, show that

$$
\begin{aligned}
&(i) \quad T_i + R_i = N_i \\
&(ii) \quad T_1 = T_2
\end{aligned}
$$