Theory and Phenomenology of Superconductivity Homework 3

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Problem 1. Consider two reservoirs for electrons at thermal equilibrium. Refer to them as left L and right R leads which extend in the x direction. Imagine we apply small voltages to the two leads which tunes their chemical potential by eV_L and eV_R.

- Starting from the scattering matrix approach, relate the states entering and leaving each lead at the interface.
- Within the second quantization formalism, write the formula for the electrical current. **Hint:** it will be useful later to write it as an energy integration.
- Taking advantage of the elements of the scattering matrix, identify in the previous formula the transmission function.
- Identify the equilibrium conductance

$$G = \frac{e^2}{h} \operatorname{Tr}\left[\mathbf{t}^\dagger(E_F)\,\mathbf{t}(E_F)\right], \tag{1}$$

  where $\mathbf{t}(E_F)$ is the transmission matrix of our system evaluated at the Fermi energy E_F. What is the meaning of the eigenvalues of the hermitian matrix $\mathbf{t}^\dagger(E_F)\mathbf{t}(E_F)$?

Proof. (a) It is necessary before answering this question to do a bit of set up work. We take our sample to extend in the z direction. The leads, on the left and right, have some eigenmodes that are plane waves in the z direction, i.e. they are proportional to $e^{\pm ikz}$. In the transverse direction, we also have some spatial wavefunctions. The total energy is given by the sum of the energies associated with each direction, $E = E_n + E_t$. The exact structure of this is not important[1]. What is important is

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[1] In principle, it is possible to take the lead to be a cube, from which we would get the transverse modes by solving the 2-dimensional particle in a box, as in the next problem. However, the point here is that it does not matter what shape it actually is, and all this information is hidden away in the S-matrix.

that there $E_n \geq 0$, and thus for each value of the total energy E there is a finite number $n(E)$ of modes for this energy in each.

First, we write down the definition of the S-matrix.

$$\begin{pmatrix} \vec{\mathbf{a}}_L^- \\ \vec{\mathbf{a}}_R^+ \end{pmatrix} = \underbrace{\begin{pmatrix} \mathbf{r} & \mathbf{t}' \\ \mathbf{t} & \mathbf{r}' \end{pmatrix}}_{S} \begin{pmatrix} \vec{\mathbf{a}}_L^+ \\ \vec{\mathbf{a}}_R^- \end{pmatrix}.$$

It is important to clarify the definitions of these coefficients $\vec{\mathbf{a}}_{L/R}^{\pm}$. The S-matrix is defined to relate probability currents, and not wavefunction amplitudes. Thus, it is important that we include a prefactor of $k^{-1/2}$ in front of the wavefunctions, i.e. that the wavefunction is formed by (up to constants)

$$\psi \propto a_{L,1}^- \frac{1}{\sqrt{k_1}} e^{-ik_1 z} + \cdots + a_{L,n_L}^- \frac{1}{\sqrt{k_{n_L}}} e^{-ik_{n_L} z} + \text{right movers.}$$

Due to the scattering matrix constraint, the Hilbert space dimension is $2n$ instead of the $4n$ that we would get from $4n$ independent modes. We write creation & annihilation operators $\hat{a}_{L/R,k}^\dagger$, $\hat{a}_{L/R,k}$ for incoming modes in the left & right leads in channel k, and $\hat{b}_{L/R,k}^\dagger$, $\hat{b}_{L/R,k}$ for the incoming modes.

It is important to note here that $\hat{a}_{L,k}^\dagger$ creates an eigenstate with energy E such that there is a probability current of 1 in the k channel in the left lead, and no incoming probability currents in the other channels, or in the right lead. Thus, $\hat{a}_{L,k}^\dagger |0\rangle$ has nonzero incoming probability amplitudes in the outgoing waves. In this language, the annihilation operators are related by

$$\begin{pmatrix} \hat{b}_{L,1} \\ \vdots \\ \hat{b}_{L,n_L} \\ \hat{b}_{R,1} \\ \vdots \\ \hat{b}_{R,n_R} \end{pmatrix} = \begin{pmatrix} \mathbf{r} & \mathbf{t}' \\ \mathbf{t} & \mathbf{r}' \end{pmatrix} \begin{pmatrix} \hat{a}_{L,1} \\ \vdots \\ \hat{a}_{L,n_L} \\ \hat{a}_{R,1} \\ \vdots \\ \hat{a}_{R,n_R} \end{pmatrix}.$$

(b) In general, the electrical current can be determined through the derivative $j^\mu = \frac{\delta S[A]}{\delta A^\mu}$, and leads to the expression for free particles coupled to an electric field

$$\vec{\mathbf{J}} = \vec{\mathbf{J}}^{\boldsymbol{\nabla}} + \vec{\mathbf{J}}^{\vec{\mathbf{A}}}$$

$$\vec{\mathbf{J}}^{\boldsymbol{\nabla}} = \frac{\hbar}{2mi}\left[\psi^\dagger \boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^\dagger)\psi\right]$$
$$\vec{\mathbf{J}}^{\vec{\mathbf{A}}} = -\frac{q}{m}\vec{\mathbf{A}}\psi^\dagger\psi$$

In the case of a DC current, we usually have an electric field but no magnetic field. Hence, we can set $\vec{\mathbf{A}} = 0$. We can write this as the current operator

$$\mathbf{J} = \frac{\hbar}{2mi}\left[\vec{\partial} + \overleftarrow{\partial}\right]$$

where the very dumb arrow denotes that the derivative acts to the left or to the right, because we have to write it as a matrix before second quantising it :((

To rewrite this as a field operator, we can promote the wavefunction ψ into an operator valued measure (field), and integrate the current density to obtain the current[2]:

$$\hat{I}_L(z,t) = \frac{\hbar e}{2mi}\int\left[\hat{\Psi}_L^\dagger(\vec{\mathbf{r}},t)\frac{\partial}{\partial z}\hat{\Psi}_L(\vec{\mathbf{r}},t) - \left(\frac{\partial}{\partial z}\hat{\Psi}_L^\dagger(\vec{\mathbf{r}},t)\right)\hat{\Psi}_L(\vec{\mathbf{r}},t)\right]\mathrm{d}\vec{\mathbf{r}}_\perp\,.$$

We would like to write our algebra in terms of the creation and annihilation operators for the energy eigenbasis. We know that the change of basis formula in second quantisation is

$$\hat{a}_\mu = \sum_\nu \langle\tilde{\psi}_\mu|\psi_\nu\rangle\,\hat{a}_\nu,$$

and thus the field operators are given by

$$\hat{\Psi}_L(\vec{\mathbf{r}},t) = \int e^{-iEt/\hbar}\sum_{m=1}^{n_L(E)}\frac{\chi_{L,m}(\vec{\mathbf{r}}_\perp)}{\sqrt{2\pi\hbar v_{L,m}(E)}}\left[\hat{a}_{L,m}e^{ik_{L,m}z} + \hat{b}_{L,m}e^{-ik_{L,m}z}\right]\mathrm{d}E$$
$$\hat{\Psi}_L^\dagger(\vec{\mathbf{r}},t) = \int e^{iEt/\hbar}\sum_{m=1}^{n_L(E)}\frac{\chi_{L,m}^*(\vec{\mathbf{r}}_\perp)}{\sqrt{2\pi\hbar v_{L,m}(E)}}\left[\hat{a}_{L,m}^\dagger e^{-ik_{L,m}z} + \hat{b}_{L,m}^\dagger e^{ik_{L,m}z}\right]\mathrm{d}E\,.$$

Here, $\chi_{L,k}$ is the perpendicular part of the wavefunction, the prefactor of $e^{-iEt/\hbar}$ comes from the time evolution of an energy eigenstate, and $v_{L,k}(E) = \hbar k_{L,m}/m$ is the velocity. We note that the funny factor down there reproduces the desired normalisation.

We are now ready to substitute this back into the expression for the current. However, it is necessary to have a bit of foresight first. Later, we will make the assumption that the leads are thermalised. Thus, the correlation functions will be that of

[2] Here, we only evaluate the current in the left lead. However, the current in both leads is identical, as can be proven using the unitarity of the S-matrix

the pure thermal system

$$\langle \hat{b}^{\dagger}_{\lambda,\eta} \hat{b}_{\lambda',\eta'} \rangle = \delta_{\eta\eta'} \delta_{\lambda\lambda'} f_{\mu_\eta}(E_\lambda).$$

The function f_μ is the Fermi function

$$f_\mu(x) = \frac{1}{e^{\beta(x-\mu)} + 1}$$

and the chemical potentials are

$$\mu_{L/R} = eV_{L/R}.$$

Thus, when expanding, it is not necessary to keep cross terms. This is important as the $\mathrm{d}\vec{\mathbf{r}}_\perp$ integral is not a full scalar product and is not guaranteed to kill all cross terms, and thus we would in principle need to keep all terms in. Thus, we have

$$\begin{aligned}
\hat{\Psi}^\dagger \frac{\partial \hat{\Psi}}{\partial z} &= \frac{1}{h} \int \mathrm{d}E \sum_{m=1}^{n_L(E)} \frac{i|\chi_{L,m}|^2 k_{L,m}}{v_{L,m}(E)} (\hat{a}^\dagger_{L,m} \hat{a}_{L,m} - \hat{b}^\dagger_{L,m} \hat{b}_{L,m}) + \text{cross terms} \\
\left(\frac{\partial \hat{\Psi}^\dagger}{\partial z} \right) \hat{\Psi} &= -\frac{1}{h} \int \mathrm{d}E \sum_{m=1}^{n_L(E)} \frac{i|\chi_{L,m}|^2 k_{L,m}}{v_{L,m}(E)} (\hat{a}^\dagger_{L,m} \hat{a}_{L,m} - \hat{b}^\dagger_{L,m} \hat{b}_{L,m}) + \text{cross terms}
\end{aligned}$$

Substituting this in the formula for the current and integrating out $\iint |\chi_{L,m}(\vec{\mathbf{r}}_\perp)|^2 \, \mathrm{d}\vec{\mathbf{r}}_\perp = 1$, we get[3]

$$\begin{aligned}
\hat{I}_L(t) &= \frac{e}{h} \int \mathrm{d}E \sum_{m=1}^{n_L} \left[\hat{a}^\dagger_{L,m} \hat{a}_{L,m} - \hat{b}^\dagger_{L,m} \hat{b}_{L,m} \right] \\
\hat{b}_{L,\smiley} &= \sum_{\frownie=1}^{n_L} \mathbf{r}_{\smiley\frownie} \hat{a}_{L,\frownie} + \sum_{\eighthnote=1}^{n_R} \mathbf{t}'_{\smiley\eighthnote} \hat{a}_{R,\eighthnote} \\
\hat{I}_L(t) &= \frac{e}{h} \int \mathrm{d}E \sum_{m=1}^{n_L} \left[\hat{a}^\dagger_{L,m} \hat{a}_{L,m} - \left(\sum_{\smiley=1}^{n_L} \mathbf{r}^*_{m\smiley} \hat{a}^\dagger_{L,\smiley} + \sum_{\frownie=1}^{n_L} (\mathbf{t}')^*_{m\frownie} \hat{a}^\dagger_{R,\frownie} \right) \right. \\
&\qquad \left. \left(\sum_{\eighthnote=1}^{n_L} \mathbf{r}_{m\eighthnote} \hat{a}_{L,\eighthnote} + \sum_{\quarternote=1}^{n_R} (\mathbf{t}')_{m\quarternote} \hat{a}_{R,\quarternote} \right) \right] \\
&= \frac{e}{h} \int \mathrm{d}E \sum_{m=1}^{n_L} \left[\hat{a}^\dagger_{L,m} \hat{a}_{L,m} - \sum_{\smiley=1}^{n_L} |\mathbf{r}_{m\smiley}|^2 \hat{a}^\dagger_{L,\smiley} \hat{a}_{L,\smiley} - \sum_{\frownie=1}^{n_L} |\mathbf{t}'_{m\frownie}|^2 \hat{a}^\dagger_{R,\frownie} \hat{a}_{R,\frownie} \right]
\end{aligned}$$

Now, it remains to do some massaging. Noting that we will replace $\hat{a}^\dagger_{L/R,\smiley} \hat{a}_{L/R,\smiley}$ with the Fermi function after taking the expectation value since these states all

[3] There were too many sums and I ran out of symbols.

have the same energy later, we compute

$$\sum_{☺,☹=1}^{n_L} |\mathbf{t}'_{☺☹}|^2 = \sum_{☺,☹=1}^{n_L} (\mathbf{t}')^\dagger_{☹☺} \mathbf{t}_{☺☹}$$
$$= \mathrm{Tr}\Big((\mathbf{t}')^\dagger \mathbf{t}'\Big)$$

We then note that $\mathrm{Tr}\big((\mathbf{t}')^\dagger \mathbf{t}'\big) = \mathrm{Tr}\big(\mathbf{t}^\dagger \mathbf{t}\big)$ due to the unitarity of the S-matrix:

$$SS^\dagger = \begin{pmatrix} \mathbf{r} & \mathbf{t}' \\ \mathbf{t} & \mathbf{r}' \end{pmatrix} \begin{pmatrix} \mathbf{r}^\dagger & \mathbf{t}^\dagger \\ \mathbf{t}'^\dagger & \mathbf{r}'^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{r}\mathbf{r}^\dagger + \mathbf{t}'\mathbf{t}'^\dagger & \mathbf{r}\mathbf{t}^\dagger + \mathbf{t}'\mathbf{r}'^\dagger \\ \mathbf{t}\mathbf{r}^\dagger + \mathbf{r}'\mathbf{t}'^\dagger & \mathbf{t}\mathbf{t}^\dagger + \mathbf{r}'\mathbf{r}'^\dagger \end{pmatrix} = \mathbb{1}$$
$$S^\dagger S = \begin{pmatrix} \mathbf{r}^\dagger & \mathbf{t}^\dagger \\ \mathbf{t}'^\dagger & \mathbf{r}'^\dagger \end{pmatrix} \begin{pmatrix} \mathbf{r} & \mathbf{t}' \\ \mathbf{t} & \mathbf{r}' \end{pmatrix} = \begin{pmatrix} \mathbf{r}^\dagger\mathbf{r} + \mathbf{t}^\dagger\mathbf{t} & \mathbf{r}^\dagger\mathbf{t}' + \mathbf{t}^\dagger\mathbf{r}' \\ \mathbf{t}'^\dagger\mathbf{r} + \mathbf{r}'^\dagger\mathbf{t} & \mathbf{t}'^\dagger\mathbf{t}' + \mathbf{r}'^\dagger\mathbf{r}' \end{pmatrix} = \mathbb{1}$$

Looking at the upper left diagonal component, which is the identity matrix, and taking its transpose, we find that

$$\mathbf{t}'\mathbf{t}'^\dagger = \mathbf{t}^\dagger\mathbf{t}$$

and hence using the properties of the trace we get

$$\mathrm{Tr}\Big(\mathbf{t}'^\dagger\mathbf{t}'\Big) = \mathrm{Tr}\Big(\mathbf{t}^\dagger\mathbf{t}\Big).$$

We do the same for the the other term. Nearing the end, we must look at the top left component of the equation $S^\dagger S = \mathbb{1}$ equation again to find

$$\mathbb{1} - \mathbf{r}^\dagger\mathbf{r} = \mathbf{t}^\dagger\mathbf{t}$$

and hence

$$n_L - \mathrm{Tr}\Big(\mathbf{r}^\dagger\mathbf{r}\Big) = \mathrm{Tr}\Big(\mathbf{t}^\dagger\mathbf{t}\Big).$$

Thus, after taking the expectation value, we get

$$I_L = \langle \hat{I}_L(t) \rangle = \int \frac{e}{h} \mathrm{Tr}\Big(\mathbf{t}^\dagger\mathbf{t}\Big) \left[f_L(E) - f_R(E) \right] \mathrm{d}E\,.$$

(c) The transmission function is the trace expression in the previous equation.

(d) The conductance can be evaluated at 0 temperature and for small voltage differences as follows: At small temperatures, the fermi function is a step function. f_L goes to 0 at $E_F + eV_L$, while f_R goes to 0 at $E_F + eV_R$. If V_L is higher than V_R, then

f_L goes to 0 earlier than f_R. This is the only part where $f_L - f_R$ does not vanish, and it has width $e(V_L - V_R) =: eV$, with V the potential difference. Additionally, if the voltages are small, we can take the integrand to be constant and evaluate it at E_F. Thus,

$$I_L = \frac{e^2 V}{h} \operatorname{Tr}\left(\mathbf{t}^\dagger \mathbf{t}\right).$$

Identifying this with the classical ohmic expression

$$I_L = VG,$$

we arrive at the expression

$$G = \frac{e^2}{h} \operatorname{Tr}\left(\mathbf{t}^\dagger \mathbf{t}\right).$$

□

Problem 2. Consider a wide conductor along x, e.g. width in y direction is large W while the height in z direction is small. The length in the x direction is large L.

Given information: The density of states of a 2D spin degenerate system is

$$\mathcal{D}_0 = \frac{m}{\pi \hbar^2}.$$

The transmission through a wire with length L is

$$T = \frac{L_0}{L + L_0},$$

where L_0 is the mean free path. The conductivity is

$$\sigma = e^2 \mathcal{D}_0 D,$$

where

$$D = \frac{v_F L_0}{\pi}$$

is the diffusion coefficient and v_F is the Fermi velocity.

Using this information, relate the previous results for conductance G with Ohm's law. I.e., does the relationship between G and conductivity σ correspond to Ohm's law?

Proof. We begin by recalling the results for the eigenenergies of a particle in a 1-dimensional box:

$$E_n = \frac{\hbar^2 k_n^2}{2m}, \qquad k_n = \frac{n\pi}{L}.$$

Since the height in the z direction is very small, the k values are very high and spaced very far apart. Thus, we can assume that we are only in the lowest mode in the z direction.

Now, we want to count the number of conducting modes. The total Hamiltonian is

$$H = \frac{1}{2m}(p_x^2 + p_y^2).$$

We seek to choose wavenumbers $k_x,\ k_y$ such that

$$k_x^2 + k_y^2 = k_F^2.$$

Since the length in x is very large, for each k_y, we should be able to pick a k_x such that $k_x^2 + k_y^2 \approx k_F^2$. Thus, we simply seek to count the k_y such that

$$|k_y| \leq |k_F|$$

or

$$\frac{n\pi}{W} \leq |k_F|.$$

Thus, the total number of modes is

$$N = \frac{k_F W}{\pi}.$$

The total conductivity is given by (initial 2 from spin degeneracy)

$$\begin{aligned}
G &= \frac{2e^2}{h}\left(\frac{k_F W}{\pi}\right)\underbrace{\frac{L_0}{L+L_0}}_{T} \\
&= \frac{2e^2}{h}\frac{W}{\pi}\frac{mv_F}{\hbar}\frac{L_0}{L+L_0} \\
&= \frac{e^2 W m v_F}{\pi^2\hbar^2}\frac{L_0}{L+L_0} \\
&\approx \frac{e^2 W m v_F}{\pi^2\hbar^2}\frac{L_0}{L} \\
&= \left(\frac{e^2 L_0 m v_F}{\pi^2\hbar^2}\right)\frac{W}{L}
\end{aligned}$$

We have used the diffusive limit $L \gg L_0$ here. From Ohm's law, we identify the term in parentheses as the conductivity. We can also evaluate the given expression

$$\sigma = e^2\mathcal{D}D$$

$$= e^2 \left(\frac{m}{\pi \hbar^2} \right) \left(\frac{v_F L_0}{\pi} \right)$$
$$= \frac{e^2 L_0 m v_F^2}{\pi^2 \hbar^2}$$

This agrees with the conductivity derived earlier from the total conductance and Ohm's law. Thus, we conclude that our result is consistent with Ohm's law. $\square$