Exercise sheet 9 – Solutions (15.12.22)

1. 2D step junction

Find the scattering matrix $\hat{S}$ for a 2D step junction with $W_R = 2W_L$.

**Solution**

We start from the general solution

$$\psi_{LE}^±(r) = \sum_n A_{n±} \sin \left( \frac{\pi n x}{W_L} \right) e^{±ik_n z}, \quad \hbar k_n = \sqrt{2m(E - E_n)}, \quad z < 0,$$

$$\psi_{RE}^±(r) = \sum_m B_{m±} \sin \left( \frac{\pi m x}{W_R} \right) e^{±ik_m z}, \quad \hbar k_m = \sqrt{2m(E - E_m)}, \quad z > 0.$$  \hspace{1cm} (1)

For the closed left channels ($E < E_n$) or closed right channels ($E < E_m$) we should take only normalized modes $a_n e^{\kappa_n z}$ at $z < 0$, and $b_m e^{-\kappa_m z}$ at $z > 0$.

The boundary conditions at $z = 0$ include the continuity of the wavefunction and its $z$ derivative

$$\psi_{RE}(z = 0) + \psi_{RE}^+(z = 0) = \psi_{LE}(z = 0) + \psi_{LE}^+(z = 0),$$

$$\frac{d\psi_{RE}}{dz}(z = 0) + \frac{d\psi_{RE}^+}{dz}(z = 0) = \frac{d\psi_{LE}}{dz}(z = 0) + \frac{d\psi_{LE}^+}{dz}(z = 0).$$ \hspace{1cm} (3)

$$\sum_m (B_{m+} + B_{m-}) \sin \left( \frac{\pi m x}{W_R} \right) + \sum_{m'} b_{m'} \sin \left( \frac{\pi m' x}{W_R} \right) =$$

$$= \left\{ \begin{array}{ll}
\sum_n (A_{n+} + A_{n-}) \sin \left( \frac{\pi n x}{W_L} \right) + \sum_{n'} a_{n'} \sin \left( \frac{\pi n' x}{W_L} \right), & 0 < x < W_L, \\
0, & W_L < x < W_R. \end{array} \right.$$

$$\sum_m (-ik_m B_{m+} + ik_m B_{m-}) \sin \left( \frac{\pi m x}{W_R} \right) - \sum_{m'} \kappa_{m'} b_{m'} \sin \left( \frac{\pi m' x}{W_R} \right) =$$

$$= \sum_n (ik_n A_{n+} - ik_n A_{n-}) \sin \left( \frac{\pi n x}{W_L} \right) + \sum_{n'} \kappa_{n'} a_{n'} \sin \left( \frac{\pi n' x}{W_L} \right) 0 < x < W_L.$$ \hspace{1cm} (5)
The next step is to multiply these equations by \( \sin \left( \frac{\pi l x}{W_L} \right) \) and integrate over \( 0 < x < W_L \).

The key property is
\[
\frac{2}{W_L} \int_0^{W_L} \sin \left( \frac{\pi n x}{W_L} \right) \sin \left( \frac{\pi l x}{W_L} \right) \, dx = \delta_{nl}. \tag{7}
\]

and we get the following equations
\[
\sum_m (B_m^+ + B_m^-) C_{ml} + \sum_{m'} b_{m'} C_{m'l} = \sum_n (A_n^+ + A_n^-) \delta_{nl} + \sum_n a_n \delta_{n'l}, \tag{8}
\]
\[
\sum_m (-ik_m B_m^+ + ik_m B_m^-) C_{ml} - \sum_{m'} \kappa_{m'} b_{m'} C_{m'l} = \sum_n (ik_n A_n^+ - ik_n A_n^-) \delta_{nl} + \sum_n \kappa_n a_n \delta_{n'l}, \tag{9}
\]
where we introduced the coefficients
\[
C_{nl} = \frac{2}{W_L} \int_0^{W_L} \sin \left( \frac{\pi n x}{W_R} \right) \sin \left( \frac{\pi l x}{W_L} \right) \, dx. \tag{10}
\]

The boundary conditions for open left channels \( l \) are
\[
\sum_m (B_m^+ + B_m^-) C_{ml} + \sum_{m'} b_{m'} C_{m'l} = (A_{l^+} + A_{l^-}), \tag{11}
\]
\[
\sum_m (-ik_m B_m^+ + ik_m B_m^-) C_{ml} - \sum_{m'} \kappa_{m'} b_{m'} C_{m'l} = (ik_l A_{l^+} - ik_l A_{l^-}). \tag{12}
\]

For closed left channels \( l \) we have additionally
\[
\sum_m (B_m^+ + B_m^-) C_{ml} + \sum_{m'} b_{m'} C_{m'l} = a_l, \tag{13}
\]
\[
\sum_m (-ik_m B_m^+ + ik_m B_m^-) C_{ml} - \sum_{m'} \kappa_{m'} b_{m'} C_{m'l} = \kappa_l a_l. \tag{14}
\]

Besides, we can integrate Eq. (5) over \( W_L < x < W_R \), introducing the coefficients
\[
D_{nk} = \frac{2}{W_R} \int_{W_L}^{W_R} \sin \left( \frac{\pi n x}{W_R} \right) \sin \left( \frac{\pi k x}{W_R} \right) \, dx. \tag{15}
\]
\[
\sum_m (B_m^+ + B_m^-) D_{mk} + \sum_{m'} b_{m'} D_{m'k} = 0. \tag{16}
\]

The channel mixing is described by coefficients \( C_{nl} \) and \( D_{nl} \).

In the case \( W_R = W_L \) one gets \( C_{nl} = \delta_{nl} \) and \( D_{nl} = 0 \) and come back to single channels.

For a numerical solution, the number of channels must be truncated to some reasonable value.

To find the scattering matrix, we need to fix \( A_{n^+} \) and \( B_{m^+} \), and find \( A_{n^-} \), \( B_{m^-} \), \( a_n \), \( b_m \) – all together \( N_R + N_L \) variables, where we count both open and closed channels. The number of equations is \( 2N_L + N_X \), \( N_X \) is the number of equations (13). Thus we need the relation \( N_R - N_L = N_X \) to have a correct system.

At \( W_R = 2W_L \) the coefficients \( C_{nl} \) and \( D_{nl} \) can be found in a simple algebraic form.
2. Channel mixing in adiabatic junctions

Estimate the corrections $\Delta_n$ in the equation

\[
\left\{ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + E_n(z) \right\} \psi_{nE}(z) = E\psi_{nE}(z) + \Delta_n,
\]  

(17)

leading to mixing of the channels with different $n$.

**Solution**

Let’s start from the full Schrödinger equation

\[
\left\{ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + U(x, y, z) \right\} \Psi_E(x, y, z) = E\Psi_E(x, y, z),
\]  

(18)

where $U(x, y, z)$ is the external potential, defining the geometry of the junction.

$\phi_n(x, y; z)$ is the solution of the “transverse” Schrödinger equation

\[
\left\{ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x, y, z) \right\} \phi_n(x, y) = E_n\phi_n(x, y).
\]  

(19)

Now we find a solution in the form

\[
\Psi_E(x, y, z) = \sum_m \phi_m(x, y; z)\psi_{mE}(z).
\]  

(20)

Substituting to (18), we get

\[
\sum_m \left\{ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + U(x, y, z) \right\} \phi_m(x, y; z)\psi_{mE}(z) = E \sum_m \phi_m(x, y; z)\psi_{mE}(z),
\]

\[
\sum_m \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + E_m(z) \right\} \phi_m(x, y; z)\psi_{mE}(z) = E \sum_m \phi_m(x, y; z)\psi_{mE}(z),
\]

\[
\sum_m \phi_m(x, y; z) \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + E_m(z) \right\} \psi_{mE}(z) + \sum_m \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2 \phi_m(x, y; z)}{\partial z^2} - \frac{\hbar^2}{2m} \frac{\partial \phi_m(x, y; z)}{\partial z} \right\} \psi_{mE}(z) = E \sum_m \phi_m(x, y; z)\psi_{mE}(z).
\]  

(21)

Now we can multiply by $\phi^*_n(x, y; z)$ and integrate over $x$ and $y$, the result is

\[
\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + E_n(z) \right\} \psi_{nE}(z) = E\psi_{nE}(z) + \Delta_n,
\]  

(22)

\[
\Delta_n = \sum_m \left\{ \frac{\hbar^2}{m} \int \phi^*_n(x, y; z) \frac{\partial \phi_m(x, y; z)}{\partial z} dxdy \right\} \frac{\partial}{\partial z} \psi_{mE}(z) +
\]

\[
+ \sum_m \left\{ \frac{\hbar^2}{2m} \int \phi^*_n(x, y; z) \frac{\partial^2 \phi_m(x, y; z)}{\partial z^2} dxdy \right\} \psi_{mE}(z).
\]  

(23)

The $\Delta_n$ term describe the coupling of the channel with index $n$ to other channels, it corresponds to interchannel scattering. These terms are proportional to spatial gradients in the longitudinal direction, which are small in the adiabatic approximation.
3. Landauer formula from scattering states

Use the current density expression

\[ j = \frac{i e \hbar}{2m} \left[ \psi(r) \nabla \psi^*(r) - \psi^*(r) \nabla \psi(r) \right], \tag{24} \]

and the expression for the scattering state

\[ \Psi_{LnE}(r) = \sum_m t_{mn}(E) \sqrt{2\pi \hbar \nu_{Rm}} \phi_{Rm}(x, y) e^{ik_m' z}, \ z > z_R, \tag{25} \]

to get the multichannel Landauer formula.

Solution

Direct application of the current density expression gives the following answer for the \( z \)-component of the current density coming to the right electrode from the \( n \)-th left channel

\[ j_{LnE}^z = \frac{i e \hbar}{2m} \left[ \psi_{LnE}(r) \frac{\partial \psi_{LnE}^*(r)}{\partial z} - \psi_{LnE}^*(r) \frac{\partial \psi_{LnE}(r)}{\partial z} \right], \tag{26} \]

\[ \psi_{LnE}(r) = \sum_{m'} \frac{t_{m'm}(E)}{\sqrt{2\pi \hbar \nu_{Rm'}}} \phi_{Rm'}(x, y) e^{-ik_{m'} z}, \ z > z_R, \tag{27} \]

\[ j_{LnE}^z = \frac{i e \hbar}{2m} \sum_{mm'} \frac{t_{mn} t_{m'n}^*}{\sqrt{2\pi \hbar \nu_{Rm} \nu_{Rm'}}} \phi_{Rm}(x, y) \phi_{Rm'}^*(x, y) (e^{-ik_{m'} z} - i k_{m'} e^{ik_m z}. \tag{28} \]

And integrating over \((x, y)\) and using the orthogonality property

\[ \int \phi_{Rm}(x, y) \phi_{Rm'}(x, y) \, dx \, dy = \delta_{mm'}, \tag{29} \]

we get

\[ I_{LnE} = \frac{e}{\hbar} \sum_m |t_{mn}|^2 = \frac{e}{\hbar} \left( \bar{t} \hat{i} \right)_{nn}. \tag{30} \]

We can summarize over transport channels, and obtain the Landauer formula

\[ I(V) = \frac{e}{\hbar} \int_{-\infty}^{\infty} T(E, V) [f_0(E - eV) - f_0(E)] \, dE, \tag{31} \]

with

\[ T(E, V) = \sum_n \left( \bar{t} \hat{i} \right)_{nn} = \text{Tr} \left( \bar{t} \hat{i} \right) = \sum_{nm} T_{mn} = \sum_{nm} |t_{mn}|^2. \tag{32} \]
4. $G_{sp}$ and $G'_{sp}$ conductance matrices

The current can be written through conductance matrices $G_{sp}$ or $G'_{sp}$

$$I_s = \sum_p [G_{ps}V_s - G_{sp}V_p] = \sum_p G'_{sp}V_p,$$

(33)

Prove the following relation at $T = 0$

$$G'_{sp} = \frac{e^2}{h} N_s \delta_{sp} - G_{sp}. \quad (34)$$

**Solution**

Consider the first term in (37)

$$\sum_p G_{ps}V_s = \left( \sum_q G_{qs} \right) V_s = \sum_p \left( \sum_q G_{qp} \right) V_p \delta_{sp}, \quad (35)$$

$$\sum_q G_{qp} = \frac{e^2}{h} \sum_q T_{qp} = \frac{e^2}{h} N_p, \quad (36)$$

where $N_p$ is the number of channels in $p$-th electrode. Indeed, $T_{qp}$ is the sum of transmission probabilities of *all channels* from $p$-th electrode to $q$-th electrode. Including the reflection probability $T_{pp}$. If we some over all electrodes, this some is unity for one incoming channel and $N_p$ for all channels.

Now return back to the the current

$$I_s = \sum_p [G_{ps}V_s - G_{sp}V_p] = \sum_p \left[ \frac{e^2}{h} N_p \delta_{sp} - G_{sp} \right] V_p = \sum_p G'_{sp}V_p. \quad (37)$$

Finally, we can replace $N_p \delta_{sp}$ to $N_s \delta_{sp}$ and get (34).
5. 4-terminal junction

Consider the 4-terminal junction and assume that electrodes 3 and 4 are weakly coupled voltage probes. Prove the relation

\[ V_{34} = \frac{T_{31}T_{42} - T_{32}T_{41}}{(T_{31} + T_{32})(T_{41} + T_{42})} V_{12}. \]

**Solution**

First of all, for weak coupled voltage probes

\[ I = I_1 = I_2 = G_{12}(V_1 - V_2) = G_{12}V. \]  \(\text{(38)}\)

Then, the conditions of zero current are

\[ I_3 = G_{31}(V_3 - V_1) + G_{32}(V_3 - V_2) + G_{34}(V_3 - V_4) = 0, \]  \(\text{(39)}\)

\[ I_4 = G_{41}(V_4 - V_1) + G_{42}(V_4 - V_2) + G_{43}(V_4 - V_3) = 0. \]  \(\text{(40)}\)

In the weak coupling limit \(G_{34}, G_{43} \ll G_{31}, G_{32}, G_{41}, G_{42}\), thus

\[ I_3 = G_{31}(V_3 - V_1) + G_{32}(V_3 - V_2) = 0, \]  \(\text{(41)}\)

\[ I_4 = G_{41}(V_4 - V_1) + G_{42}(V_4 - V_2) = 0. \]  \(\text{(42)}\)

\[ V_3 = \frac{G_{31}V_1 + G_{32}V_2}{G_{31} + G_{32}}, \quad V_4 = \frac{G_{41}V_1 + G_{42}V_2}{G_{41} + G_{42}}. \]  \(\text{(43)}\)

\[ V_3 - V_4 = \frac{(G_{31}V_1 + G_{32}V_2)(G_{41} + G_{42}) - (G_{41}V_1 + G_{42}V_2)(G_{31} + G_{32})}{(G_{31} + G_{32})(G_{41} + G_{42})} = \frac{G_{31}G_{42}V_1 + G_{32}G_{41}V_2 - G_{41}G_{32}V_1 - G_{42}G_{31}V_2}{(G_{31} + G_{32})(G_{41} + G_{42})} = \frac{(G_{31}G_{42} - G_{32}G_{41})(V_1 - V_2)}{(G_{31} + G_{32})(G_{41} + G_{42})}. \]  \(\text{(44)}\)