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Tutorial V
Quantum electron transport

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1 S and M matrices

We consider a one-dimensional conductor with a single scattering center characterized by the potential $\mathcal{V}(x)$ which is non-zero between the points $x = -a$ and $x = +a$. Due to its presence, incoming plane waves A^{ikx} ($A'e^{-ikx}$) propagating towards the scatterer in the domain $x < -a$ ($x > +a$) give rise to outgoing plane waves propagating away from the scatterer (we take $k > 0$). A stationary state of this scattering problem with energy $E = \hbar^2 k^2/2m$ can be written as :

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < -a, \\ B'e^{ikx} + A'e^{-ikx} & \text{for } x > a. \end{cases} \tag{1.1}$$

Knowing the coefficients A and A' of the incoming waves, the solution of Schrödinger equation allows for the determination of the coefficients B and B' of the outgoing waves. The S matrix expresses the amplitudes of the outgoing waves as a function of the amplitudes of the incoming waves :

$$\begin{pmatrix} B \\ B' \end{pmatrix} = S \begin{pmatrix} A \\ A' \end{pmatrix}, \tag{1.2}$$

where one can write in full generality :

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \tag{1.3}$$

1. A stationary state defined by the wave-function $\Psi(x)$ is associated with the particle current density

$$j(x) = \frac{\hbar}{2mi}\left(\Psi^*(x)\frac{\mathrm{d}\Psi(x)}{\mathrm{d}x} - \Psi(x)\frac{\mathrm{d}\Psi^*(x)}{\mathrm{d}x}\right), \tag{1.4}$$

and the current density $J(x) = ej(x)$. Calculate the current density associated with the incident and outgoing waves, as well as that of the state defined in Eq. (1.1).

- $x < -a$,

$$\begin{aligned} j(x) &= \frac{\hbar}{2mi}\left(\left[A^*e^{-ikx} + B^*e^{ikx}\right] ik \left[Ae^{ikx} - Be^{-ikx}\right] - \left[Ae^{ikx} + Be^{-ikx}\right] ik \left[-A^*e^{-ikx} + B^*e^{ikx}\right]\right) \\ &= \frac{\hbar k}{2m}\left[|A|^2 - A^*Be^{-2ikx} + B^*Ae^{2ikx} - |B|^2 + |A|^2 - AB^*e^{2ikx} + A^*Be^{-2ikx} - |B|^2\right] \\ &= \frac{\hbar k}{m}[|A|^2 - |B|^2] \end{aligned}$$

- $x > +a$ similarly,

$$j(x) = -\frac{\hbar k}{m}[-|A'|^2 + |B'|^2]$$

Thus, we can write,

$$J(x) = ej(x) = \begin{cases} +\dfrac{e\hbar k}{m}\left[|A|^2 - |B|^2\right] \text{ for } x < -a \\ -\dfrac{e\hbar k}{m}\left[-|A'|^2 + |B'|^2\right] \text{ for } x > +a \end{cases}$$

2. Defining the column matrices

$$\mathcal{I} = \begin{pmatrix} A \\ A' \end{pmatrix} \quad \text{and} \quad \mathcal{O} = \begin{pmatrix} B \\ B' \end{pmatrix}, \tag{1.5}$$

show that current conservation leads to $\mathcal{O}^\dagger\mathcal{O} = \mathcal{I}^\dagger\mathcal{I}$, and thus to the unitarity of the scattering matrix, *i.e.* $S^\dagger S = I$. Establish the resulting relations between the scattering amplitudes r, r', t and t'. Express the reflection ($\mathcal{R}$) and the transmission ($\mathcal{T}$) probabilities in terms of the scattering amplitudes and establish the relationship between $\mathcal{R}$ and $\mathcal{T}$ that results from current conservation.

From current conservation we can write,

$$J(x)\Big|_{x<-a} = J(x)\Big|_{x>+a} \implies \frac{e\hbar k}{m}[|A|^2 - |B|^2] = -\frac{e\hbar k}{m}[-|A'|^2 + |B'|^2]$$

Leading us to write,

$$|A|^2 + |A'|^2 = |B|^2 + |B'|^2$$

and we recognize that

$$\mathcal{I}^\dagger\mathcal{I} = |A|^2 + |A'|^2 \qquad \mathcal{O}^\dagger\mathcal{O} = |B|^2 + |B'|^2$$

So we get,

$$\mathcal{I}^\dagger\mathcal{I} = \mathcal{O}^\dagger\mathcal{O}$$

from Eq. (1.2) we know that,

$$\begin{pmatrix} B \\ B' \end{pmatrix} = S\begin{pmatrix} A \\ A' \end{pmatrix}$$

Which can can be written in two ways,

$$\mathcal{O} = S\mathcal{I}, \qquad \mathcal{O}^\dagger = \mathcal{I}^\dagger S^\dagger$$

Thus,

$$\mathcal{O}^\dagger\mathcal{O} = (\mathcal{I}^\dagger S^\dagger)(S\mathcal{I}) = \mathcal{I}^\dagger\mathcal{I}$$

implying that indeed,

$$S^\dagger S = \mathrm{Id} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now, plugging in the form of S in that equation lead us to,

$$\begin{pmatrix} r^* & t^* \\ t'^* & r'^* \end{pmatrix} \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Giving us the following equations,

$$\left| \begin{array}{c} |r|^2 + |t|^2 = 1 \\ r^* t' + r' t^* = 0 \\ r t'^* + r'^* t = 0 \\ |t'|^2 + |r'|^2 = 1 \end{array} \right.$$

If now we define $\mathcal{R} = |r|^2$ and $\mathcal{T} = |t|^2$ we indeed get the current conservation in the form of

$$\mathcal{R} + \mathcal{T} = 1$$

3. One can also define the transfer matrix M through the relation :

$$\begin{pmatrix} B' \\ A' \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} \tag{1.6}$$

Express the matrix elements of M, as a function of r, r', t and t'.

We know that

$$\begin{pmatrix} B' \\ A' \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} B \\ B' \end{pmatrix} = S \begin{pmatrix} A \\ A' \end{pmatrix}$$

defining,

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \qquad S = \begin{pmatrix} r & t' \; t & r' \end{pmatrix}$$

This allows us to write,

$$\begin{cases} B' = M_{11} A + M_{12} B \\ A' = M_{21} A + M_{22} B \end{cases} \qquad \begin{cases} B' = rA + t'A' \\ B = tA + r'A' \end{cases}$$

$$B' = M_{11} A + M_{12} B = M_{11} A + M_{12} [rA + t'A'] = (M_{11} + r M_{12}) A + M_{12} t' A'$$

which, we can identify with $B' = tA + r'A'$ leading us to,

$$\begin{cases} M_{11} = t - rM_{12} = t - \dfrac{rr'}{t'} \\ M_{12} = \dfrac{r'}{t'} \end{cases}$$

And now for the other relation,

$$A' = M_{21}A + M_{22}B$$

which can be rewritten in

$$B = \frac{A'}{M_{22}} - \frac{M_{21}}{M_{22}}A$$

which can be identified with $B = rA + t'A'$ leading to,

$$\begin{cases} M_{22} = \dfrac{1}{t'} \\ M_{21} = -\dfrac{r}{t'} \end{cases}$$

The whole transfer matrix M is then,

$$M = \begin{pmatrix} t - \frac{rr'}{t'} & \frac{r'}{t'} \\ -\frac{r}{t'} & \frac{1}{t'} \end{pmatrix}$$

4. Consider the case where $a \to 0$ with a very high potential, which can be assimilated to $\mathcal{V}(x) = a\delta(x)$. Integrating the Schrödinger equation in the interval $[0^-, 0^+]$, obtain the discontinuity of $\mathrm{d}\Psi(x)/\mathrm{d}x$ at $x = 0$, and calculate the scattering ans transfer matrices characterizing this scatterer.

2 Landauer formula

We consider a one dimensional configuration of a scatterer, defined by a potential $\mathcal{V}(x)$ and an associated scattering matrix S, connected through scatter-free leads to two particle reservoirs labeled by 1 and 2. The latter are at equilibrium at a temperature T, and have, respectively, chemical potentials μ_1 and μ_2. The scattering state $\Psi_k^{(1,2)}(x)$ is generated by an incoming wave from the left (right) side of the scatterer with wave-vector k, *i.e.* it corresponds to the stationary state (1.1) with $A' = 0$ ($A = 0$). These scattering states are populated by the left (right) reservoir with a probability given by the Fermi distribution $f_{1,2}(\epsilon) = 1/(1 + e^{(\epsilon - \mu_{1,2})/k_B T})$.

1. Give the current density for $x > 0$ associated with the scattering state generated by an incoming state arising from the left with wave-vector k.

We can write any plane wave coming from left or right as a superposition,

$$\psi(x) \propto \frac{1}{\sqrt{L}}(e^{ikx} + e^{ikx})$$

If now we consider a wave coming from the left, this means that we have

$$\psi(x) = \frac{1}{\sqrt{L}}e^{ikx}$$

and thus,

$$j(x) = \frac{\hbar}{m}\frac{k}{L}$$

leading to,

$$J(x) = ej(x) = \frac{e\hbar k}{mL}$$

2. Choosing a boundary condition for the leads allows to normalize the incoming waves and quantize the values of k. Taking then the continuum limit in the sum of k, the total current at $x > 0$ arising from the left reservoir can be written as

$$I_{1\to 2} = 2e\int_0^{+\infty}\frac{\mathrm{d}k}{2\pi}\frac{\hbar k}{m}\mathcal{T}(k)f_1\left(\frac{\hbar^2k^2}{2m}\right) = 2e\int_0^{+\infty}\mathrm{d}\varepsilon v(\epsilon)g(\epsilon)\mathcal{T}(\epsilon)f_1(\epsilon). \qquad (2.1)$$

The factor of 2 stands for spin-degeneracy, v is the velocity of the incoming electrons, g the density of states of the one-dimensional lead, and $\mathcal{T}$ is the transmission probability. Comment on the change of variables allowing to go between the two integrals of Eq. (2.1), in particular identifying the different terms of the two integrands.

We can write the current as,

$$I_{1\to 2} = g_s\frac{e}{L}\sum_k v_k\mathcal{T}(k)f_1\left(\frac{\hbar^2k^2}{2m}\right)$$

with $g_s = 2$ the spin degeneracy and $v_k = \hbar k/m$ the mode velocity. We know the density of state of a 1D lead,

$$g(\varepsilon) = \frac{2}{\pi}\frac{\partial\varepsilon}{\partial k} = \frac{2}{\pi\hbar v(\varepsilon)}$$

Now we can make the continuum limit,

$$\begin{aligned} I_{1\to 2} &= 2\frac{e}{L}\sum_k v_k\mathcal{T}(k)f_1\left(\frac{\hbar^2k^2}{2m}\right) \\ &\longrightarrow 2e\int_0^{+\infty}\frac{\mathrm{d}k}{2\pi}\frac{\hbar k}{m}\mathcal{T}(k)f_1\left(\frac{\hbar^2k^2}{2m}\right) \\ &= 2e\int_0^{+\infty}v(\varepsilon)g(\varepsilon)\mathcal{T}(\varepsilon)f_1(\varepsilon)\mathrm{d}\varepsilon \\ &= \frac{2e}{h}\int_0^{+\infty}\mathrm{d}\varepsilon\mathcal{T}(\varepsilon)f_1(\varepsilon) \end{aligned}$$

3. Calling $I_{2\to1}$ the total current at $x<0$ arising from the right reservoir (using the sign convention that currents towards the right are positive), calculate the net current

$$I_{\text{tot}} = I_{1\to2} + I_{2\to1} \tag{2.2}$$

Similarly, we can write,

$$I_{2\to1} = -\frac{2e}{h}\int_0^{+\infty} \mathrm{d}\varepsilon \mathcal{T}(\varepsilon) f_2(\varepsilon)$$

Thus the total read,

$$I_{\text{tot}} = I_{1\to2} + I_{2\to1} = \frac{2e}{h}\int_0^{+\infty} \mathrm{d}\varepsilon \mathcal{T}(\varepsilon)\left[f_1(\varepsilon) - f_2(\varepsilon)\right]$$

which is the known one channel, two terminals current.

4. The applied bias voltage V is related to the difference between the chemical potentials of the reservoirs by $\mu_1 - \mu_2 = eV$. Noting ϵ_{F} the Fermi energy of the reservoirs in the absence of a bias voltage, and assuming that $eV \ll k_B T \ll \epsilon_{\mathrm{F}}$, show that the conductance can be written by the Landauer formula :

$$G = \frac{2e^2}{h}\mathcal{T}(\epsilon_{\mathrm{F}}). \tag{2.3}$$

We can perform two approximations,

— Low temperature approximation, thus, the Fermi-Dirac distribution can be approximated by an Heaviside function.

— $|\mu_1 - \mu_2| \ll E_F$ thus, we can approximate

$$f_1(\varepsilon) - f_2(\varepsilon) \approx \frac{\partial f}{\partial \varepsilon}\mathrm{d}\varepsilon$$

and for the low-temperature limit, this derivative is $-\delta(\varepsilon)$

Considering low temperature,

$$I_{\text{tot}} = \frac{2e}{h}\int_{\mu_1}^{\mu_2} \mathrm{d}\varepsilon \mathcal{T}(\varepsilon)$$

And assuming a small potential difference, we get $\mathcal{T}(\varepsilon) \approx \mathcal{T}(E_F)$, leading us to,

$$G = \frac{I}{V} = \frac{2e^2}{h}\mathcal{T}(E_F)$$

3 Multimode conductor and quantum point contact (bonus)

In the case of a two or three dimensional conductor, several transverse mode can contribute to the transport of the electrical current. They correspond to the quantization of the motion along the directions orthogonal to the direction of propagation (the one dimensional conductor thus corresponds to the case of a single mode conductor). The scattering of a conductor with N transverse modes can still be described by a scattering matrix as the one defined in Eq. (1.3) by replacing the coefficients r, r', t and t' by matrices of dimension $N \times N$.

1. Provide the multimode generalization of Landauer formula Eq. (2.3) (no detailed derivation is requested).

If we consider a 2D geometry, with a length L and width W,

$$\psi(x, y) = \sqrt{\frac{2}{LW}} \sin(k_y y) e^{ik_x x}$$

where k_y is quantized following $k_y = n_y \frac{\pi}{W}$ with $n_y \in \mathbb{N}^*$. We can then write,

$$\varepsilon = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 n_y^2 \pi^2}{2mW^2}$$

How many transverse modes do we get? we have $\varepsilon < \varepsilon_F$ thus,

$$n_y < \mathrm{int}\left(\frac{k_F W}{\pi}\right) \equiv N_{\text{modes}}$$

we see that we get the maximum number of modes for $k = 0$. We can write the current in mode a as follow,

$$I_a = \sum_b I_{a,b}$$

with

$$I_{a,b} = \frac{2e^2}{h} \mathcal{T}_{a,b}(V_1 - V_2)$$

and with $\mathcal{T}_{a,b} = |t_{a,b,}|^2$ that connect the a and b modes. Thus the total current read,

$$I_{\text{tot}} = \sum_{a,b} I_{a,b} = \frac{2e^2}{h}(V_1 - V_2) \sum_{a,b} \mathcal{T}_{a,b}$$

$t_{a,b}$ is a $N \times N$ matrix,

$$\sum_{a,b} \mathcal{T}_{a,b} = \sum_{a,b} t_{a,b} t^*_{a,b} = \sum_{a,b} t_{a,b} t^*_{b,a} = \sum_a (tt^\dagger)_{aa} = \mathrm{Tr}(tt^\dagger)$$

Thus,

$$G = \frac{2e^2}{h}\mathrm{Tr}(tt^\dagger)$$

with $h/e^2 \approx 25.8\ \Omega$. In the balistic regime, $\mathcal{T}_{a,b} = \delta_{a,b}$ (meaning no transport from mode a to b) and thus,

$$G = \frac{2e^2}{h}\sum_{\text{modes}}\Theta(E_F - E_a) = \frac{2e^2}{h}N_{\text{modes}}$$

where E_a is the energy of the mode a.

2. The quantization of the conductance has first been observed in a quantum point contact defined in a two-dimensional electron gas within a GaAlAs-GaAs heterostructure. Two electroced (called gates) deposited at the surface of the sample are used to deplete the electron gas through the application of a negative DC gate voltage V_g (see Fig.2). The width of the constriction can then be controlled by changing V_g. Explain how the experimental data of Fig.2 constitute a proof of the applicability of the multimode Landauer formula to quantum transport.