Lecture 8. Landauer Formula

Electric current flow is often viewed as an electron (or charged carriers) response to an applied electric field. Alternatively, Landauer viewed current flow as a transmission process, or a consequence of the injection of carriers at contacts and probability of the carriers to reach the other end. This approach has proven to be extremely useful for transport properties of nanostructured materials and devices, including molecular systems.

Landauer’s original result was obtained for a system of two one-dimensional leads connecting to a sample. The two leads are connected to two macroscopic electrodes or electron reservoirs (Fig. 1). The sample is where scattering can take place and characterized by a transmission function \( T(E) \). The conductance \( (G) \) of the system at a small applied bias voltage \( (V) \) is given by

\[
G = \frac{I}{V} = \frac{2e^2}{h}T(E_F) , \quad (1)
\]

where \( e \) is the electron charge and \( h \) is the Planck constant.

Here is a simple way to see how the simple formula arises. Let us consider an ideal one-dimensional sample of length \( L \). The density of state between \( k \) and \( k + dk \), including electron spin, is

\[
n(k)dk = 2 \frac{1}{L} \frac{L}{2\pi} dk , \quad (2)
\]

and the electron group velocity is

\[
\nu = \frac{\hbar k}{m} . \quad (3)
\]

The current flow through such a system is
The conductance, $G$, is thus,

$$G = \frac{2e^2}{h} = (12.9 \text{ kohm})^{-1}. \quad (5)$$

In general, the sample is not ideal and the transmission is not 100% due to scattering. In this case, Eq. 5 becomes

$$G = \frac{2e^2}{h} T(E_F), \quad (6)$$

which is what we saw in Eq. 1. This result is for one-dimensional systems in which only one conduction channel or mode exists in the direction normal to the propagation. If the sample has a finite width, electrons in the transverse direction form a series of quantum modes. For a two-dimensional wire, the number of quantum modes is simply determined by the ratio of the width ($W$) of the wire and the half the Fermi wavelength ($\lambda_F$), $N = \text{INT}\left(\frac{2W}{\lambda_F}\right)$. For a three-dimensional wire, $N \sim \left(\frac{\pi R}{\lambda_F}\right)^2$, $R$ is the radius of the circular cross section of the sample. In this case, the Landauer formula can be generalized to the form of

$$G = \frac{2e^2}{h} \sum_{i,j} T_{ij}(E_F), \quad (7)$$
where $T_{ij}$ is the probability that a carrier (e.g. electron) transmits from the $i^{th}$ mode at the left of the sample to the $j^{th}$ mode at the right of the sample. Eq. 7 is strictly right only for a small bias voltage. More generally, the current for a finite bias voltage is given by

$$I = \int_{0}^{\infty} \frac{dE}{e} [f(E + eV) - f(E)]G(E), \quad (8)$$

where $G(E) = \frac{2e^2}{\hbar} \sum_{i,j} T_{ij}(E)$. \quad (9)

Eqs. 8 and 9 provide a convenient starting point to calculate electron transport though a molecular junction in which a molecule is coupled between two metal electrodes. The Hamiltonian of the system is written as $H = H_0 + V$, where $H_0$ is the Hamiltonian of uncoupled molecule and the two electrodes, and $V$ represents the coupling between the molecule and the electrodes. In the weak coupling limit, the $T$ operator is

$$T(E) = V + VG(E)V, \quad (10)$$

where $G(E) = \frac{1}{E - H + i\Gamma}$ is the Green function (see Lecture 6). The first term represents direct electron transport from the left electrode to the right electrode, which is small if electron transport through molecule dominates the total transport current. For a linear molecule consisting of $N$ bridge sites, we have

$$T_{lr}(E) = \langle l | V G(E) V | r \rangle = \langle l | V | 1 \rangle \langle 1 | G(E) | N \rangle \langle N | V | r \rangle. \quad (11)$$

Note that the $T$ operator in eqs. 10 and 11 is related to but different from $T_{ij}$ in the Landauer formula. in Eq. 9. They are related by the following identity (Homework)

$$\sum_{i,j} T_{ij}(E) = 4\pi^2 \sum_{l,r} T_{lr}^2 \delta(E - E_l)\delta(E - E_r). \quad (11)$$
At zero temperature, Eq. 9 can be written as (See reference 1)

\[ G(E) = \frac{2e^2}{h} \sum_{i,j} T_{ij}(E) = \Gamma_1^{(L)} \Gamma_N^{(R)} | G_{1N}(E_F) |^2. \]  (12)

\( G_{1N} \) in the above equation is a matrix element of the reduced Green’s function (the molecule),

\[ G(E) = \frac{1}{E - H_M + \Sigma_M(E)}, \]  (13)

where \( H_M \) is the Hamiltonian and \( \Sigma_M \) is the self energy of the molecule. Each of them is given as follows

\[ H_M = H_M^0 + V_B = \sum_{n} E_n | n > < n | + \sum_{n} \sum_{n'} V_{nn'} | n > < n'| \]  (14)

and

\[ \Sigma_{nn'}(E) = \delta_{nn'}(\delta_{n1} + \delta_{nN})[\Lambda_{n}(E) - (1/2)i\Gamma_{n}(E)], \]  (15)

where

\[ \Gamma_n(E) = 2\pi \sum_{l} |V_{ln}|^2 \delta(E_l - E) + 2\pi \sum_{r} |V_{rn}|^2 \delta(E_r - E) \]

\[ \equiv \Gamma_n^{(L)}(E) + \Gamma_n^{(R)}(E) \]  (16)

\[ \Lambda_{n}(E) = \frac{1}{2\pi} P \int_{-\infty}^{+\infty} dE' \frac{\Gamma_{n}(E')}{E - E'}. \]  (17)

\( \Gamma_n \) is the broadened line width of the molecular energy level due to the coupling between the molecule and the electrodes, and \( \Sigma \) is the associated shift in the energy level. In order to calculate the conductance of the molecular junction, we can use Eq. 12 together with Eq. 16 for \( \Gamma_n^{(L)} \) and \( \Gamma_n^{(R)} \) and Eq. 13 (with Eqs. 14-17) to determine \( G_{1N}(E_F) \). In many cases, we want to determine the current \( I \) as a function of applied bias voltage \( E \). This can be achieved using Eq. 8 instead of Eq. 12. If we use the tight binding model for the molecule, \( G_{1N} \) is given by
\[ G_{1N}(E) = \frac{1}{(E - E_1 + \Sigma_1(E))(E - E_N + \Sigma_N(E))} \prod_{j=2}^{N-1} \frac{V_{j,j+1}}{E - E_j}. \]  

(18)


**Homework**

8-1. Show \( \sum_{i,j} T_{ij}(E) = 4\pi^2 \sum_{l,r} |T_{lr}|^2 \delta(E - E_l)\delta(E - E_r) \).