Nanoscience MCC026, Quantum Transport Theory
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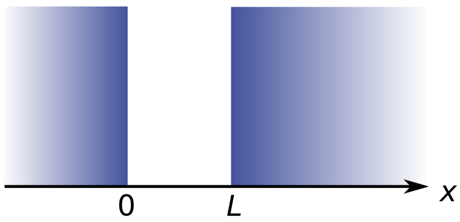
Exercise 1: Reminder 1 – Particle in a box



Consider a 1-dimensional box of length L with hard-wall boundary conditions. Solve the Schrödinger equation to find the energy eigenfunctions inside the box. Employing boundary conditions, find the possible values for k (and as a consequence for E).

Quantization in one or two spatial dimensions plays an important role in quantum transport. The quantized energies found here are examples for possible offset energies of energy bands for different propagating modes in a waveguide.

Exercise 2: Reminder 2 – Density of states

Consider a 1–,2–, or 3–dimensional conductor, characterized by dimensions L_x (and possibly L_y and L_z) and a volume V. The energy dispersion is given by

$$E = E_\mathrm{b} + \frac{\hbar^2|\boldsymbol{k}|^2}{2m} \tag{1}$$

Assume periodic boundary conditions, leading to quantized k-values as found in Exercise 1.

a.) Determine the space occupied by each $\boldsymbol{k}$-state and the volume of the Fermi sphere for the 1–,2–, or 3–dimensional conductor. This allows you to calculate the total number N of $\boldsymbol{k}$-states.

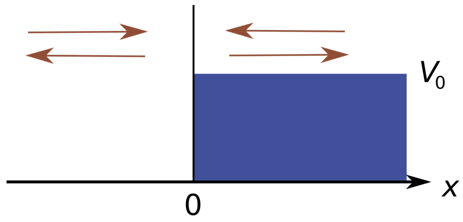
b.) Find the density of states per volume by dividing N by the respective volume and calculating the derivative with respect to energy.

Exercise 3: Scattering at a potential barrier

We consider a 1-dimensional potential landscape described by the potential

$$V(x) = V_0\theta(x) + v_0\delta(x) \tag{2}$$

with the Heaviside function $\theta(x)$ and the Dirac delta function $\delta(x)$. The explicit shape of this potential is required only for exercise c.).



a.) We take the (conveniently normalized) scattering states (transmitted and reflected) for a plane wave incoming from the left

$$\psi^1_E(x) = \begin{cases} \frac{1}{\sqrt{2\pi v}} \left[e^{ikx} + r_1(E)e^{-ikx}\right] & \text{for } x < 0 \\ \frac{1}{\sqrt{2\pi v'}} t_1(E)e^{ik'x} & \text{for } x > 0 \end{cases} \tag{3}$$

and for a plane wave incoming from the right

$$\psi^2_E(x) = \begin{cases} \frac{1}{\sqrt{2\pi v}} t_2(E)e^{-ikx} & \text{for } x < 0 \\ \frac{1}{\sqrt{2\pi v'}} \left[e^{-ik'x} + r_2(E)e^{ik'x}\right] & \text{for } x > 0 \end{cases} . \tag{4}$$

Calculate the probability currents (per energy E) on the left and on the right side of the potential associated to these states. Show what current conservation, $j_{\mathrm{L}}(E) = j_{\mathrm{R}}(E)$, requires for the relation between $R_1 = |r_1|^2, T_1 = |t_1|^2$ (respectively $R_2 = |r_2|^2, T_2 = |t_2|^2$).

b.) Now derive the full current expressions by writing down the integral over all energies (without actually solving it!!). Different incoming states are weighted by different Fermi functions! Using the fact that at equilibrium (electrochemical potentials $\mu_{\mathrm{L}} = \mu_{\mathrm{R}}$ and temperatures $T_{\mathrm{L}} = T_{\mathrm{R}}$) no current flows, $I_{\mathrm{L}} = I_{\mathrm{R}} = 0$, also determine the relations between T_1 and T_2 (respectively R_1 and R_2).

c.) Find the scattering states (transmitted and reflected) given above, explicitly. To do so, solve the Schrödinger equation and impose continuity of the wave function and its derivative at $x = 0$.

Also extract the transmission and reflection probabilities from the obtained results. With this, you can explicitly verify the relations between scattering amplitudes (or probabilities) found above.