Applied Quantum Mechanics

Homework #4, due Monday Feb 4, 2008

Problem 1: Read pp. 140-143 of the book.

Problem 2: (Levi , Problem 3.5) Calculate the transmission and reflection flux coefficient for an electron of energy E, moving from left to right, impinging normal to the plane of a semiconductor heterojunction potential barrier of energy V_0, where the effective electron mass on the left-hand side is m_1 and the effective electron mass on the right-hand side is m_2.
If the potential barrier energy is V_0=1.5eV and the ratio of effective electron mass on either side of heterointerface is m_1/m_2=3, at what particle energy is the transmission flux coefficient unity? What is the transmission flux coefficient in the limit that particle energy $E \rightarrow \infty$?

Hint: Use what you learned in problem 1!

Levi, pp. 140-143:

3.8.2 Scattering from a potential step when $m_1 \neq m_2$

In this case, we assume that m_j varies from region to region. At the boundary between regions 1 and 2 we require continuity in the wave function ψ and the derivative $(1/m_j) \cdot d\psi/dx$, so that

$$\psi_1|_{x_0} = \psi_2|_{x_0} \tag{3.98}$$

$$\frac{1}{m_1}\frac{d}{dx}\psi_1\bigg|_{x_0} = \frac{1}{m_2}\frac{d}{dx}\psi_2\bigg|_{x_0} \tag{3.99}$$

Inadequacies in our model force us to choose a boundary condition that ensures conservation of current $j_x \propto ep_x/m$ rather than $d\psi_1/dx|_{x_0} = d\psi_2/dx|_{x_0}$ (more accurate models satisfy both of these conditions).

These conditions and Eqn (3.81) and Eqn (3.82) give, for $x_0 = 0$,

$$A + B = C + D \tag{3.100}$$

$$A - B = \frac{m_1 k_2}{m_2 k_1} C - \frac{m_1 k_2}{m_2 k_1} D \tag{3.101}$$

If we know that the particle is incident from the left, then $A = 1$ and $D = 0$, giving

$$1 + B = C \tag{3.102}$$

$$1 - B = \frac{m_1 k_2}{m_2 k_1} C \tag{3.103}$$

We now solve for the transmission probability $|C|^2$ and the reflection probability $|B|^2$. The result is

$$|C|^2 = \frac{4}{\left(1 + \dfrac{m_1 k_2}{m_2 k_1}\right)^2} \tag{3.104}$$

$$|B|^2 = \frac{\left(1 - \dfrac{m_1 k_2}{m_2 k_1}\right)^2}{\left(1 + \dfrac{m_1 k_2}{m_2 k_1}\right)^2} \tag{3.105}$$

Compared with Eqn (3.96) and Eqn (3.97), the ratio m_1/m_2 appearing in Eqn (3.104) and Eqn (3.105) gives an extra degree of freedom in determining transmission and reflection probability. It is this extra degree of freedom that will allow us to engineer the transmission and reflection probability in device design. Having established this, we now proceed to calculate probability current density for an electron scattering from a potential step.

3.8.3 Probability current density for scattering at a step

Probability current density for transmission and reflection is different from transmission and reflection probability. We will be interested in calculating the incident current $\mathbf{J}_\mathrm{I}$, reflected current $\mathbf{J}_\mathrm{R}$, and transmitted current $\mathbf{J}_\mathrm{T}$, shown schematically in Fig. 3.10.

From our work in Section 3.8.2, the solution for the wave function will be of the form

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \tag{3.106}$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \tag{3.107}$$

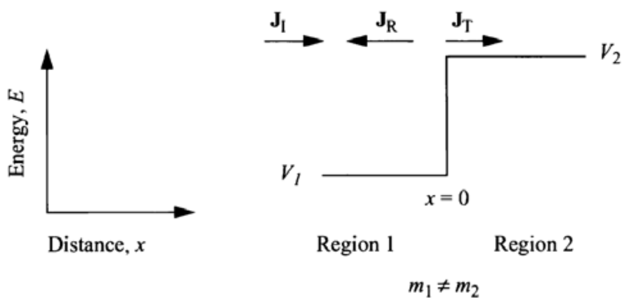

Fig. 3.10. Sketch of a one-dimensional, rectangular potential step. In region 1 the potential energy is V_1 and particle mass is m_1. In region 2 the potential energy is V_2 and particle mass is m_2. The transition between region 1 and region 2 occurs at position $x = x_{12}$. Incident probability current density $\mathbf{J}_\mathrm{I}$, reflected probability current density $\mathbf{J}_\mathrm{R}$, and transmitted probability current density $\mathbf{J}_\mathrm{T}$ are indicated.

For a particle incident from the left, we had $|A|^2 = 1, |D|^2 = 0$. Adopting the boundary conditions

$$\psi_1|_{x=0} = \psi_2|_{x=0} \tag{3.108}$$

$$\left.\frac{1}{m_1}\frac{d}{dx}\psi_1\right|_{x=0} = \left.\frac{1}{m_2}\frac{d}{dx}\psi_2\right|_{x=0} \tag{3.109}$$

gives reflection probability

$$|B|^2 = \frac{(1 - m_1 k_2/m_2 k_1)^2}{(1 + m_1 k_2/m_2 k_1)^2} \tag{3.110}$$

and transmission probability

$$|C|^2 = \frac{4}{(1 + m_1 k_2/m_2 k_1)^2} \tag{3.111}$$

We now calculate current using the current operator

$$\mathbf{J} = \frac{-ie\hbar}{2m}(\psi^* \nabla \psi - \psi \nabla \psi^*)$$

The incident current is

$$\mathbf{J}_\mathrm{I} = \frac{e\hbar k_1}{m_1}|A|^2 \tag{3.112}$$

The reflected current is

$$\mathbf{J}_\mathrm{R} = \frac{-e\hbar k_1}{m_1}|B|^2 \tag{3.113}$$

and the transmitted current is

$$\mathbf{J}_\mathrm{T} = \frac{e\hbar k_2}{m_2}|C|^2 \tag{3.114}$$

The reflection coefficient for the particle flux is

$$Refl = -\frac{\mathbf{J}_R}{\mathbf{J}_I} = \left|\frac{B}{A}\right|^2 = \left(\frac{(1 - m_1 k_2/m_2 k_1}{(1 + m_1 k_2/m_2 k_1)}\right)^2 \tag{3.115}$$

where the minus sign indicates current flowing in the negative x direction. This is the same as the reflection probability given by Eqn (3.105), because the ratio of velocity terms that contribute to particle flux is unity. The transmission coefficient for the particle flux is

$$Trans = \frac{\mathbf{J}_T}{\mathbf{J}_I} = \frac{m_1 k_2}{m_2 k_1}\left|\frac{C}{A}\right|^2 = \frac{4k_1 k_2/m_1 m_2}{\left(\frac{k_1}{m_1} + \frac{k_2}{m_2}\right)^2} = 1 - Refl \tag{3.116}$$

where we note that $Trans + Refl = 1$. The fact that $Trans + Refl = 1$ is expected since current conservation requires that the incident current must equal the sum of the transmitted and reflected current.

Impedance matching for unity transmission across a potential step

In this section we continue our discussion of particle scattering at the potential step shown schematically in Fig. 3.10. Suppose we want a flux transmission probability of unity for a particle of energy $E > V_2$ approaching the potential step from the left. Since momentum $p = \hbar k = mv$ we can identify velocity $v_j = \hbar k_j/m_j$ as the physically significant quantity in the expression for the transmission coefficient. Substituting v_j into Eqn (3.116) gives

$$Trans = \frac{m_1 k_2}{m_2 k_1}\left|\frac{C}{A}\right|^2 = \frac{m_1 k_2}{m_2 k_1}\frac{4}{(1 + v_2/v_1)^2} = \frac{v_2}{v_1}\frac{4}{(1 + v_2/v_1)^2} \tag{3.117}$$

If $Trans = 1$, then Eqn (3.117) can be rewritten

$$1 = \frac{v_2}{v_1}\frac{4}{(1 + v_2/v_1)^2} \tag{3.118}$$

which shows that unity transmission occurs when the velocity of the particle in the two regions is matched[2] in such a way that $v_2/v_1 = 1$. In microwave transmission line theory, this is called an impedance matching condition. To figure out when impedance matching occurs as a function of particle energy, we start with

$$\frac{v_2}{v_1} = \frac{m_1 k_2}{m_2 k_1} = \frac{m_1}{m_2}\cdot\left(\frac{2m_2\hbar^2(E - V_2)}{2m_1\hbar^2(E - V_1)}\right)^{1/2} = \left(\frac{m_1(E - V_2)}{m_2(E - V_1)}\right)^{1/2} \tag{3.119}$$

[2] J. F. Müller, A. F. J. Levi, and S. Schmitt-Rink, *Phys. Rev.* **B38**, 9843 (1988) and T. H. Chiu and A. F. J. Levi, *Appl. Phys. Lett.* **55**, 1891 (1989).

so that impedance matching ($v_2/v_1 = 1$) will occur when

$$\boxed{1 = \frac{m_1}{m_2} \cdot \frac{E - V_2}{E - V_1}} \tag{3.120}$$

or

$$\boxed{\frac{m_2}{m_1} = \frac{E - V_2}{E - V_1}} \tag{3.121}$$

Clearly, for an electron incident on the potential step with energy E, the value of E for which $Trans = 1$ depends upon the ratio of effective electron mass in the two regions and the difference in potential energy between the steps. To see what this means in practice, we now consider a specific example.

For a potential step of 1 eV we set $V_1 = 0$ eV and $V_2 = 1$ eV. We assume that the electron mass is such that $m_1 = 10 \times m_2$, so that the particle flux transmission coefficient $Trans = 1$ when

$$\frac{m_2}{m_1} = \frac{E - V_2}{E - V_1} = \frac{E - 1}{E} = \frac{1}{10} \tag{3.122}$$

Hence the particle energy when $Trans = 1$ is

$$E = \frac{10}{9} = 1.11 \text{ eV} \tag{3.123}$$

When $m_1 = 2 \times m_2$, the particle flux transmission coefficient $Trans = 1$ when

$$\frac{m_2}{m_1} = \frac{E - V_2}{E - V_1} = \frac{E - 1}{E} = \frac{1}{2} \tag{3.124}$$

so that the particle energy is $E = 2.00$ eV.

We can also calculate $Trans$ in the limit when energy E goes to infinity. In this case

$$v_2/v_1|_{E\to\infty} = \sqrt{\frac{m_1}{m_2}} \tag{3.125}$$

and

$$Trans|_{E\to\infty} = \lim_{E\to\infty} (v_2/v_1) \frac{4}{(1 + v_2/v_1)^2} \tag{3.126}$$

For the case $m_1/m_2 = 10$

$$Trans|_{E\to\infty} = (\sqrt{10}) \frac{4}{(1 + \sqrt{10})^2} = 0.73 \tag{3.127}$$

and when $m_1/m_2 = 2$ one finds

$$Trans|_{E\to\infty} = (\sqrt{2}) \frac{4}{(1 + \sqrt{2})^2} = 0.97 \tag{3.128}$$