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Physics

Physics at Nanoscale – IV

Perpendicular transport in single and multiple heterostructures

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Subject Name	Physics
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Table of Contents

4.5 Perpendicular transport in single and multiple heterostructures

4.5.1 Perpendicular transport in single heterostructures

For transport through the heterstructures, there are two situations: when the carrier energy is greater than or less than the conduction band minimum within the barrier region. These two conditions are shown in Figure 4.19. When the electron has energy greater than the potential barrier, it simply moves from one region into the other with no chance of reflection.

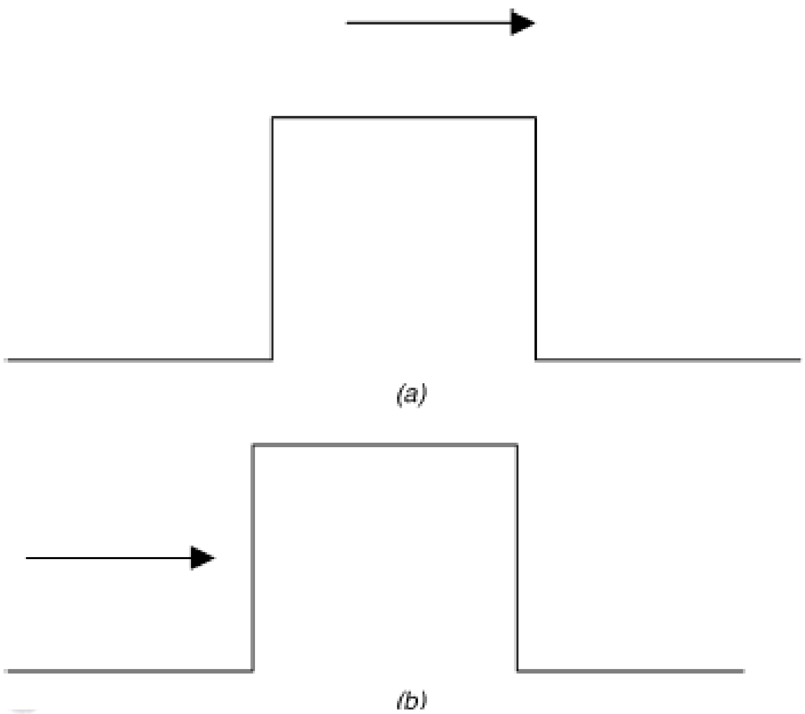

Figure 4.19 *The energy of the carriers with respect to height of the potential barrier for two separate cases: (a) carrier energy greater than the potential barrier height; (b) carrier energy less than the barrier height.*

However, if the electron energy is less than the potential barrier in the second region, the electron is reflected from the barrier back into the same layer. But the situation is different, when the problem is treated quantum mechanically. If the problem is treated classically i.e. when electrons suffer no reflection at the hetero interface. With this assumption, it is relatively straightforward to calculate the final electron state after crossing the interface. The electron energy should be conserved upon crossing the hetero barrier. The electron transmission at a potential energy step can be obtained quantitatively.

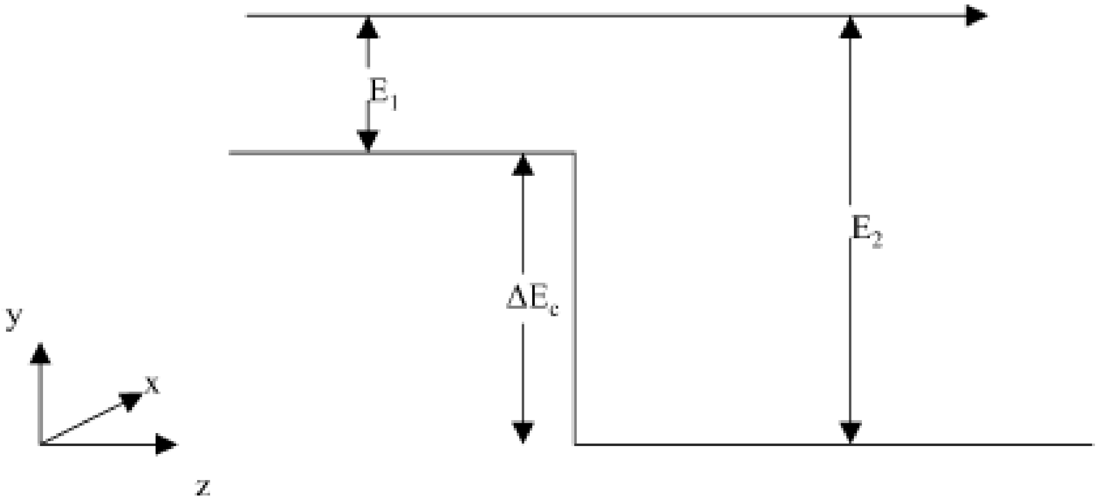

Figure 4.20 *Heterostructure system with a band offset of* ΔE_c *. The energy of the carriers in the left side (wide gap semiconductor) and right side (narrow gap semiconductor) of the heterostructure are* E_1 *and* E_2*, respectively.*

Assuming parabolic energy bands, the conservation of energy requirement demands that

$$E_2 = E_1 + \Delta E_c$$

$$\frac{\hbar^2 {k_2}^2}{2m_2} = \frac{\hbar^2 k^2}{2m_1} + \Delta E_c \qquad (4.48)$$

where k_2 and k_1 are k-vectors, and m_2 and m_1 are the effective masses of carriers in the narrow- and wide-gap semiconductor layers, respectively. If the z direction is direction perpendicular to the hetero structure, conservation of linear momentum leads to

$$k_{1x} = k_{2x} \qquad k_{1y} = k_{2y} \qquad (4.49)$$

Let us assume that the electron is confined completely to the x–z plane. Using Eqs. 4.49 and 4.48

$$\frac{\hbar^2}{2m_1}\left({k_{1x}}^2 + {k_{1z}}^2\right) + \Delta E_c = \frac{\hbar^2}{2m_2}\left({k_{1x}}^2 + {k_{2z}}^2\right) \qquad (4.50)$$

If the energy of the incident carriers is known, only unknown in Eq. 4.50 is k_{2z} which can be given by

$$k_{2z}{}^2 = \left[\frac{m_2}{m_1}\left(k_{1x}{}^2 + k_{1z}{}^2\right) - k_{1x}{}^2\right] + \frac{2m_2\Delta E_c}{\hbar^2} \qquad (4.51)$$

Hence, the final state of the electron in the narrow-gap semiconductor layer is given as

$$E_2 = E_1 + \Delta E_c$$

$$k_{2x} = k_{1x}$$

$$k_{2z} = \sqrt{\left[\frac{m_2}{m_1}\left(k_{1x}{}^2 + k_{1z}{}^2\right) - k_{1x}{}^2\right] + \frac{2m_2\Delta E_c}{I^2}} \qquad (4.52)$$

This formulation applies, if electrons are treated classically and is important in those cases where the carrier traverses a single potential barrier and reflective loss at the barrier is negligible. However, an electron is a quantum particle, so there is some probability that the electron will be reflected as well as transmitted. Whether the electron is incident from the wide-gap semiconductor into the narrow-gap semiconductor, or vice versa, there is a nonzero probability that it will undergo reflection at the hetero interface. It can be shown that when the mass is different between the two semiconductor layers, the transmission and reflection coefficients can be given by

$$T = \frac{4\left(\frac{k_{2z}}{k_{1z}}\right)\left(\frac{m_1}{m_2}\right)}{\left[1+\left(\frac{k_{2z}}{k_{1z}}\right)\left(\frac{m_1}{m_2}\right)\right]^2} \qquad (4.53)$$

$$R = \frac{\left[1-\left(\frac{k_{2z}}{k_{1z}}\right)\left(\frac{m_1}{m_2}\right)\right]^2}{\left[1+\left(\frac{k_{2z}}{k_{1z}}\right)\left(\frac{m_1}{m_2}\right)\right]^2} \qquad (4.54)$$

T and R in Eqs. 4.53 and 4.54 correspond to the transmission and reflection coefficients for particle flux at the hetero interface, respectively. In case where the electron is incident from the narrow-gap layer into the wide-gap layer so that the energy of electrons is less than the potential barrier height formed by the wide-gap semiconductor material, classically, the electron would be reflected at the interface, but the transmission of electrons into the other side of the potential barrier would be zero. However, quantum mechanically, there would be always a nonzero probability of the transmission of electrons into the other side of the barrier even when its energy is less than the barrier height due the phenomena known as *tunneling*. When the energy of the electrons is less than the potential barrier height, the transmission and reflection coefficients can be given by

$$T = \left[1 + \frac{V_0{}^2 sinh^2 k_2 b}{4E(v_0 - E)}\right]^{-1} \qquad R = \left[1 + \frac{4E(v_0 - E}{V_0{}^2 sinh^2 k_2 b}\right]^{-1} \qquad (4.55)$$

It is clear from above expressions that there is a nonzero probability of the electron being transmitted through the barrier when its energy is less than the barrier height. An interesting condition occurs when two barriers are used to enclose a small potential well, known as quantum well, as discussed before. When the energy of the electrons matches with the one of the quantized energy level in quantum well, the transmission coefficient approaches unity. This effect is known as *resonant tunneling*.

The results obtained above can be extended to the case of a repeated periodic potential by growing multiple quantum well along z-direction. Two different situations can again be considered, (i) when the carrier has energy greater than the potential barrier height, and (ii) when it has energy less than the potential barrier height. In both situation, the Schrodinger¨ equation can be solved throughout the structure with appropriate boundary conditions at each interface. The solution for the transmission coefficient of the entire system is then obtained using a transfer matrix approach. Let us we consider the case when the electron energies exceed the potential barrier in a multi quantum-well system.

The Schrodinger equation for a hetero structure in case where energy exceeds the potential barrier can be solved for the incident, transmitted, and reflected electron wave functions as

$$\psi_i = Ae^{i(k_{ix}+k_{iy})}$$

$$\psi_t = Be^{i(k_{tx}+k_{ty})} \qquad (4.56)$$

$$\psi_r = Ae^{i(k_{rx}+k_{ry})}$$

respectively, where A, B, and C are the amplitudes and x is the direction of propagation. The continuity of the wave function across the hetero interface implies that

$$\psi_i(o,y) + \psi_r(o,y) = \psi_t(o,y) \qquad (4.57)$$

Since the y components of each k vector are equal (i.e$k_{iy} = k_{1y} = k_{ry}$), Eq. 4.57 implies that

$$A + C = B \;\; \text{or} \qquad I + r = t \qquad (4.58)$$

where r = C/A is the reflectivity and t = B/A is the transmissivity. The probability current density normal to the interface, j_x is conserved, which yields

$$j_{ix} + j_{rx} = j_{tx} \qquad (4.59)$$

J_{ix},j_{tx},j_{rx} are given as

$$j_{ix} = \frac{I}{m_1} AA^* k_{ix}$$

$$j_{tx=} \frac{I}{m_2} BB^* k_{tx} \qquad (4.60)$$

$$j_{rx=} \frac{I}{m_1} CC^* k_{rx}$$

Substituting Eqs. 4.60 into Eq.4.59 and recognizing that k_{rx}= k_{ix} yields

$$\frac{m_1}{k_{ix}} \frac{k_{tx}}{m_2} t^2 + r^2 = 1 \qquad (4.61)$$

Combining Eqs. 4.58 and 4.61, the electron amplitude transmissivity becomes

$$t = \frac{2(\frac{m_2}{k_{tx}})}{\left(\frac{m_2}{k_{tx}}\right) + \left(\frac{m_1}{k_{ix}}\right)} \qquad (4.62)$$

And the electron reflectivity is

$$r = \frac{\left(\frac{m_2}{k_{tx}}\right) - \left(\frac{m_1}{k_{ix}}\right)}{\left(\frac{m_2}{k_{tx}}\right) - \left(\frac{m_1}{k_{ix}}\right)} \qquad (4.63)$$

recognizing that $k_{ix}=k_i\cos\theta_i$, $k_{tx}=k_t\cos\theta_t$. Eqs. 4.62 and 4.63 give for the transmission and reflection amplitudes,

$$t = \frac{2\sqrt{\frac{E}{m_1}}cos\theta_i}{\sqrt{\frac{E}{m_1}}cos\theta_i + \sqrt{\frac{E-V}{m_2}}cos\theta_t} \qquad (4.64)$$

$$r = \frac{\sqrt{E/m_1}cos\theta_i - \sqrt{\frac{E-V}{m_2}}cos\theta_t}{\sqrt{E/m_1}cos\theta_i + \sqrt{\frac{E-V}{m_2}}cos\theta_t} \qquad (4.65)$$

4.5.2 Perpendicular transport in multiple heterostructures

Using the results above one can now determine the transmission coefficient for a multi quantum-well stack under the condition that the incident electron energy is greater than the potential barrier height. If there are a system of M layers comprising a multi quantum-well structure, the solution can be obtained by solving the Schrodinger equation in each layer and matching the appropriate boundary conditions at the interface. The general expression for the probability amplitudes for the m layer in terms of the (m + 1)th layer is then given as

$$\begin{bmatrix}\Psi_{i,m}\\ \Psi_{r,m}\end{bmatrix} = \frac{1}{t_m}\begin{bmatrix}1 & r_m\\ r_m & 1\end{bmatrix}\begin{bmatrix}e^{ik_m d_m cos\theta_m} & 0\\ 0 & e^{-ik_m d_m cos\theta_m}\end{bmatrix} \qquad (4.66)$$

where t_m and r_m are the amplitude transmissivity and reflectivity at the m-1 and m interfaces as described by Eqs. 4.64 and 4.65, k_m is the magnitude of the electron wave vector in layer m, d_m is the thickness of layer m, and $\theta_m$is the angle of the wave vector direction in layer m. For the entire stack of M layers, the total normalized transmitted electron wave amplitude, $\psi_{t,M+1}$ the final region is M + 1 after the Mth stack), and the total normalized reflected electron wave amplitude, $\psi_{Rr,0}$ (in region 0), are obtained through chain multiplication of the total M + 1 versions of Eq. 4.66. The resultant expression is

$$\begin{bmatrix} 1 \\ \Psi_{r,0} \end{bmatrix} = \prod_{m=1}^{M} \frac{1}{t_m} \begin{bmatrix} 1 & r_m \\ r_m & 1 \end{bmatrix} \begin{bmatrix} e^{ik_m d_m cos\theta_m} & 0 \\ 0 & e^{-ik_m d_m cos\theta_m} \end{bmatrix} \times \frac{1}{t_{M+1}} \begin{bmatrix} 1 & r_{M+1} \\ r_{M+1} & 1 \end{bmatrix} \begin{bmatrix} \Psi_{t,M+1} \\ 0 \end{bmatrix} \quad (4.67)$$

This can be solved directly for amplitude transmissivity and reflectivity. Using Eq. 4.67, t is possible to calculate what the transmissivity of an electron at an arbitrary angle of incidence is on a multi quantum-well stack under the condition that the electron energy exceeds the potential barrier height. One can design multilayered hetero structure stacks, often referred to as *super-lattices*, such that the transmissivity can be maximized for certain electron energies. Alternatively, super lattice filter designs can be made that only pass electrons with certain specific incident energies, rejecting all others. These super lattice filters have direct analogy to thin-film optical interference filters. Therefore, many different super lattice structures can be made that mimic optical thin-film interference filters and perform for electrons functions similar to those performed for light.