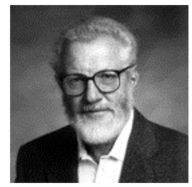
Handout 25

Semiconductor Heterostructures

In this lecture you will learn:

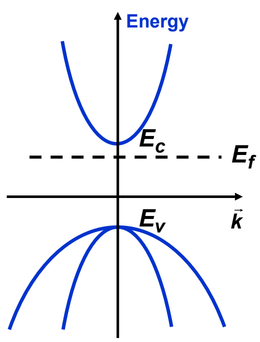
- Energy band diagrams in real space
- Semiconductor heterostructures and heterojunctions
- Electron affinity and work function
- Heterojunctions in equilibrium
- Electrons at Heterojunctions



Herbert Kroemer (1920-)
Nobel Prize 2000 for the Semiconductor Heterostructure Laser

Band Diagrams in Real Space - I

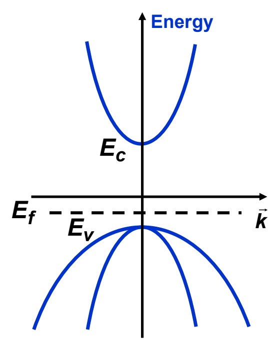
N-type semiconductor



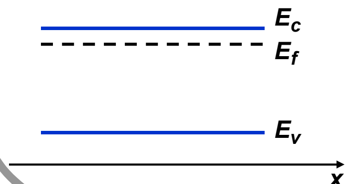
$$n = N_c \, e^{-(E_c - E_f)/KT}$$

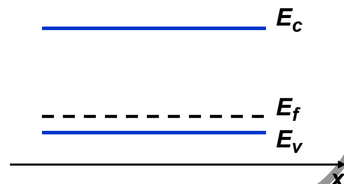
$$p = N_v \, e^{-(E_f - E_v)/KT}$$

P-type semiconductor



For devices, it is useful to draw the conduction and valence band edges in real space:





Band Diagrams in Real Space - II

Electrostatic potential and electric field:

An electrostatic potential (and an electric field) can be present in a crystal:

$$\phi(\vec{r}) \qquad \text{and} \qquad \vec{E}(\vec{r}) = -\nabla\phi(\vec{r})$$

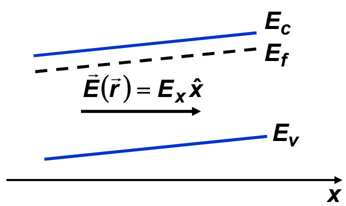
The total energy of an electron in a crystal is then given not just by the energy band dispersion $E_n(\vec{k})$ but also includes the potential energy coming from the potential:

$$E_n(\vec{k}) \rightarrow E_n(\vec{k}) - e\phi(\vec{r})$$

Therefore, the conduction and valence band edges also become position dependent:

$$E_c \rightarrow E_c - e\phi(\vec{r}) \qquad\qquad E_v \rightarrow E_v - e\phi(\vec{r})$$

Example: Uniform x-directed electric field

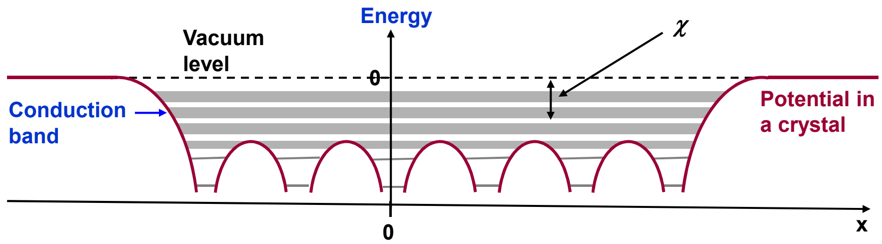


$$\vec{E}(\vec{r}) = E_x\hat{x}$$
$$\phi(\vec{r}) = \phi(x=0) - E_x x$$
$$E_c(x) = E_c(x=0) + eE_x x$$

N-type semiconductor

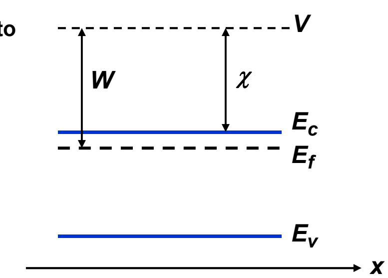
Electron Affinity and Work Function

Electron affinity "χ" is the energy required to remove an electron from the bottom of the conduction band to outside the crystal, i.e. to the vacuum level



Work function "W" is the energy required to remove an electron from the Fermi level to the vacuum level

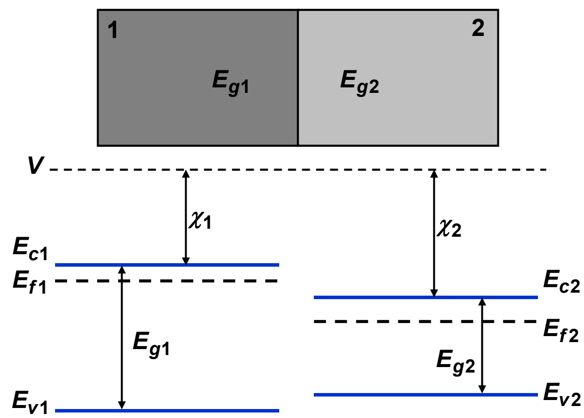
• Work function changes with doping but affinity is a constant for a given material



Semiconductor N-N Heterostructure: Electron Affinity Rule

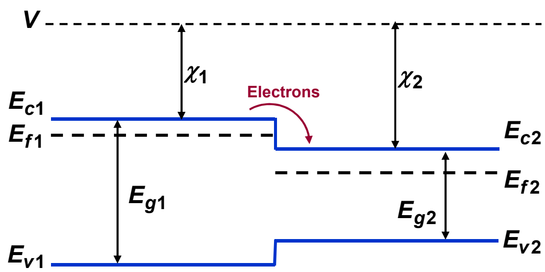
Heterostructure: A semiconductor structure in which more than one semiconductor material is used and the structure contains interfaces or junctions between two different semiconductors

Consider the following heterostructure interface between a wide bandgap and a narrow bandgap semiconductor (both n-type):



The **electron affinity rule** tells how the energy band edges of the two semiconductors line up at a hetero-interface

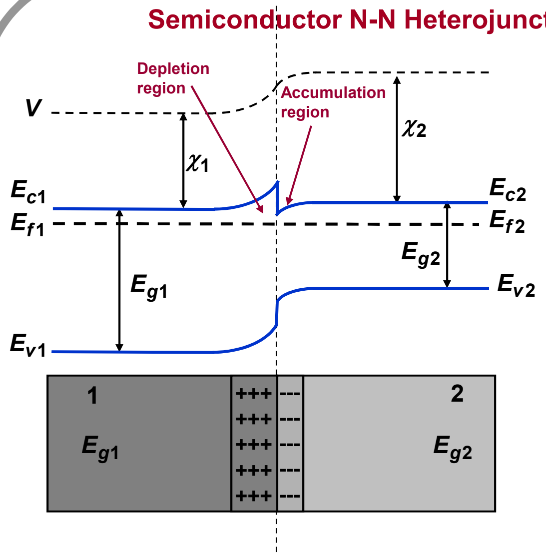
Semiconductor N-N Heterojunction



Something is wrong here: the Fermi level (the chemical potential) has to be the same everywhere in equilibrium (i.e. a flat line)

• Once a junction is made, electrons will flow from the side with higher Fermi level (1) to the side with lower Fermi level (2)

Semiconductor N-N Heterojunction: Equilibrium

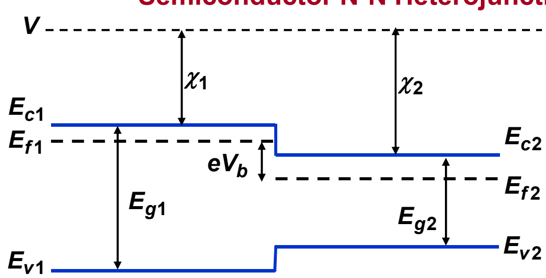


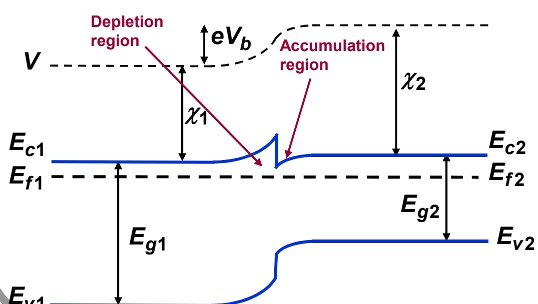
- Electrons will flow from the side with higher Fermi level (1) to the side with lower Fermi level (2)
- Electron flow away from semiconductor (1) will result in a region at the interface which is depleted of electrons (depletion region). Because of positively charged donor atoms, the depletion region has net positive charge density
- Electron flow into semiconductor (2) will result in a region at the interface which has an accumulation of electrons (accumulation region). The accumulation region has net negative charge density

Note: the vacuum level follows the electrostatic potential:

$$V(x) = V(x=0) - e\,[\,\phi(x) - \phi(x=0)\,]$$

Semiconductor N-N Heterojunction: Equilibrium

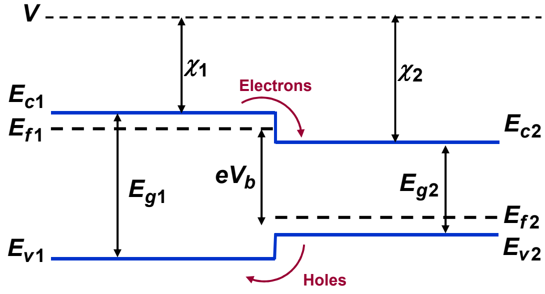




- Electron flow from semiconductor (1) to semiconductor (2) continues until the electric field due to the formation of depletion and accumulation regions becomes so large that the Fermi levels on both sides become the same
- In equilibrium, because of the electric field at the interface, there is a potential difference between the two sides – called the built-in voltage
- The built-in voltage is related to the difference in the Fermi levels before the equilibrium was established:

$$eV_b = E_{f1} - E_{f2}$$

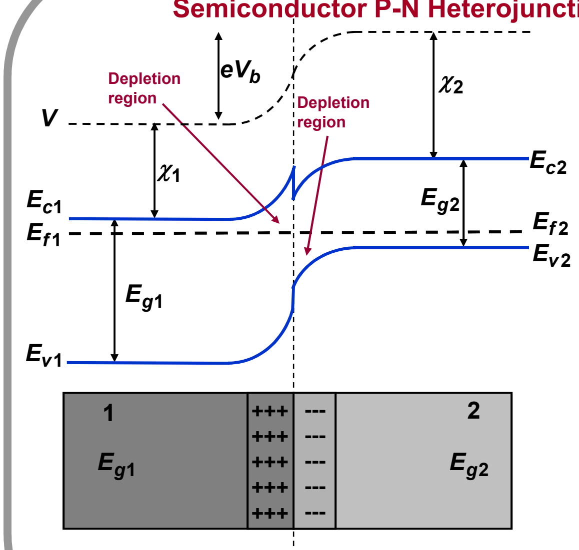
Semiconductor P-N Heterojunction



Once a junction is made:

- Electrons will flow from the side with higher Fermi level (1) to the side with lower Fermi level (2)
- Holes will flow from the side with lower Fermi level (2) to the side with higher Fermi level (1)

Semiconductor P-N Heterojunction: Equilibrium

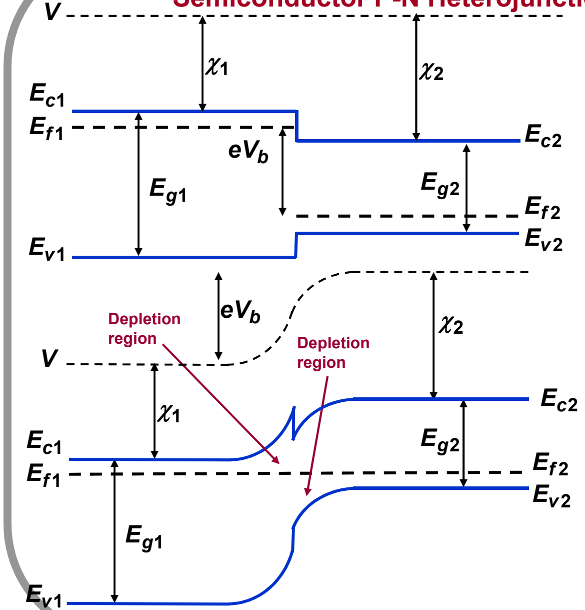


- Electron flow away from semiconductor (1) will result in a region at the interface which is depleted of electrons (depletion region). Because of positively charged donor atoms, the depletion region has net positive charge density
- Hole flow away from semiconductor (2) will result in a region at the interface which is depleted of holes (depletion region). Because of negatively charged acceptor atoms, the depletion region has net negative charge density

Note: the vacuum level follows the electrostatic potential:

$$V(x) = V(x=0) - e\,[\,\phi(x) - \phi(x=0)\,]$$

Semiconductor P-N Heterojunction: Equilibrium



- Electron flow from semiconductor (1) to semiconductor (2) and hole flow from semiconductor (2) to semiconductor (1) continues until the electric field due to the formation of depletion regions becomes so large that the Fermi levels on both sides become the same

- The built-in voltage is related to the difference in the Fermi levels before the equilibrium was established:

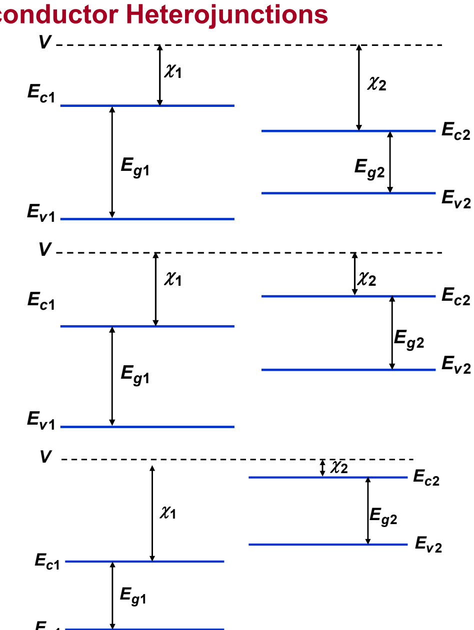
$$eV_b = E_{f1} - E_{f2}$$

Types of Semiconductor Heterojunctions

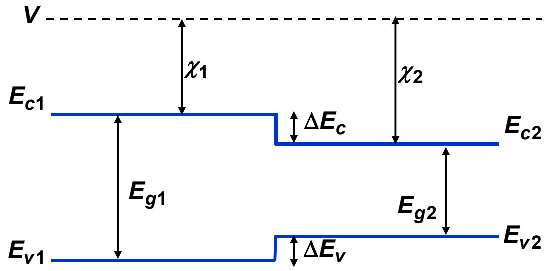
Type-I: Straddling gap

Type-II: Staggered gap

Type-III: Broken gap



Band Offsets in Heterojunctions

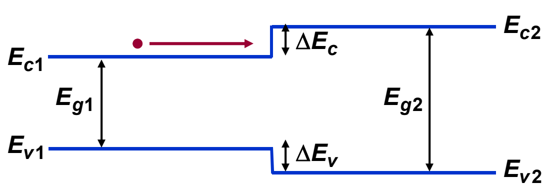


The conduction and valence band offsets are determined as follows:

$$\Delta E_c = \chi_2 - \chi_1$$

$$\Delta E_v = \Delta E_g - \Delta E_c = (E_{g1} - E_{g2}) - \Delta E_c$$

Electrons at Heterojunctions



Question: What happens to the electron that approaches the interface (as shown)? How does it see the band offset? Does it bounce back? Does it go on the under side?

The **effective mass equation** can be used to answer all the above questions

In semiconductor 1:

$$\psi_1(\vec{r}) = \phi_1(\vec{r})\ \psi_{c1,\vec{k}_o}(\vec{r})$$

$$\left[\hat{E}_{c1}(\vec{k}_o - i\nabla) + U(\vec{r})\right]\phi_1(\vec{r}) = E\ \phi_1(\vec{r})$$

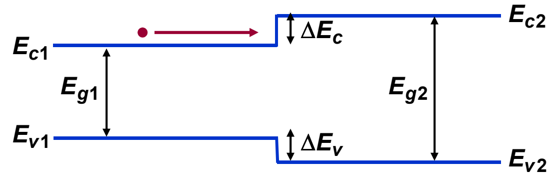
In semiconductor 2:

$$\psi_2(\vec{r}) = \phi_2(\vec{r})\ \psi_{c2,\vec{k}_o}(\vec{r})$$

$$\left[\hat{E}_{c2}(\vec{k}_o - i\nabla) + U(\vec{r})\right]\phi_2(\vec{r}) = E\ \phi_2(\vec{r})$$

Electrons at Heterojunctions; Effect of Band Offsets

$U(\vec{r}) = 0$



Assume for the electron in the conduction band of semiconductor 1:

$$E_{c1}(\vec{k}) = E_{c1} + \frac{\hbar^2 k^2}{2m_{e1}} \qquad \psi_1(\vec{r}) = \phi_1(\vec{r})\ \psi_{c1,\vec{k}_o=0}(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m_{e1}}\nabla^2 + E_{c1} \right] \phi_1(\vec{r}) = E\ \phi_1(\vec{r})$$

And for the electron in semiconductor 2:

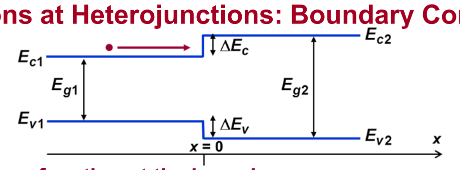
$$E_{c2}(\vec{k}) = E_{c2} + \frac{\hbar^2 k^2}{2m_{e2}} \qquad \psi_2(\vec{r}) = \phi_2(\vec{r})\ \psi_{c2,\vec{k}_o=0}(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m_{e2}}\nabla^2 + E_{c2} \right] \phi_2(\vec{r}) = E\ \phi_2(\vec{r})$$

Notice that the conduction band edge energy (i.e. E_{c1} or E_{c2}) appears as a constant potential in the effective mass Schrodinger equation

Conduction band offset at the heterojunction therefore appears like a potential step to the electron

Electrons at Heterojunctions: Boundary Conditions



(1) Continuity of the wavefunction at the boundary:

$$\psi_1(\vec{r})\big|_{x=0} = \psi_2(\vec{r})\big|_{x=0}$$

If one assumes: $\psi_{c1,\vec{k}_o}(\vec{r}) \approx \psi_{c2,\vec{k}_o}(\vec{r})$ $\Rightarrow$ $\phi_1(\vec{r})\big|_{x=0} = \phi_2(\vec{r})\big|_{x=0}$

(2) Continuity of the normal component of the probability current at the boundary:

In text book quantum mechanics the probability current is defined as:

$$\vec{J}(\vec{r}) = \psi^*(\vec{r})\frac{\hbar}{2im}\nabla\psi(\vec{r}) + c.c. = \psi^*(\vec{r})\frac{\hbar}{2im}\nabla\psi(\vec{r}) - \psi(\vec{r})\frac{\hbar}{2im}\nabla\psi^*(\vec{r})$$

Or in shorter component notation:

$$J_\alpha(\vec{r}) = \psi^*(\vec{r})\frac{\hbar}{2im}\partial_\alpha\psi(\vec{r}) + c.c.$$

Probability current is always continuous across a boundary

We need an expression for the probability current in terms of the envelope function

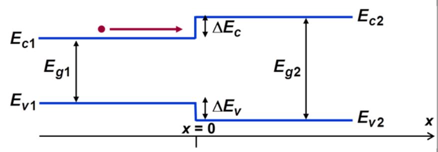
Electrons at Heterojunctions: Boundary Conditions

Probability Current: In a material with energy band dispersion given by:

$$E_n(\vec{k}) = E_n + \frac{\hbar^2}{2}(\vec{k}-\vec{k}_o).M^{-1}.(\vec{k}-\vec{k}_o) = E_n + \sum_{\alpha,\beta} \frac{\hbar^2}{2m_{\alpha\beta}}(k_\alpha - k_{o\alpha})(k_\beta - k_{o\beta})$$

The expression for the electron probability current (in terms of the envelope function) is:

$$J_\alpha(\vec{r}) = \sum_\beta \phi^*(\vec{r}) \frac{\hbar}{2im_{\alpha\beta}} \partial_\beta \phi(\vec{r}) + c.c.$$



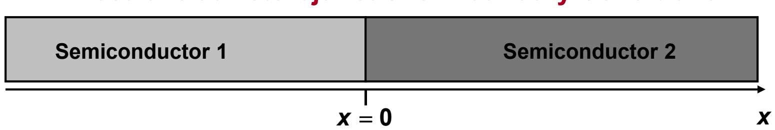
Continuity of the probability current:

The continuity of the normal component of the probability current across a heterojunction gives another boundary condition for the envelope function:

$$\sum_\beta \frac{1}{m_{x\beta 1}} \partial_\beta \phi_1(\vec{r})\Big|_{x=0} = \sum_\beta \frac{1}{m_{x\beta 2}} \partial_\beta \phi_2(\vec{r})\Big|_{x=0}$$

For: $M^{-1} = \begin{bmatrix} 1/m_{xx} & & \\ & 1/m_{yy} & \\ & & 1/m_{zz} \end{bmatrix} \Longrightarrow \frac{1}{m_{xx1}} \frac{\partial \phi_1(\vec{r})}{\partial x}\Big|_{x=0} = \frac{1}{m_{xx2}} \frac{\partial \phi_2(\vec{r})}{\partial x}\Big|_{x=0}$

Electrons at Heterojunctions: Boundary Conditions



(1) Continuity of the envelope function at the boundary:

$$\phi_1(\vec{r})\big|_{x=0} = \phi_2(\vec{r})\big|_{x=0}$$

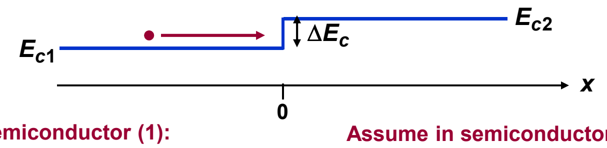
(2) Continuity of the normal component of the probability current at the boundary:

$$\sum_\beta \frac{1}{m_{x\beta 1}} \partial_\beta \phi_1(\vec{r})\Big|_{x=0} = \sum_\beta \frac{1}{m_{x\beta 2}} \partial_\beta \phi_2(\vec{r})\Big|_{x=0}$$

If in both the materials the inverse effective mass matrix is diagonal then this boundary condition becomes:

$$M^{-1} = \begin{bmatrix} 1/m_{xx} & & \\ & 1/m_{yy} & \\ & & 1/m_{zz} \end{bmatrix} \Longrightarrow \frac{1}{m_{xx1}} \frac{\partial \phi_1(\vec{r})}{\partial x}\Big|_{x=0} = \frac{1}{m_{xx2}} \frac{\partial \phi_2(\vec{r})}{\partial x}\Big|_{x=0}$$

The Effective Mass Theory for Heterojunctions



Assume in semiconductor (1):

$$\vec{k}_o = 0$$

$$E_{c1}(\vec{k}) = E_{c1} + \frac{\hbar^2 k_x^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_{y1}} + \frac{\hbar^2 k_z^2}{2m_{z1}}$$

Assume in semiconductor (2):

$$\vec{k}_o = 0$$

$$E_{c2}(\vec{k}) = E_{c2} + \frac{\hbar^2 k_x^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_{y2}} + \frac{\hbar^2 k_z^2}{2m_{z2}}$$

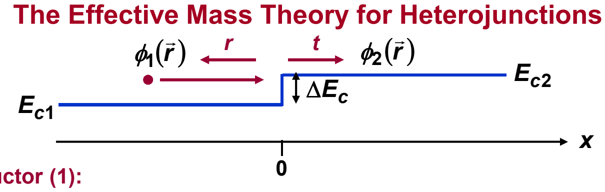
In semiconductor (1):

$$\left[\hat{E}_{c1}(\vec{k}_o - i\nabla) + U(\vec{r})\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\Rightarrow \left[\hat{E}_{c1}(-i\nabla)\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m_{x1}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{y1}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{z1}}\frac{\partial^2}{\partial z^2} + E_{c1}\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

The Effective Mass Theory for Heterojunctions



In semiconductor (1):

$$\left[-\frac{\hbar^2}{2m_{x1}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{y1}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{z1}}\frac{\partial^2}{\partial z^2} + E_{c1}\right]\phi_1(\vec{r}) = E\,\phi_1(\vec{r})$$

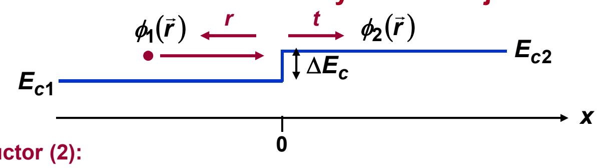
Assume a plane wave solution: $\phi_1(\vec{r}) = e^{i(k_{x1}x + k_y y + k_z z)}$

Plug it in to get: $E = E_{c1} + \frac{\hbar^2 k_{x1}^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_{y1}} + \frac{\hbar^2 k_z^2}{2m_{z1}}$ → **A plane wave solution works**

We expect a reflected wave also so we write the total solution in semiconductor (1) as:

$$\phi_1(\vec{r}) = e^{i(k_{x1}x + k_y y + k_z z)} + r\,e^{i(-k_{x1}x + k_y y + k_z z)}$$

The Effective Mass Theory for Heterojunctions



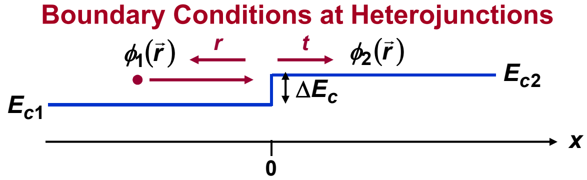
In semiconductor (2):

$$\left[-\frac{\hbar^2}{2m_{x2}}\frac{\partial^2}{\partial x^2}-\frac{\hbar^2}{2m_{y2}}\frac{\partial^2}{\partial y^2}-\frac{\hbar^2}{2m_{z2}}\frac{\partial^2}{\partial z^2}+E_{c2}\right]\phi_2(\vec{r})=E\,\phi_2(\vec{r})$$

Assume a plane wave solution: $\phi_2(\vec{r})=t\,e^{i\left(k_{x2}x+k_y y+k_z z\right)}$

Plug it in to get: $E=E_{c2}+\frac{\hbar^2k_{x2}^2}{2m_{x2}}+\frac{\hbar^2k_y^2}{2m_{y2}}+\frac{\hbar^2k_z^2}{2m_{z2}}$ ⟶ A plane wave solution works here also

Boundary Conditions at Heterojunctions



$\phi_1(\vec{r})=e^{i\left(k_{x1}x+k_y y+k_z z\right)}+r\,e^{i\left(-k_{x1}x+k_y y+k_z z\right)}$ ⟶ $E=E_{c1}+\frac{\hbar^2k_{x1}^2}{2m_{x1}}+\frac{\hbar^2k_y^2}{2m_{y1}}+\frac{\hbar^2k_z^2}{2m_{z1}}$

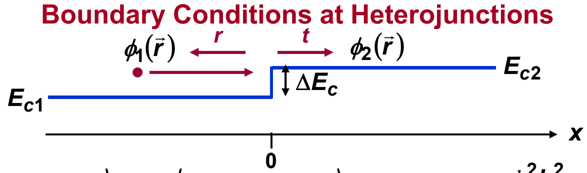
$\phi_2(\vec{r})=t\,e^{i\left(k_{x2}x+k_y y+k_z z\right)}$ ⟶ $E=E_{c2}+\frac{\hbar^2k_{x2}^2}{2m_{x2}}+\frac{\hbar^2k_y^2}{2m_{y2}}+\frac{\hbar^2k_z^2}{2m_{z2}}$

(1) Envelope functions must be continuous at the interface:

$$\phi_1(x=0)=\phi_2(x=0)$$
$$\Rightarrow e^{i\left(k_y y+k_z z\right)}+r\,e^{i\left(k_y y+k_z z\right)}=t\,e^{i\left(k_y y+k_z z\right)}$$
$$\Rightarrow 1+r=t$$

Note that this boundary condition can only be satisfied if the components of the wavevector parallel to the interface are the same on both sides

Boundary Conditions at Heterojunctions



$$\phi_1(\vec{r}) = e^{i(k_{x1}x + k_y y + k_z z)} + r\, e^{i(-k_{x1}x + k_y y + k_z z)} \longrightarrow E = E_{c1} + \frac{\hbar^2 k_{x1}^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_{y1}} + \frac{\hbar^2 k_z^2}{2m_{z1}}$$

$$\phi_2(\vec{r}) = t\, e^{i(k_{x2}x + k_y y + k_z z)} \longrightarrow E = E_{c2} + \frac{\hbar^2 k_{x2}^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_{y2}} + \frac{\hbar^2 k_z^2}{2m_{z2}}$$

Energy conservation:

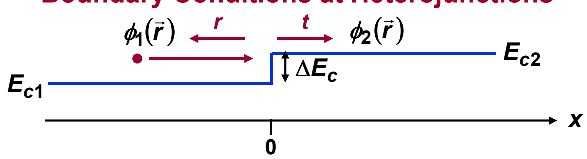
$$E = E_{c1} + \frac{\hbar^2 k_{x1}^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_{y1}} + \frac{\hbar^2 k_z^2}{2m_{z1}} = E_{c2} + \frac{\hbar^2 k_{x2}^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_{y2}} + \frac{\hbar^2 k_z^2}{2m_{z2}}$$

$$\Rightarrow \frac{\hbar^2 k_{x2}^2}{2m_{x2}} = \frac{\hbar^2 k_{x1}^2}{2m_{x1}} - \Delta E_c - \frac{\hbar^2 k_y^2}{2}\left(\frac{1}{m_{y2}} - \frac{1}{m_{y1}}\right) - \frac{\hbar^2 k_z^2}{2}\left(\frac{1}{m_{z2}} - \frac{1}{m_{z1}}\right)$$

$$\Rightarrow \frac{\hbar^2 k_{x2}^2}{2m_{x2}} = \frac{\hbar^2 k_{x1}^2}{2m_{x1}} - \Delta V_{eff}(k_y, k_z)$$

Note that the effective barrier height depends on the band offset as well as the parallel components of the wavevector

Boundary Conditions at Heterojunctions



$$\phi_1(\vec{r}) = e^{i(k_{x1}x + k_y y + k_z z)} + r\, e^{i(-k_{x1}x + k_y y + k_z z)} \longrightarrow E = E_{c1} + \frac{\hbar^2 k_{x1}^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_{y1}} + \frac{\hbar^2 k_z^2}{2m_{z1}}$$

$$\phi_2(\vec{r}) = t\, e^{i(k_{x2}x + k_y y + k_z z)} \longrightarrow E = E_{c2} + \frac{\hbar^2 k_{x2}^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_{y2}} + \frac{\hbar^2 k_z^2}{2m_{z2}}$$

(2) Probability current must be continuous at the interface:

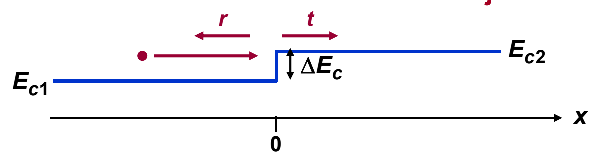
$$\frac{1}{m_{x1}} \left.\frac{\partial \phi_1}{\partial x}\right|_{x=0} = \frac{1}{m_{x2}} \left.\frac{\partial \phi_2}{\partial x}\right|_{x=0} \longrightarrow$$

Conservation of probability current at the interface

$$\Rightarrow \frac{ik_{x1}}{m_{x1}}\left(e^{i(k_y y + k_z z)} - r\, e^{i(k_y y + k_z z)}\right) = \frac{ik_{x2}}{m_{x2}}\, t\, e^{i(k_y y + k_z z)}$$

$$\Rightarrow \frac{k_{x1}}{m_{x1}}(1 - r) = \frac{k_{x2}}{m_{x2}}\, t$$

Transmission and Reflection at Heterojunctions



We have two equations in two unknowns:

$$1 + r = t \qquad \frac{k_{x1}}{m_{x1}}(1 - r) = \frac{k_{x2}}{m_{x2}} t$$

The solution is:

$$t = \frac{2}{1 + m_{x1}k_{x2} / m_{x2}k_{x1}} \qquad r = \frac{1 - m_{x1}k_{x2} / m_{x2}k_{x1}}{1 + m_{x1}k_{x2} / m_{x2}k_{x1}}$$

Where:

$$\frac{\hbar^2 k_{x2}^2}{2m_{x2}} = \frac{\hbar^2 k_{x1}^2}{2m_{x1}} - \Delta V_{eff}(k_y, k_z)$$

Special case: If the RHS in the above equation is negative, then k_{x2} becomes imaginary and the wavefunction decays exponentially for x>0 (in semiconductor 2). In this case:

$$|r| = 1$$

and the electron is completely reflected from the hetero-interface