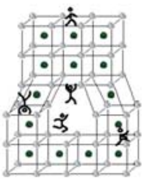
The Quantum World



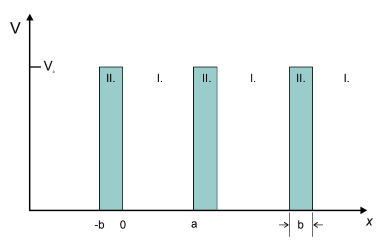
- Four Important Solutions to the Schrödinger Equation
  - Free Electrons
  - Electron in a Well
  - Tunneling
  - The Kronig-Penny Model

Monday, Oct. 27, 2003

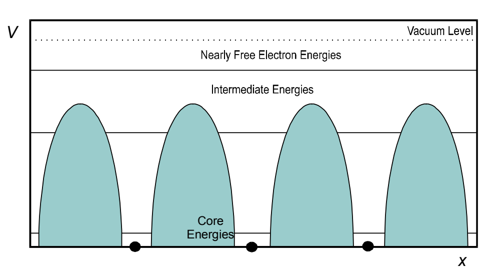
MATS275: INTRODUCTION TO MATERIALS SCIENCE

Case IV: Electrons in a Periodic Potential (the Solid State)

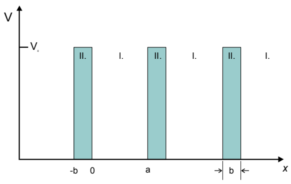
"Muffin Tin Approximation" (Kronig-Penney Model)



Actual Atomic Potential in 1D



Back to the Muffin Tin



- Region I

$$\frac{d^2\psi_I}{dx^2}+\frac{2m}{\hbar^2}E\psi_I=0$$

- Region II

$$\frac{d^2\psi_{II}}{dx^2}+\frac{2m}{\hbar^2}(E-V_0)\psi_{II}=0$$

Bloch Waves

- Bloch showed that the Schrödinger equation for a periodic potential must have solutions of the form:

$$\psi(x)=u(x)e^{ikx}$$

Using Bloch Waves

$$\psi(x)=u(x)e^{ikx}$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+(E-U)\psi=0$$

$$\frac{d\psi}{dx}=\frac{du}{dx}e^{ikx}+iku(x)e^{ikx}$$

$$\frac{d^2\psi}{dx^2}=\frac{d^2u}{dx^2}e^{ikx}+ik\frac{du}{dx}e^{ikx}+ik\frac{du}{dx}e^{ikx}-k^2u(x)e^{ikx}$$

$$=\left(\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-k^2u(x)\right)e^{ikx}$$

Region I - V = 0

(0<x<a)

I

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi$$

$$=\left[\left(\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-k^2u(x)\right)e^{ikx}\right]+\frac{2m}{\hbar^2}E\left[u(x)e^{ikx}\right]$$

$$=\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-k^2u(x)+\frac{2mE}{\hbar^2}u(x)\right]e^{ikx}$$

$$\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(k^2-\alpha^2\right)u(x)\right]=0 \qquad \alpha^2\equiv\frac{2mE}{\hbar^2}$$

Region II – V=V

(-b<x<0)

II

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi$$

$$=\left[\left(\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-k^2u(x)\right)e^{ikx}\right]+\frac{2m}{\hbar^2}(E-V)\left[u(x)e^{ikx}\right]$$

$$=\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-k^2u(x)+\frac{2m(E-V)}{\hbar^2}u(x)\right]e^{ikx}$$

$$\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(k^2+\gamma^2\right)u(x)\right]=0 \qquad \gamma^2\equiv\frac{2m(V-E)}{\hbar^2}$$

Solving the Equations

I

$$\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(k^2-\alpha^2\right)u(x)\right]=0$$

II

$$\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(k^2+\gamma^2\right)u(x)\right]=0$$

Solutions…

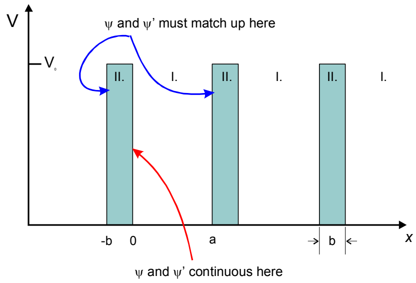
$$\psi_I=e^{-ikx}\left(Ae^{-i\alpha x}+Be^{i\alpha x}\right)$$

$$\psi_I'=-ike^{-ikx}\left(Ae^{-i\alpha x}+Be^{i\alpha x}\right)-i\alpha e^{ikx}\left(Ae^{-i\alpha x}-Be^{i\alpha x}\right)$$

$$\psi_{II}=e^{-ikx}\left(Ce^{\gamma x}+De^{-\gamma x}\right)$$

$$\psi_{II}'=-ike^{-ikx}\left(Ce^{\gamma x}+De^{-\gamma x}\right)+\gamma e^{-ikx}\left(Ce^{\gamma x}-De^{-\gamma x}\right)$$

Boundary Conditions



Setting Boundaries

$$\psi_I(0) = Ae^{-i\alpha 0} + Be^{i\alpha 0} = A + B$$

$$\psi_{II}(0) = Ce^{-i\gamma 0} + De^{i\gamma 0} = C + D$$

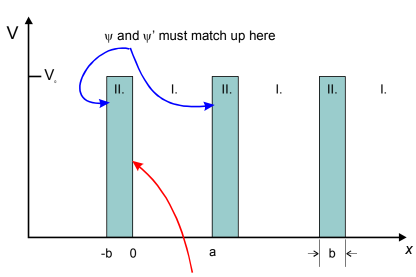
$$A + B = C + D$$

$$\psi'_I(0) = -ike^{-ik0}\left(Ae^{-i\alpha 0} + Be^{i\alpha 0}\right) - i\alpha e^{ik0}\left(Ae^{-i\alpha 0} - Be^{i\alpha 0}\right)$$
$$= (-ik - i\alpha)A + (-ik + i\alpha)B = -ik(A+B) - i\alpha(A-B)$$

$$\psi'_{II}(0) = -ike^{-ik0}\left(Ce^{\gamma 0} + De^{-\gamma 0}\right) + \gamma e^{-ik0}\left(Ce^{\gamma 0} - De^{-\gamma 0}\right)$$
$$= (-ik + \gamma)C + (-ik - \gamma)D = -ik(C+D) + \gamma(C-D)$$

$$i\alpha A - i\alpha B = \gamma C - \gamma D$$

Boundary Conditions



Setting Boundaries

$$\psi_I(a) = e^{-ika}\left(Ae^{-i\alpha a} + Be^{i\alpha a}\right)$$

$$\psi_{II}(-b) = e^{ikb}\left(Ce^{-\gamma b} + De^{\gamma b}\right)$$

$$Ae^{-i\alpha a} + Be^{i\alpha a} = \left(Ce^{-\gamma b} + De^{\gamma b}\right)e^{ik(a+b)}$$

$$\psi'_I(a) = -ike^{-ika}\left(Ae^{-i\alpha a} + Be^{i\alpha a}\right) - i\alpha e^{-ika}\left(Ae^{-i\alpha a} - Be^{i\alpha a}\right)$$

$$\psi'_{II}(-b) = -ike^{ikb}\left(Ce^{-\gamma b} + De^{\gamma b}\right) + \gamma e^{ikb}\left(Ce^{-\gamma b} - De^{\gamma b}\right)$$

$$(k+\alpha)Ae^{-i\alpha a} + (k-\alpha)Be^{i\alpha a} = \left[(k-i\gamma)Ce^{-\gamma b} + (k+i\gamma)De^{\gamma b}\right]e^{ik(a+b)}$$

Solving the Boundaries

- Using a bit of linear algebra, we can get the solution:

$$\frac{\gamma^2-\alpha^2}{2\gamma\alpha}\sin(\alpha a)\sinh(\gamma b) + \cos(\alpha a)\cosh(\gamma b) = \cos[k(a+b)]$$

Take b to 0, V_0 to ∞

$$\cosh(\gamma b) \Rightarrow 1 \qquad \alpha^2 << \gamma^2$$

$$\sinh(\gamma b) \Rightarrow \gamma b \qquad b << a$$

Solving the Boundaries

- Applying the limits

$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\sinh(\gamma b)\sin(\alpha a) + \cosh(\gamma b)\cos(\alpha a) = \cos(ka + kb)$$

$$\gamma^2 - \alpha^2 \Rightarrow \frac{2mV_0}{\hbar^2}$$

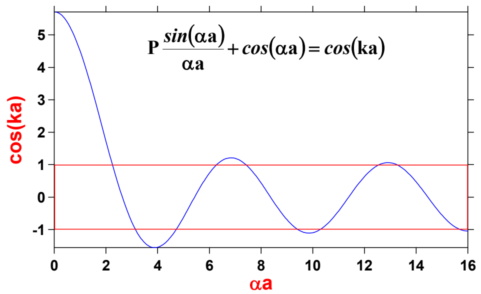
$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\gamma b\sin(\alpha a) + \cos(\alpha a) = \cos(ka)$$

$$\frac{mV_0 b}{\hbar^2\alpha}\sin(\alpha a) + \cos(\alpha a) = \cos(ka)$$

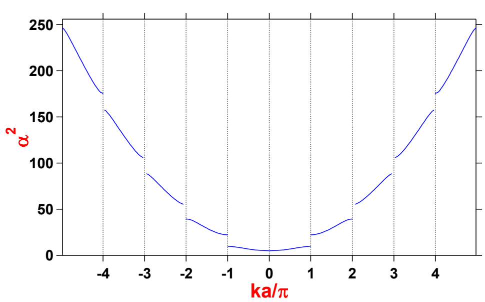
$$P \equiv \frac{maV_0 b}{\hbar^2}$$

$$\frac{P}{\alpha a}\sin(\alpha a) + \cos(\alpha a) = \cos(ka)$$

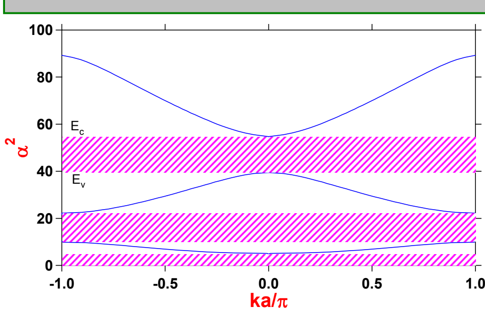
Forming Gaps



Gaps



Gaps



Band Gaps

• C	5.4 eV	indirect
• Si	1.17 eV (1.11)	indirect
• Ga	0.74 eV (0.66)	indirect
• GaAs	1.52 eV (1.43)	direct
• SiC	3.0 eV	indirect

To the Effective Mass

- The group velocity is given by:

$$v_g = \frac{dE}{dp} = \frac{1}{\hbar}\frac{dE}{dk} \qquad \vec{v}_g = \frac{1}{\hbar}\nabla_{\vec{k}} E$$

- So the acceleration is…

$$F = \hbar \frac{dk}{dt} = -eV$$

$$a = \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dE}{dk}\frac{dk}{dt}\right) \Rightarrow a = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F = \frac{F}{m^*}$$

$$m^* \equiv \frac{\hbar^2}{\nabla_{\vec{k}}^2 E}$$

Finally...