

## **Lecture 3**

# **Quantum Mechanics and relationship to electron motion in crystals**

**Reading:**

**Notes**

## Recall: Carrier Movement Within the Crystal

$$F = -qE = m_n^* \frac{dv}{dt}$$

$F \equiv$  force,  $v \equiv$  velocity,  $t \equiv$  time,

$q \equiv$  electronic charge,

$m_n^* \equiv$  electron effective mass

$$F = qE = m_p^* \frac{dv}{dt}$$

$F \equiv$  force,  $v \equiv$  velocity,  $t \equiv$  time,

$q \equiv$  electronic charge,

$m_p^* \equiv$  hole effective mass

**Table 2.1** Density of States Effective Masses at 300 K.

Material	$m_n^*/m_0$	$m_p^*/m_0$
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

Ge and GaAs have “lighter electrons” than Si  
which results in faster devices

# Introduction to Quantum Mechanics (notes only)

People RARELY get quantum mechanics of their first exposure.

Many aspects of quantum mechanics are counter intuitive and thus, “visual learners” will likely have more trouble than those that tend to think in the abstract.

We will introduce it now in hopes it will be easier the more you are exposed to it.

Parts of this discussion are taken from:

Solyman and Walsh – Electrical Properties of Materials

Neudeck and Pierret – Advanced Semiconductor Fundamentals

Dimitrijevic – Understanding Semiconductor Devices

Mayer and Lau – Electronic Materials Science

Colclaser and Diehl-Nagle – Materials and Devices for electrical engineers and physicists

Tipler – Physics for scientists and engineers V4.

# Introduction to Quantum Mechanics (notes only)

•To fully understand the origin of the energy bandgap and effective mass concepts as well as future topics of energy states in quantum wells and tunneling currents, one must have at least a basic understanding of electron motion in free space and in the presence of other sources of electrostatic potential (atomic cores for example).

•This requires an understanding of the dual wave-particle nature of electrons and in turn quantum mechanics.

•Consider the electron microscope:

•Electrons have a charge and thus can be focused...

•...but also have a phase and thus can interfere with each other destructively or constructively

Electron Source

Deflection Plates

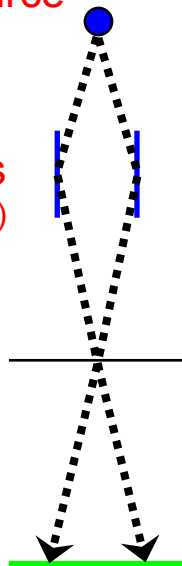
(voltage used to focus electrons)

Thin sample

(spatially varied charge creates multiple phase delayed electron paths)

Phosphor Screen

(converts electron energy to visible light – waves constructively and destructively interfere to get light and dark regions)



$$v = \frac{h}{m\lambda}$$

$$v = \frac{6.6 \times 10^{-34} \text{ Js}}{9.1 \times 10^{-31} \text{ kg} \times 10^{-11} \text{ meters}} = 7.25 \times 10^7 \text{ m/s}$$

$$KE = \frac{1}{2} m v^2 = qV$$

$$V = \frac{9.1 \times 10^{-31} (7.25 \times 10^7 \text{ m/s})^2}{2 \times 1.6 \times 10^{-19} \text{ C}} = 15,000 \text{ V}$$

15KV gives sub atomic resolution!



# Introduction to Quantum Mechanics (notes only)

- What is the wavelength of macroscopic particles? Consider a bullet (1km/s 1 gram)?

$$1000m/s = \frac{6.6 \times 10^{-34} Js}{1 \times 10^{-3} kg \times \lambda} \Rightarrow \lambda = 6.6 \times 10^{-34} m$$

- Though it acts as a wave, it's wavelength is too small to ever measure/observe.
- So an electron (or every particle) acts as a wave AND a particle simultaneously. How can we describe this?

- Other useful properties of “energy-particle waves”:  $E = hf = \left(\frac{h}{2\pi}\right)(2\pi f) = \hbar\omega = mc^2$

Or the momentum of the photon is...

$$p = mc = \frac{hf}{c} = \frac{h}{\lambda} = \hbar \left( \frac{2\pi}{\lambda} \right) = \hbar k$$

$$p = \frac{h}{\lambda} \text{ this is known as the de Broglie hypothesis}$$

Where scalar,  $k$ , is known as the wave number. If momentum,  $\mathbf{p}$  is expressed as a vector,  $\mathbf{k}$  is known as the wave vector.

# Introduction to Quantum Mechanics (notes only)

Why do we use “k” or “**k**” instead of “p” or “**p**”?

$k=2\pi/\lambda$  is independent of mass. Classically,  $\mathbf{p}=m\mathbf{v}$ . However, we will show that the “mass”\* will change with crystalline direction allowing two parameters (m and v) to change the momentum. Thus, k is simpler to consider.

\*actually the effective mass is what changes with crystalline direction.

# Introduction to Quantum Mechanics (notes only)

So how do we account for the wavelike nature of small particles like electrons?

Schrödinger Equation:

- In “Electrical Properties of Materials”, Solymar and Walsh point out that there are NO physical assumptions available to “derive” the Schrödinger Equation
- Just like Newton’s law of motion,  $F=ma$ , and Maxwell’s equations, the Schrödinger Equation was proposed to explain several observations in physics that were previously unexplained. These include the atomic spectrum of hydrogen, the energy levels of the Planck oscillator, non-radiation of electronic currents in atoms, and the shift in energy levels in a strong electric field.

$$KE + PE = E_{Total}$$

Kinetic energy “operator”  $-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = i\hbar \frac{\partial \Psi}{\partial t}$  Energy “operator”

Potential electron moves through

Other operators exist:

Table 2.1 Dynamic Variable/Operator Correspondence

Dynamic Variable ( $\alpha$ )		Mathematical Operator ( $\alpha_{op}$ )		Expectation Value— $\langle \alpha \rangle$
$x, y, z$	$\leftrightarrow$	$x, y, z$	$\dots$	$\langle x \rangle = \int_V \Psi^* x \Psi dV$
$f(x, y, z)$	$\leftrightarrow$	$f(x, y, z)$		
$p_x, p_y, p_z$	$\leftrightarrow$	$\frac{\hbar}{i} \frac{\partial}{\partial x}, \frac{\hbar}{i} \frac{\partial}{\partial y}, \frac{\hbar}{i} \frac{\partial}{\partial z}$	$\dots$	$\langle p_x \rangle = \int_V \Psi^* \frac{\hbar}{i} \frac{\partial \Psi}{\partial x} dV$
$E$	$\leftrightarrow$	$\frac{\hbar}{i} \frac{\partial}{\partial t}$		

# Introduction to Quantum Mechanics (notes only)

$\Psi(x,y,z,t)$  is called the electron “wave function”

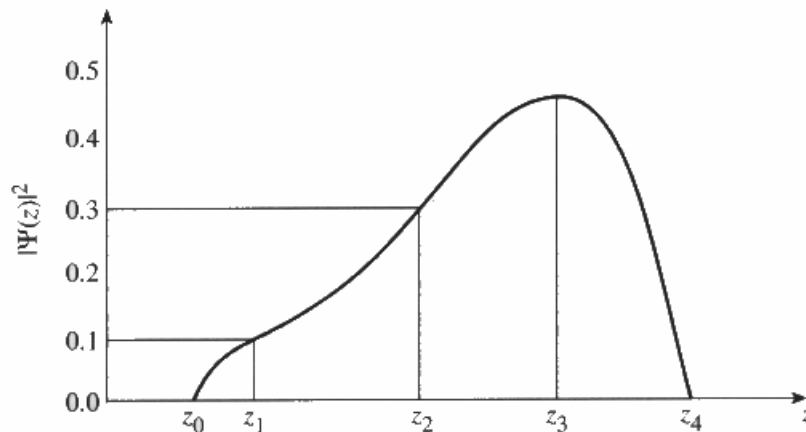
It is related to the probability of finding an electron at time  $t$  in a volume  $dxdydz$ . Specifically, this probability is:

$$|\Psi(x, y, z, t)|^2 dxdydz \text{ or } [\Psi^* \Psi dxdydz]$$

But since  $\Psi$  is a probability,

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x, y, z, t)|^2 dxdydz = 1$$

$$\text{or in 1D } \int_{-\infty}^{\infty} [\Psi^* \Psi dx] = 1$$



Introducing the concept of the wave function.  $|\psi(z)|^2 dz$  proportional to the probability that the electron may be found in the interval  $dz$  at the point  $z$ .

# Introduction to Quantum Mechanics (notes only)

To solve the Schrödinger equation one must make an assumption about the wave function. Lets assume the wave function has separate spatial and temporal components:

$$* \Psi(x, y, z, t) = \Psi(x, y, z)w(t)$$

Plugging this (\*) into the Schrödinger equation and dividing both sides by (\*) we arrive at:

$$\left( -\frac{\hbar^2}{2m} \frac{\nabla^2 \Psi}{\Psi} + V \right) = i\hbar \frac{1}{w} \frac{\partial w}{\partial t}$$

Since the left hand side varies only with position, and the right hand side varies only with time, the only way these two sides can equate is if they are equal to a constant ( we will call this constant, total energy, E). Thus, we can break this equation into two equations:

$$E = i\hbar \frac{1}{w} \frac{\partial w}{\partial t} \qquad \left( -\frac{\hbar^2}{2m} \frac{\nabla^2 \Psi}{\Psi} + V \right) = E$$

Consider first the time variable version (left side) then later we will examine the spatially variable portion. This will give us time variable solutions and a separate spatially variable solution.

# Introduction to Quantum Mechanics (notes only)

Consider the time variable solution:

$$E = i\hbar \frac{1}{w} \frac{\partial w}{\partial t}$$

$$\frac{\partial w}{\partial t} = -\left(i \frac{E}{\hbar}\right) w$$

$$w(t) = e^{\left(-\left(i \frac{E}{\hbar}\right)t\right)} \quad \text{or} \quad w(t) = e^{(-i\omega t)}$$

*where*  $E = \hbar\omega$

This equation expresses the periodic time nature of the wave equation.

# Introduction to Quantum Mechanics (notes only)

Consider the space variable solution:

$$\left( -\frac{\hbar^2}{2m} \frac{\nabla^2 \Psi}{\Psi} + V \right) = E$$

The combined  
"operator" is called  
the Hamiltonian

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = E\Psi$$
$$\hat{H} \Psi = E\Psi$$

momentum  
"operator"

$$\left( \frac{1}{2m} (-j\hbar\nabla)^2 + V \right) \Psi = E\Psi$$

$$\left( \frac{\hat{p}^2}{2m} + \hat{V} \right) \Psi = E\Psi$$

Kinetic Energy + Potential Energy = Total Energy

Classically, momentum,  $p=mv$  and kinetic energy is  $(mv^2)/2 = (p^2)/2m$

# Introduction to Quantum Mechanics (notes only)

Consider a specific solution for the free space (no electrostatic potential,  $V=0$ ) wave solution (electron traveling in the +x direction in 1D only):

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = E\Psi$$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - E\Psi = 0$$

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\text{where } k = \frac{2\pi}{\lambda} = \sqrt{\frac{2mE}{\hbar^2}} \text{ or } E = \frac{\hbar^2 k^2}{2m}$$

Since we have to add our time dependent portion (see (\*) previous) our total solution is:

$$\Psi = \Psi(x)w(t) = Ae^{-i(\omega t - kx)} + Be^{-i(\omega t + kx)}$$

This is a standard wave equation with one wave traveling in the +x direction and one wave traveling in the -x direction. Since our problem stated that the electron was only traveling in the +x direction,  $B=0$ .

Classically, momentum,  $p=mv$  and kinetic energy is  $(mv^2)/2 = (p^2)/2m$

# Introduction to Quantum Mechanics (notes only)

An interesting aside: What is the value of A?

Since  $\Psi$  is a probability,

$$\int_{-\infty}^{\infty} [\Psi^* \Psi dx] = 1$$

$$\int_{-\infty}^{\infty} A e^{ikx} A e^{-ikx} dx = 1$$

$$\int_{-\infty}^{\infty} A^2 e^{ikx-ikx} dx = 1$$

$$\int_{-\infty}^{\infty} A^2 dx = 1$$

This requires A to be vanishingly small (unless we restrict our universe to finite size) and is the same probability for all x and t. More importantly it brings out a quantum phenomena: If we know the electrons momentum, p or k, we can not know it's position! This is a restatement of the uncertainty principle:

$$\Delta p \Delta x \geq \hbar$$

Where  $\Delta p$  is the uncertainty in momentum and  $\Delta x$  is the uncertainty in position

# Introduction to Quantum Mechanics (notes only)

The solution to this free particle example brings out several important observations about the dual wave-particle nature of our universe:

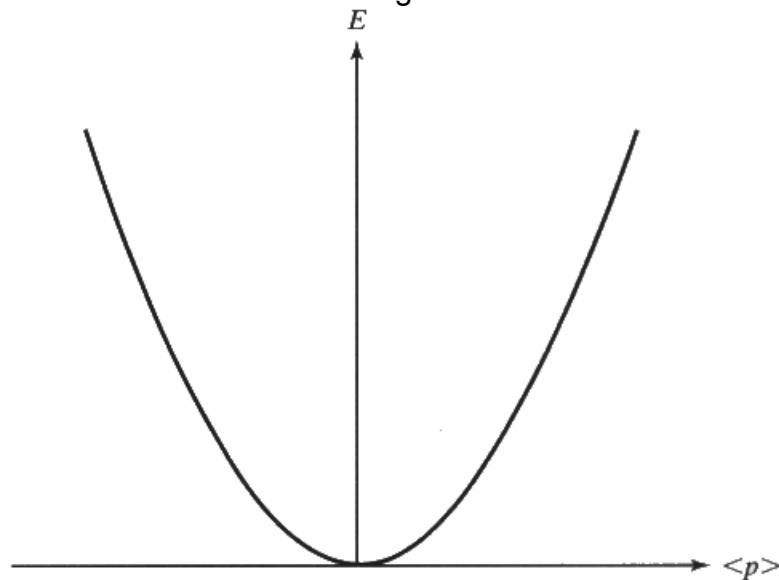
$$\Psi = \Psi(x)w(t) = Ae^{-i(\omega t - kx)}$$

While particles act as waves, their charge is carried as a particle. I.e. you can only say that there is a “probability” of finding an electron in a particular region of space, but if you find it there, it will have all of its charge there, not just a fraction.

Energy of moving particles follows a square law relationship:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\langle p \rangle^2}{2m}$$

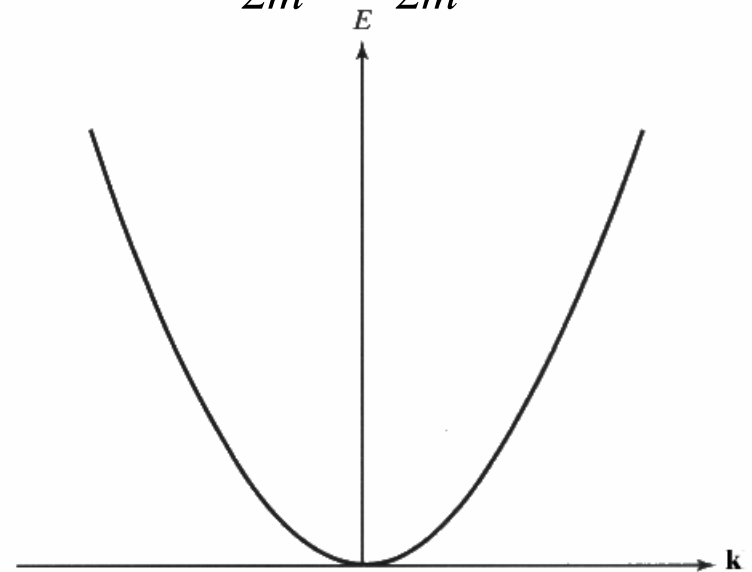
Neudeck and Pierret Fig 2.3



Energy-momentum relationship for a free particle.

Classically, momentum,  $p=mv$  and kinetic energy is  $(mv^2)/2 = (p^2)/2m$

Georgia Tech



Energy-momentum relationship for a free particle.

ECE 3080 - Dr. Alan Doolittle

# Introduction to Quantum Mechanics (notes only)

What effect does this “E-k” square law relationship have on electron velocity and mass?

The group velocity (rate of energy delivery) of a wave is:

$$v_g = \frac{dE}{dp} = \frac{1}{\hbar} \frac{dE}{dk}$$

So the “speed” of an electron in the direction defined by  $\mathbf{p}$  is found from the slope of the E-k diagram.

Similarly, since  $E = \frac{\hbar^2 k^2}{2m}$

$$m^* = \hbar^2 \left( \frac{d^2 E}{dk^2} \right)^{-1}$$

So the “effective mass” of an electron is related to the local inverse curvature of the E-k diagram

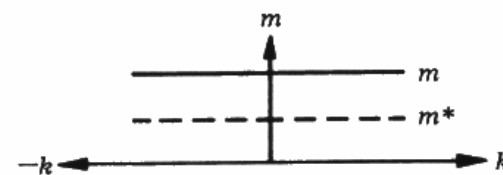
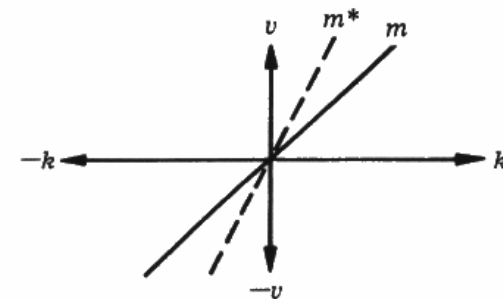
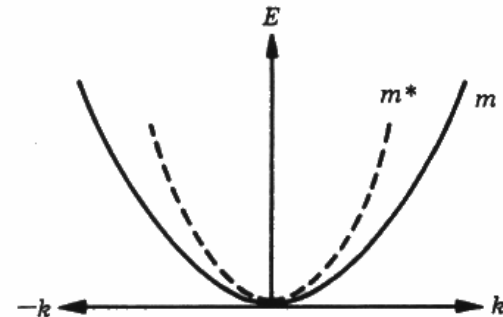


FIGURE 12.2 E-k diagram for a free electron with mass  $m$  (solid line) and a smaller mass,  $m^*$ . The parabolic E-k diagram leads to a linear  $v$  versus  $k$  relation and a constant mass.

# What effect does an electrostatic potential have on an electron?

Consider the electron moving in an electrostatic potential,  $V_o$ . The wave solution (electron traveling in the +x direction in 1D only):

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = E\Psi$$
$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - (E - V_o) \Psi = 0$$

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\text{where } k = \frac{2\pi}{\lambda} = \sqrt{\frac{2mE - V_o}{\hbar^2}} \text{ or } E = \frac{\hbar^2 k^2}{2m} - V_o$$

Since we have to add our time dependent portion (see (\*) previous) our total solution is:

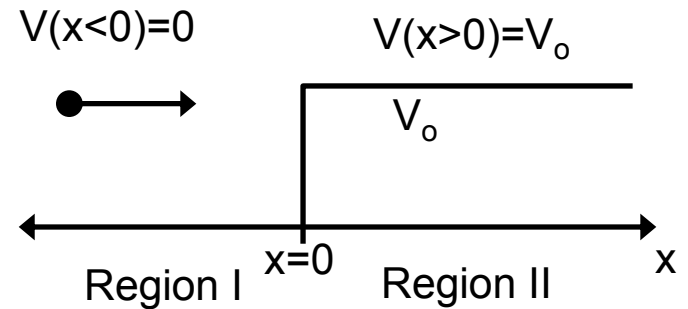
$$\Psi = \Psi(x)w(t) = Ae^{-i(\omega t - kx)} + Be^{-i(\omega t + kx)}$$

This is, again, a standard wave equation with one wave traveling in the +x direction and one wave traveling in the -x direction. Since our problem stated that the electron was only traveling in the +x direction,  $B=0$ .

***When the electron moves through an electrostatic potential, for the same energy as in free space, the only thing that changes is the “wavelength” of the electron.***

# What about an electrostatic potential step?

Consider the electron moving incident on an electrostatic potential,  $V_0$ . The wave solution (1D only):



We have already solved these in regions I and II. The total solution is:

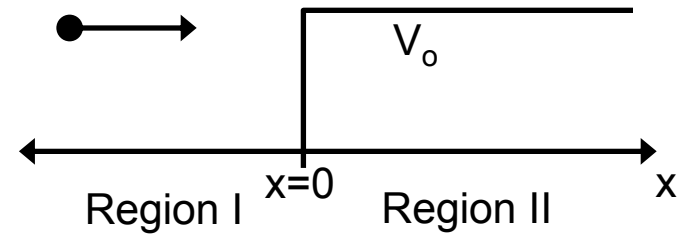
$$\Psi_I = \Psi_I(x)w_I(t) = A_I e^{-i(\omega t - k_I x)} + B_I e^{-i(\omega t + k_I x)}$$

$$\Psi_{II} = \Psi_{II}(x)w_{II}(t) = A_{II} e^{-i(\omega t - k_{II} x)} + B_{II} e^{-i(\omega t + k_{II} x)}$$

$$\text{where } k_I = \frac{2\pi}{\lambda_I} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_{II} = \frac{2\pi}{\lambda_{II}} = \sqrt{\frac{2mE - V_0}{\hbar^2}}$$

# What about an electrostatic potential step?

cont'd...



$$\Psi_I = \Psi_I(x)w_I(t) = A_I e^{-i(\omega t - k_I x)} + B_I e^{-i(\omega t + k_I x)}$$

$$\Psi_{II} = \Psi_{II}(x)w_{II}(t) = A_{II} e^{-i(\omega t - k_{II} x)} + B_{II} e^{-i(\omega t + k_{II} x)}$$

$$\text{where } k_I = \frac{2\pi}{\lambda_I} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_{II} = \frac{2\pi}{\lambda_{II}} = \sqrt{\frac{2mE - V_o}{\hbar^2}}$$

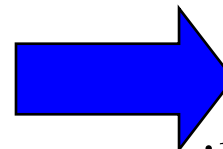
**When the “wave” is incident on the barrier, some of it is reflected, some of it is transmitted. However, since there is nothing at  $x=+\infty$  to reflect the wave back,  $B_{II}=0$ .**

**Since  $\psi$  is a wave, both  $\psi$  and its first derivative must be continuous across the boundary at  $x=0$  for all time,  $t$ . Thus,**

$$\Psi_I(x=0) = \Psi_{II}(x=0)$$

and

$$\frac{\partial \Psi_I(x=0)}{\partial x} = \frac{\partial \Psi_{II}(x=0)}{\partial x}$$



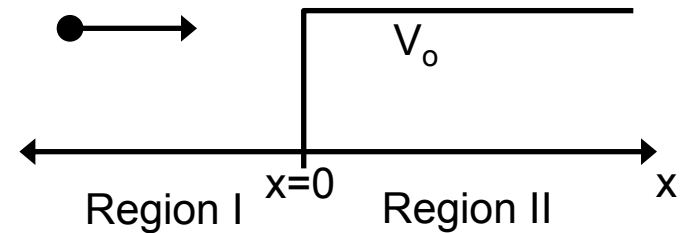
$$A_I + B_I = A_{II}$$

and

$$ik_I(A_I - B_I) = ik_{II}A_{II}$$

# What about an electrostatic potential step?

cont'd...



**We can define a “reflection coefficient” as the amplitude of the reflected wave relative to the incident wave,**

$$R \equiv \frac{B_I}{A_I} = \frac{k_I - k_{II}}{k_I + k_{II}}$$

**And likewise, we can define a transmission coefficient as the amplitude of the transmitted wave relative to the incident wave,**

$$T \equiv \frac{A_{II}}{A_I} = \frac{2k_I}{k_I + k_{II}}$$

**The probability of a reflection is  $R^*R$  while the probability of transmission is  $T^*T$**

$$k_I = \frac{2\pi}{\lambda_I} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_{II} = \frac{2\pi}{\lambda_{II}} = \sqrt{\frac{2mE - V}{\hbar^2}}$$

# What about an electrostatic potential step?

cont'd...

Consider 2 cases: Case 1:  $E > V$

Both  $k_I$  and  $k_{II}$  are real and thus, the particle moves with a wave of different wavelength in the two regions.

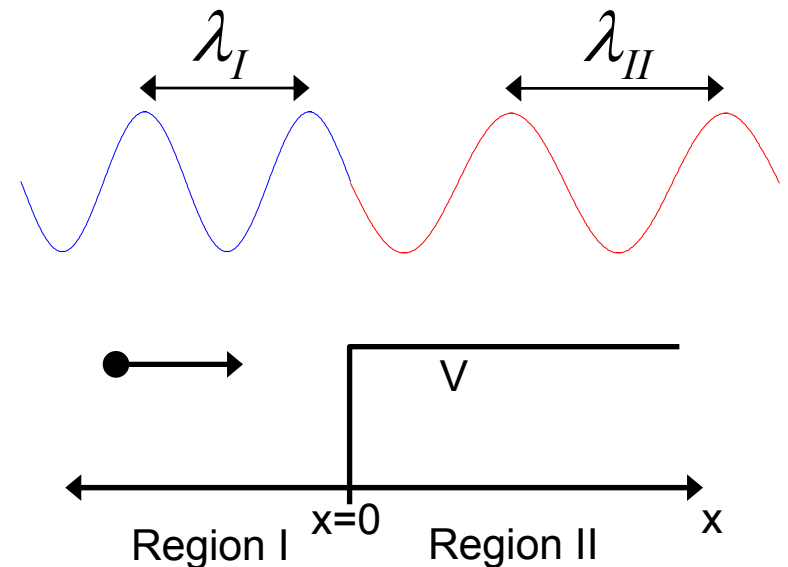
However,  $R \neq 0$  is finite. Thus, even though the electron has an energy,  $E$ , greater than  $V$  it will have a finite probability of being reflected by the potential barrier.

If  $E \gg V$ , this probability of reflection reduces to  $\sim 0$  ( $k_I \rightarrow k_{II}$ )

$$R \equiv \frac{B_I}{A_I} = \frac{k_I - k_{II}}{k_I + k_{II}}$$

$$T \equiv \frac{A_{II}}{A_I} = \frac{2k_I}{k_I + k_{II}}$$

$$k_I = \frac{2\pi}{\lambda_I} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_{II} = \frac{2\pi}{\lambda_{II}} = \sqrt{\frac{2mE - V}{\hbar^2}}$$



# What about an electrostatic potential step?

cont'd...

Case 2:  $E < V$

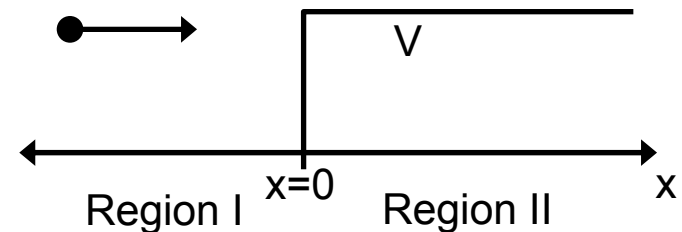
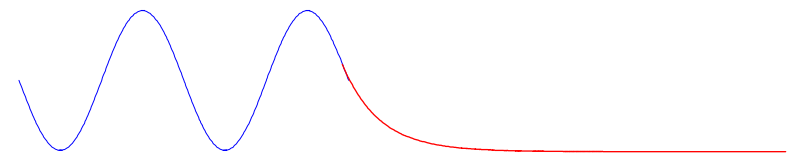
$k_I$  is real but  $k_{II}$  is imaginary. When an imaginary  $k_{II}$  is placed inside our exponential,  $\exp(ik_{II}x)$ , a decaying function of the form,  $\exp(-ax)$  results in region II.

However,  $T^*T$  is now finite, so even though the electron has an energy,  $E$ , less than  $V$  it will have a finite probability of being found within the potential barrier. The probability of finding the electron deep inside the potential barrier is  $\sim 0$  due to the rapid decay of  $\psi$ .

$$R \equiv \frac{B_I}{A_I} = \frac{k_I - k_{II}}{k_I + k_{II}}$$

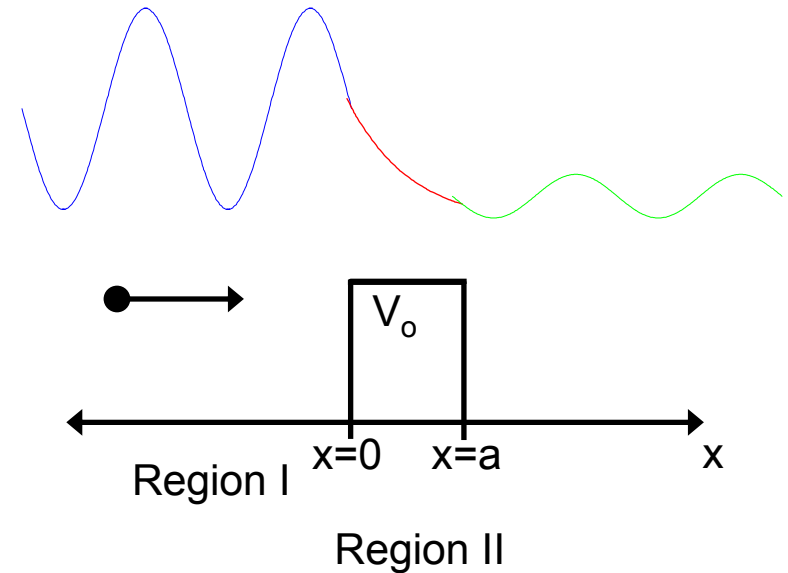
$$T \equiv \frac{A_{II}}{A_I} = \frac{2k_I}{k_I + k_{II}}$$

$$k_I = \frac{2\pi}{\lambda_I} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_{II} = \frac{2\pi}{\lambda_{II}} = \sqrt{\frac{2mE - V}{\hbar^2}}$$



# What about an electrostatic potential step?

Without proof (see homework), consider the following potential profile with an electron of energy  $E < V_0$ .



The electron has a finite probability to “tunnel” through the barrier and will do so if the barrier is thin enough. Once through, it will continue traveling on it’s way.

# Now consider an periodic potential in 1D

## Kronig-Penney Model

Consider what potentials an electron would see as it moves through the lattice (limited to 1D for now). The electrostatic potential,  $V(x)$  is periodic such that  $V(x+L)=V(x)$ .

The Bloch theorem states that since the potential repeats every “L” lengths, the magnitude of the wavefunction (but not necessarily the phase) must also repeat every “L” lengths. This is true because the probability of finding an electron at a given point in the crystal must be the same as found in the same location in any other unit cell.

Since  $V(x + L) = V(x)$

$$\Psi(x + L) = e^{ikL}\Psi(x)$$

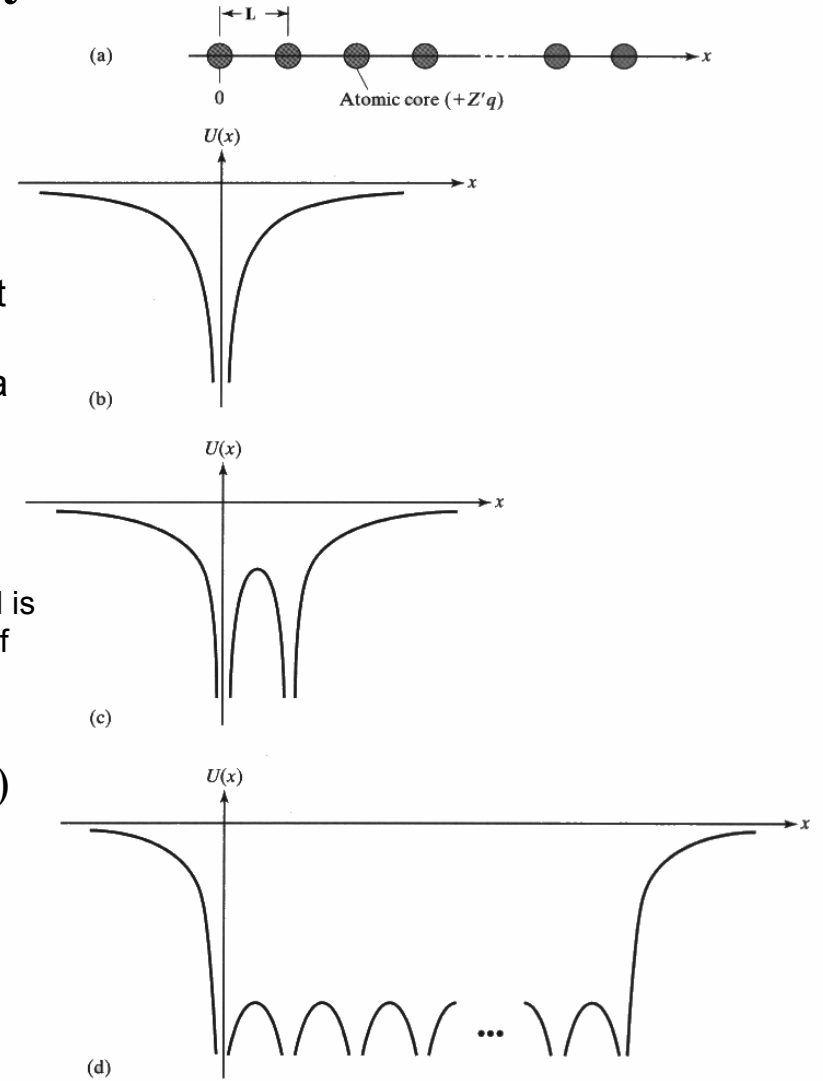


The wavefunction in one unit cell is merely a phase shifted version of the wavefunction in an adjacent unit cell.

$$\Psi^*(x + L)\Psi(x + L) = e^{-ikL}\Psi^*(x)e^{ikL}\Psi(x) = \Psi^*(x)\Psi(x)$$

We **MUST** have standing waves in the crystal that have a period equal to a multiple of the period of the crystal's electrostatic potential. (Similar to a multilayer antireflection coating in optics)

It is important to note that since, the wavefunction repeats each unit cell, we only have to consider what happens in one unit cell to describe the entire crystal. Thus, we can restrict ourselves to values of  $k$  such that  $-\pi/a$  to  $+\pi/a$  (implying  $ka \leq 1$  or  $(2\pi/\lambda)a \leq 1$ )



(a) One-dimensional crystalline lattice. (b-d) Potential energy of an electron inside the lattice considering (b) only the atomic core at  $x = 0$ , (c) the atomic cores at both  $x = 0$  and  $x = a$ , and (d) the entire lattice chain.

# Now consider an periodic potential in 1D

## Kronig-Penney Model

Assumptions of Kronig-Penney Model:

- Simplifying the potential to that shown here:

- 1D only

- Assume electron is a simple plane wave of the form,

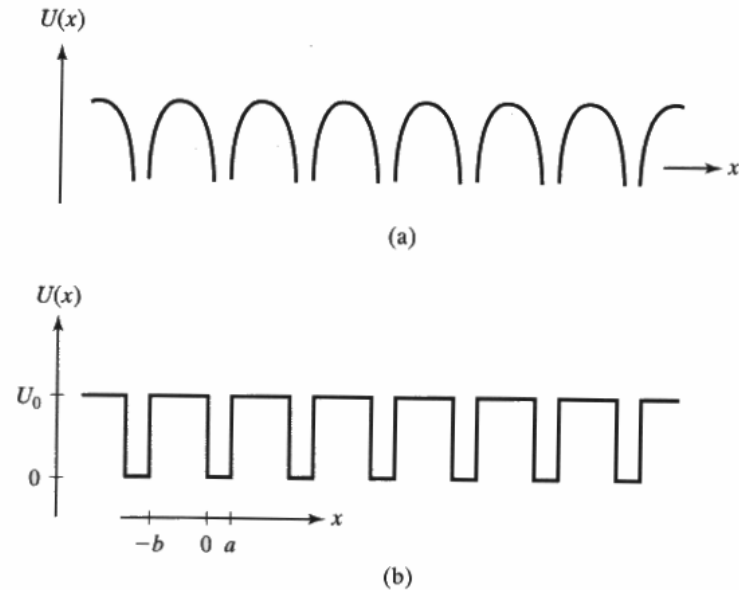
$$e^{ikx}$$

...modulated by the periodic crystalline potential,  $U(x)$

- The crystalline potential is periodic,  $U(x)=U(x+L)$

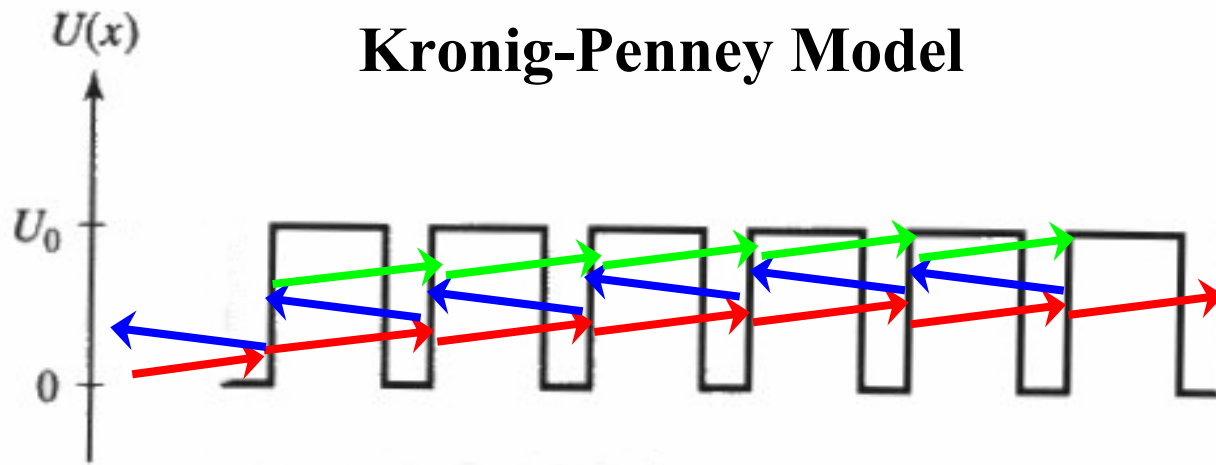
- Thus the wave function is a simple plain wave modulated by the periodic crystalline potential:

$$\Psi(x) = U(x)e^{ikx}$$



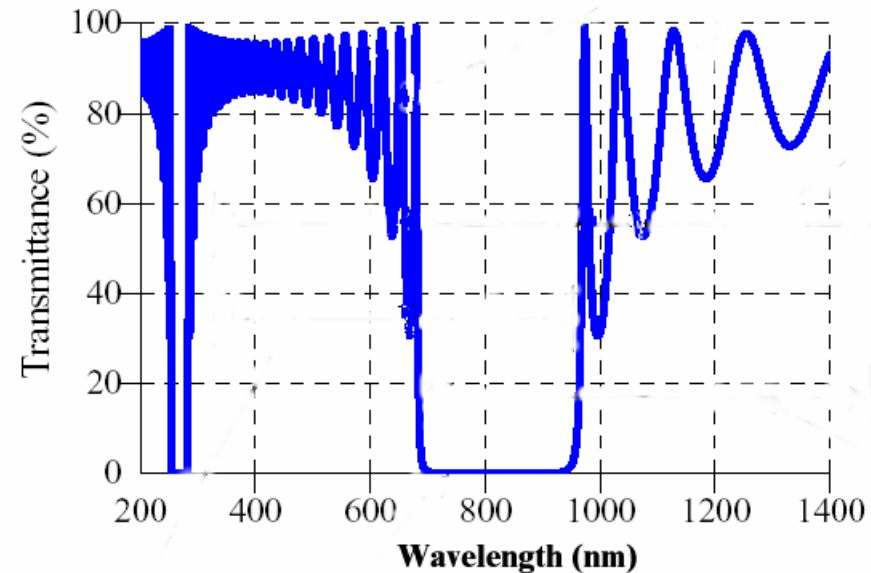
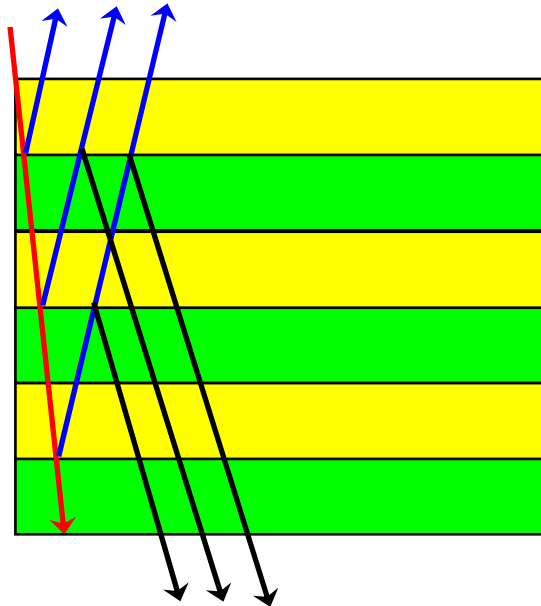
**Figure 3.2** Kronig-Penney idealization of the potential energy associated with a one-dimensional crystalline lattice. (a) One-dimensional periodic potential. (b) Kronig-Penney model.

# Kronig-Penney Model



Resonant reflectance/transmission creates “standing waves” in the crystal. Only certain wavelengths (energies) can pass through the 1D crystal.

By analogy, a multiple layer optical coating has similar reflection/transmission characteristics. The result is the same, only certain wavelengths (energies) are transmitted through the optical stack. In a sense, we have an “optical bandgap”.



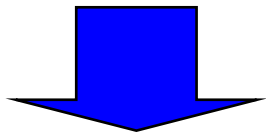
# Kronig-Penney Model

For  $0 < x < a$ :

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + \cancel{V} \right) \Psi = E\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \alpha^2 \Psi = 0$$

$$\text{where } \alpha = \sqrt{\frac{2mE}{\hbar^2}}$$



$$\Psi_a(x) = A \sin(\alpha x) + B \cos(\alpha x)$$

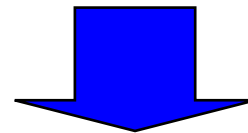
For  $-b < x < 0$ :

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = E\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \beta^2 \Psi = 0$$

$$\beta = \sqrt{\frac{2m(E - U_o)}{\hbar^2}} \text{ for } E > U_o$$

$$\beta = \sqrt{\frac{2m(U_o - E)}{\hbar^2}} \text{ for } 0 < E < U_o$$



$$\Psi_b(x) = C \sin(\beta x) + D \cos(\beta x)$$

# Kronig-Penney Model

For  $0 < x < a$ :

$$\Psi_a(x) = A \sin(\alpha x) + B \cos(\alpha x)$$

For  $-b < x < 0$ :

$$\Psi_b(x) = C \sin(\beta x) + D \cos(\beta x)$$

Applying the following boundary conditions:

$$\Psi_a(x) = \Psi_b(x)$$
$$\left. \frac{d\Psi_a(x)}{dx} \right|_{x=0} = \left. \frac{d\Psi_b(x)}{dx} \right|_{x=0}$$

**BC for continuous  
wave function at the  
boundary**

$$\Psi_a(x = a) = e^{ik(a+b)} \Psi_b(x = -b)$$
$$\left. \frac{d\Psi_a(x)}{dx} \right|_{x=a} = e^{ik(a+b)} \left. \frac{d\Psi_b(x)}{dx} \right|_{x=-b}$$

**BC for periodic wave  
function at the  
boundary**

# Kronig-Penney Model

Applying the boundary conditions, we get:

$$B = D$$

$$\alpha A = \beta C$$

$$A \sin(\alpha a) + B \cos(\alpha a) = e^{ik(a+b)} [-C \sin(\beta b) + D \cos(\beta b)]$$

$$\alpha A \cos(\alpha a) + \alpha B \sin(\alpha a) = e^{ik(a+b)} [\beta C \cos(\beta b) + \beta D \sin(\beta b)]$$

Eliminating the variables C and D using the above equations, we get:

$$A \left[ \sin(\alpha a) + \left( \frac{\alpha}{\beta} \right) e^{ik(a+b)} \sin(\beta b) \right] + B \left[ \cos(\alpha a) - e^{ik(a+b)} \cos(\beta b) \right] = 0$$

$$A \left[ \alpha \cos(\alpha a) - \alpha e^{ik(a+b)} \cos(\beta b) \right] + B \left[ -\alpha \sin(\alpha a) - \beta e^{ik(a+b)} \sin(\beta b) \right] = 0$$

This equation set forms a matrix of the form:

$$\begin{bmatrix} w & x \\ y & z \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

A and B are only non-zero (non-trivial solution) when the determinate of the above set is equal to zero.

# Kronig-Penney Model

Taking the determinate and simplifying we get:

$$-\left(\frac{\alpha^2 + \beta^2}{2\alpha\beta}\right) \sin(\alpha a) \sin(\beta b) + \cos(\alpha a) \cos(\beta b) = \cos(k(a + b))$$

Plugging in the definitions for  $\alpha$  and  $\beta$  we get:

$$\left(\frac{1 - 2\frac{E}{U_o}}{2\sqrt{\frac{E}{U_o}\left(\frac{E}{U_o} - 1\right)}}\right) \sin\left(a\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\frac{E}{U_o}}\right) \sin\left(b\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\left(\frac{E}{U_o} - 1\right)}\right) + \cos\left(a\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\frac{E}{U_o}}\right) \cos\left(b\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\left(\frac{E}{U_o} - 1\right)}\right) = \cos(k(a + b)) \text{ for } E > U_o.$$

$$\left(\frac{1 - 2\frac{E}{U_o}}{2\sqrt{\frac{E}{U_o}\left(1 - \frac{E}{U_o}\right)}}\right) \sin\left(a\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\frac{E}{U_o}}\right) \sinh\left(b\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\left(1 - \frac{E}{U_o}\right)}\right) + \cos\left(a\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\frac{E}{U_o}}\right) \cosh\left(b\sqrt{\frac{2mU_o}{\hbar^2}}\sqrt{\left(1 - \frac{E}{U_o}\right)}\right) = \cos(k(a + b)) \text{ for } 0 < E < U_o.$$

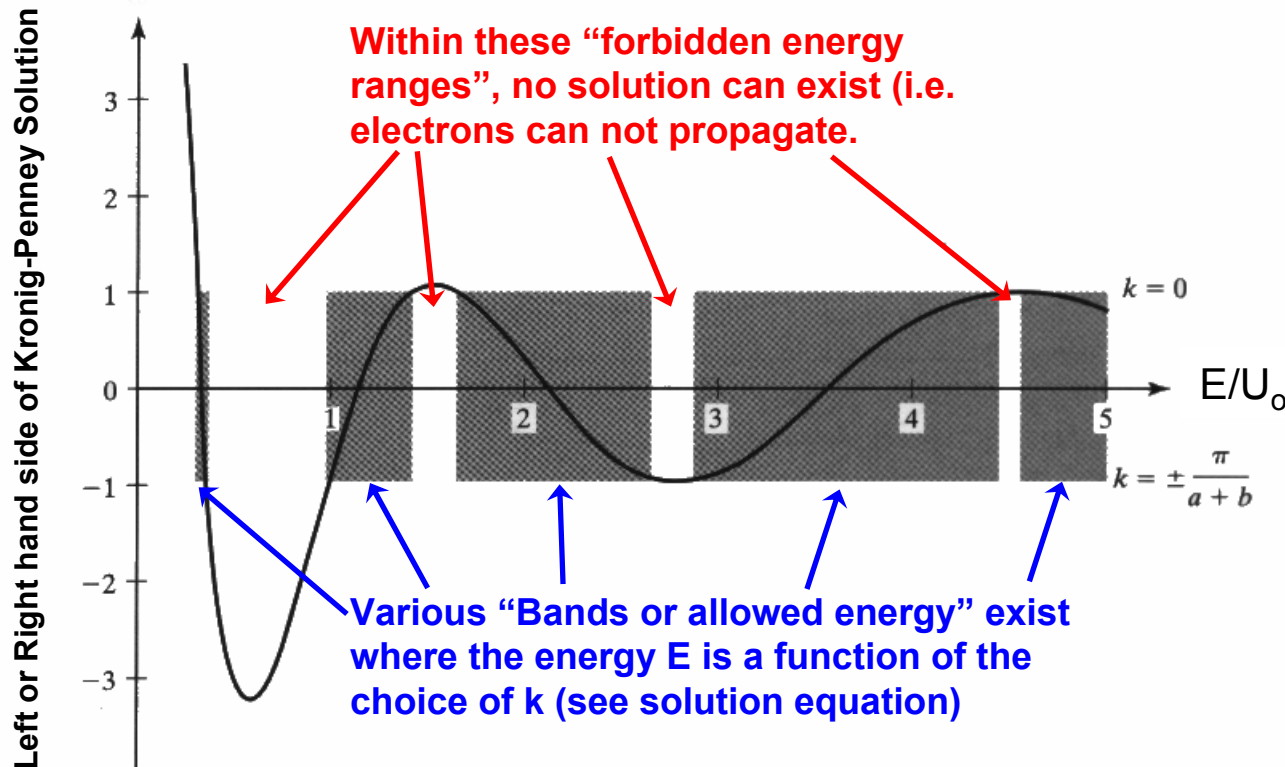
The right hand side is constrained to a range of +/- 1 and is a function of k only. The limits of the right hand side (+/- 1) occurs at k=0 and +/-  $\pi/(a+b)$  where a+b is the period of the crystal potential.

The left hand side is NOT constrained to +/- 1 and is a function of energy only.

# Kronig-Penney Model

The right hand side is constrained to a range of  $\pm 1$  and is a function of  $k$  only. The limits of the right hand side ( $\pm 1$ ) occurs at  $k=0$  to  $\pm \pi/(a+b)$ .

The left hand side is NOT constrained to  $\pm 1$  and is a function of energy only.



Graphical determination of allowed electron energies. The left-hand side of the Eqs. (3.18) Kronig-Penney model solution is plotted as a function of  $\xi = E/U_0$ . The shaded regions where  $-1 \leq f(\xi) \leq 1$  identify the allowed energy states for the specific case where,

$$a\sqrt{\frac{2mU_0}{\hbar^2}} = b\sqrt{\frac{2mU_0}{\hbar^2}} = \pi$$

# Kronig-Penney Model

Replotting the previous result in another form recognizing the lower k limit is shared by + and  $-\pi/(a+b)$  while the upper limit is for  $k=0$ .

There are at most 2 k-values for each allowed energy, E

The slope,  $dE/dK$  is zero at the k-zone boundaries at  $k=0$ ,  $k= -\pi/(a+b)$  and  $k= +\pi/(a+b)$   
Thus we see that the velocity of the electrons approaches zero at the zone boundaries.  
This means that the electron trajectory/momentum are confined to stay within the allowable k-zones.

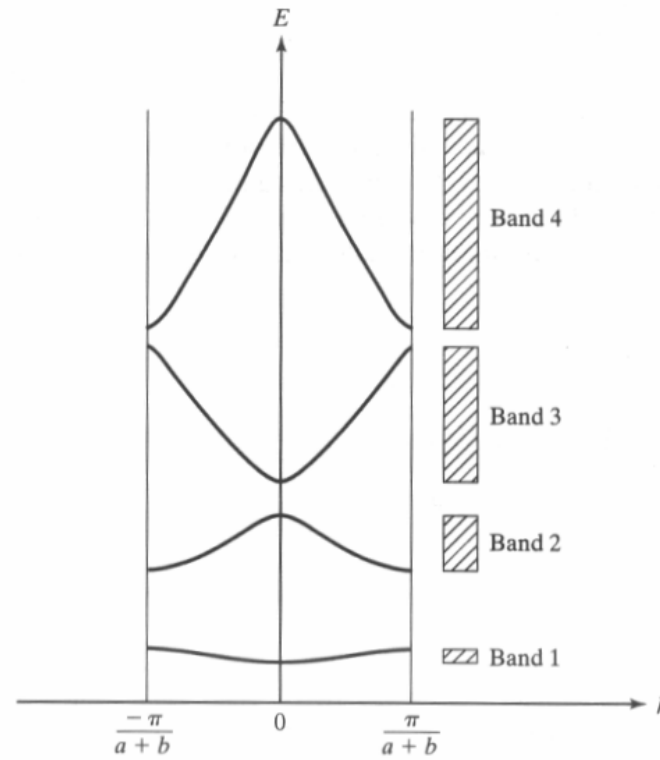
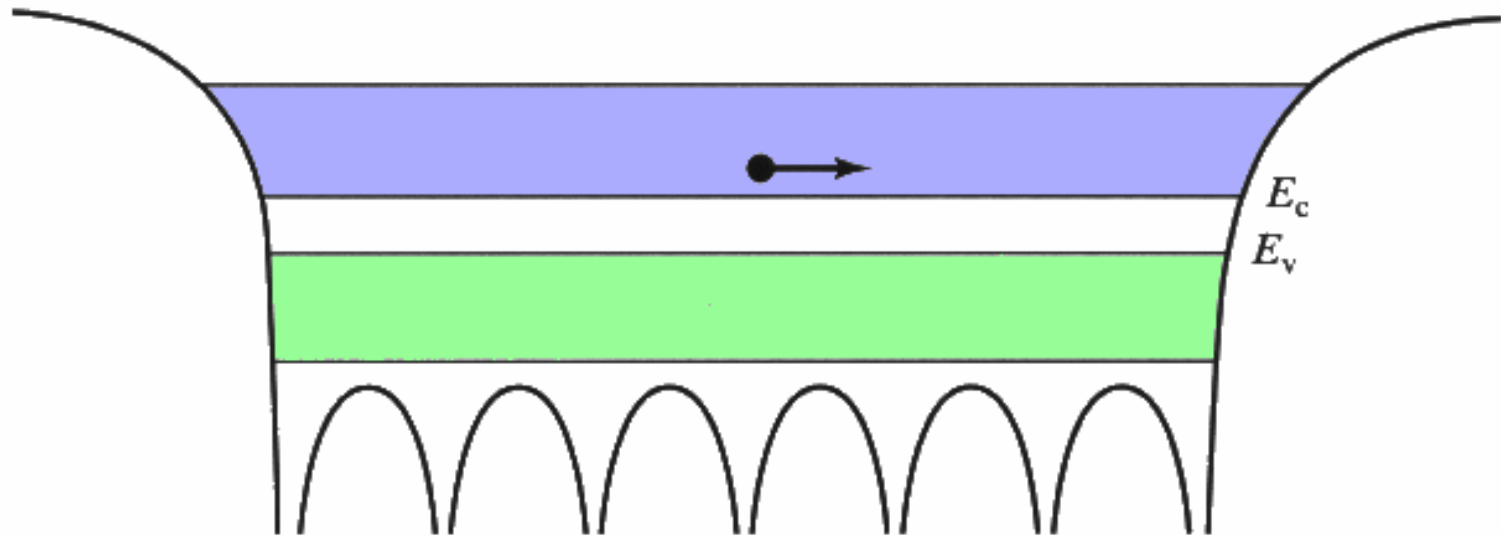


Figure 3.5 Reduced-zone representation of allowed  $E$ - $k$  states in a one-dimensional crystal

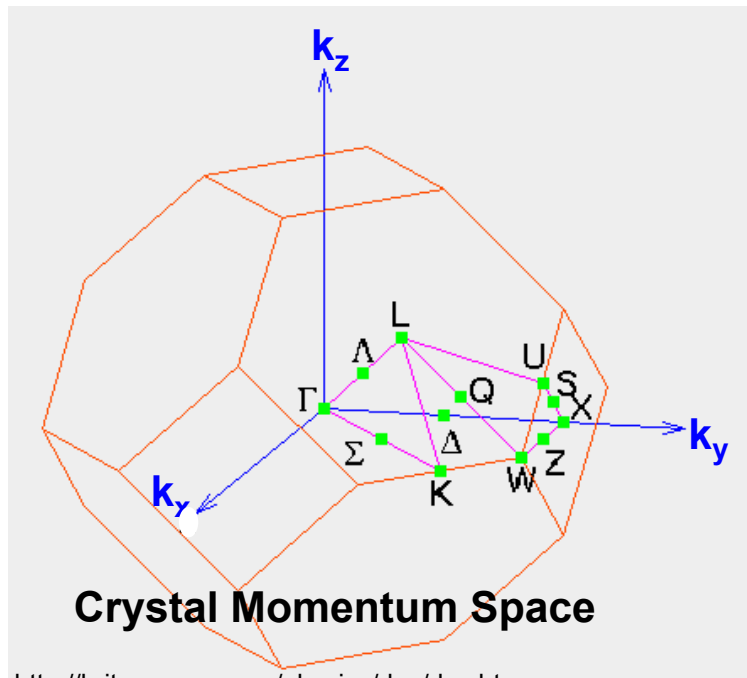
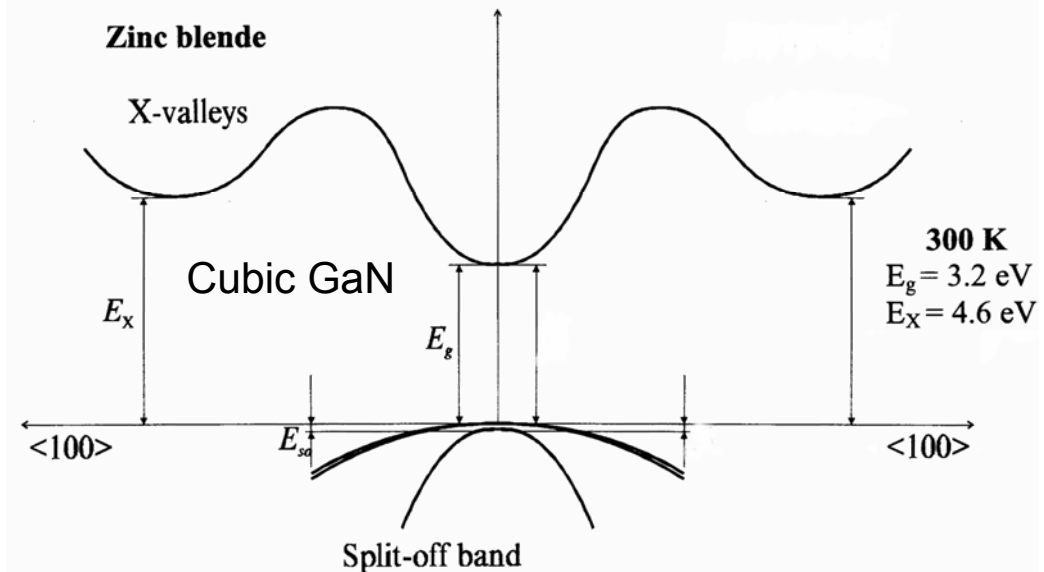
# Now consider an periodic potential in 1D Kronig-Penney Model



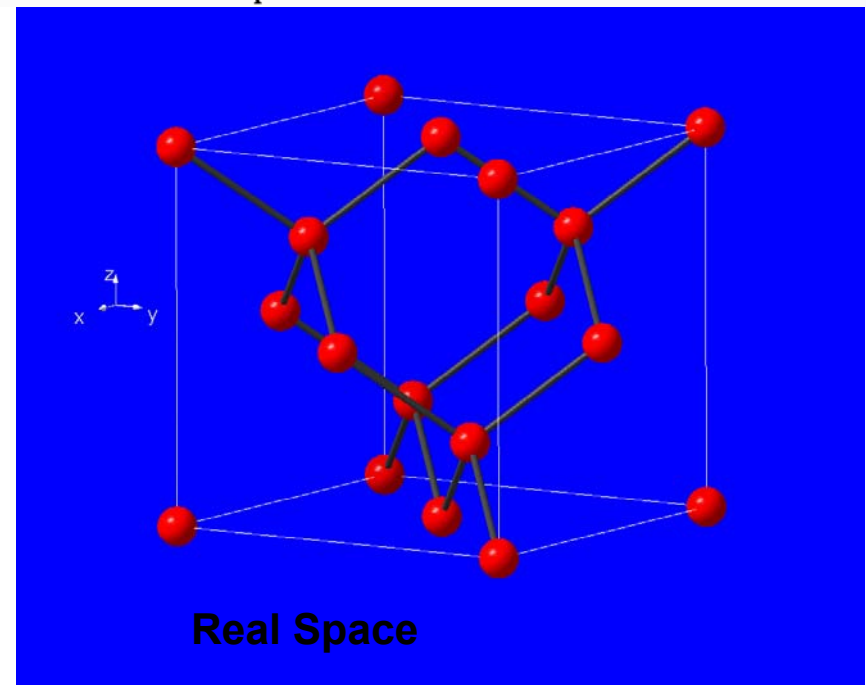
Visualization of a conduction band electron moving in a crystal.

# Now consider the 3D periodic potential in a cubic crystal

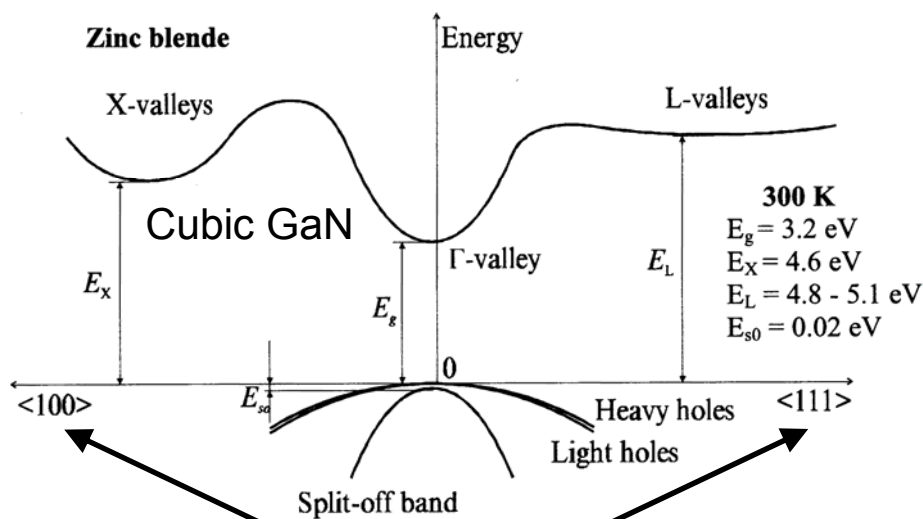
- Different potentials exist in different directions
- Electron wavelength and crystal momentum,  $k=2\pi/\lambda$ , differs with direction
- Many different parabolic E-k relationships exist depending on our crystalline momentum



<http://britneyspears.ac/physics/dos/dos.htm>

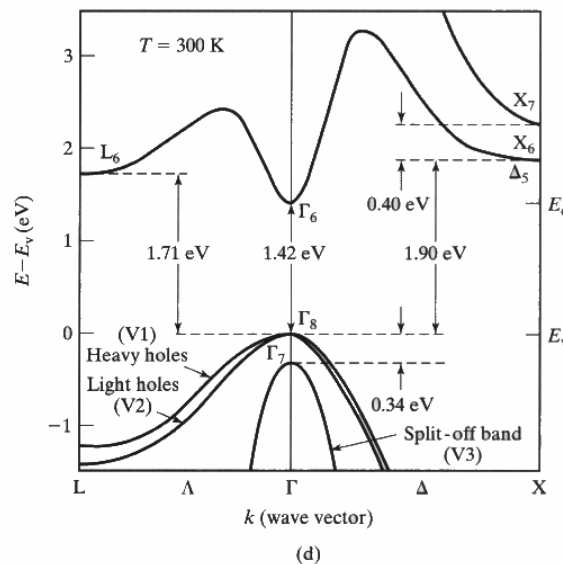
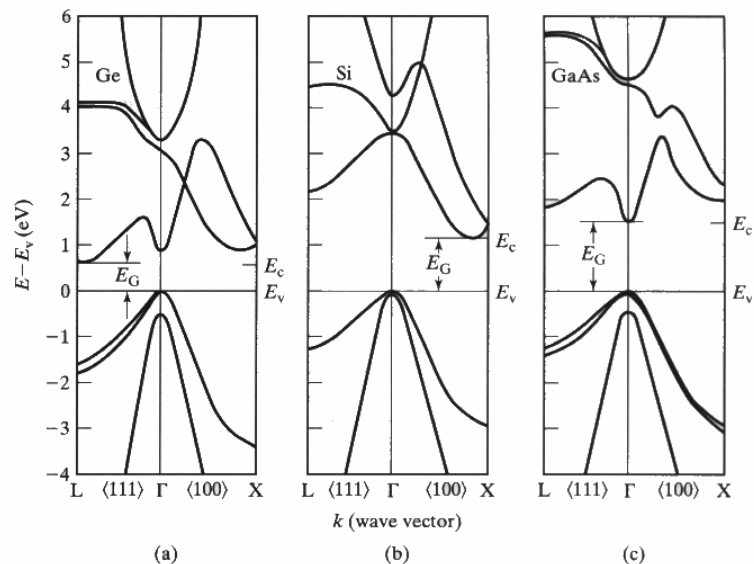


# Now consider the 3D periodic potential in a cubic crystal



**300 K**  
 $E_g = 3.2$  eV  
 $E_x = 4.6$  eV  
 $E_L = 4.8 - 5.1$  eV  
 $E_{s0} = 0.02$  eV

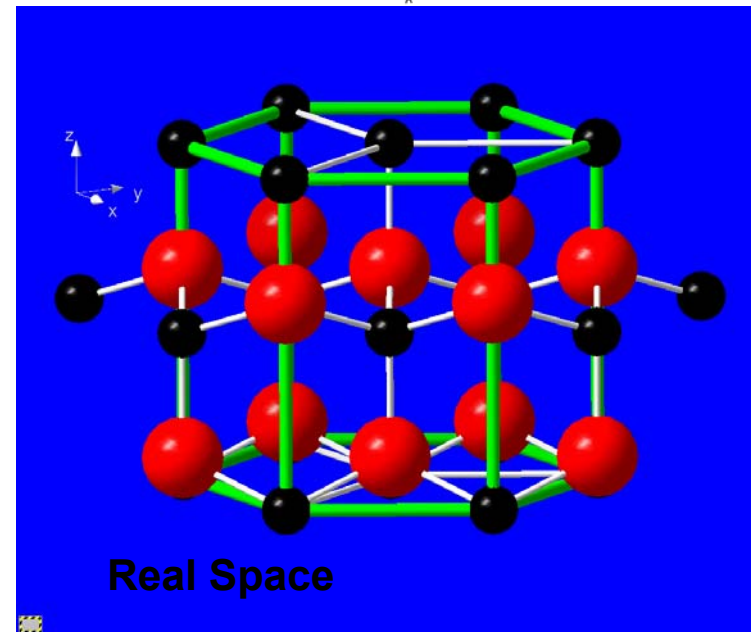
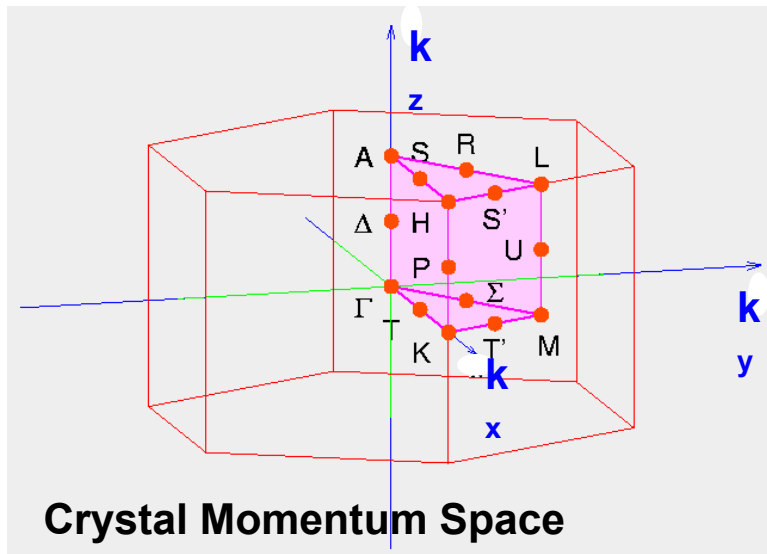
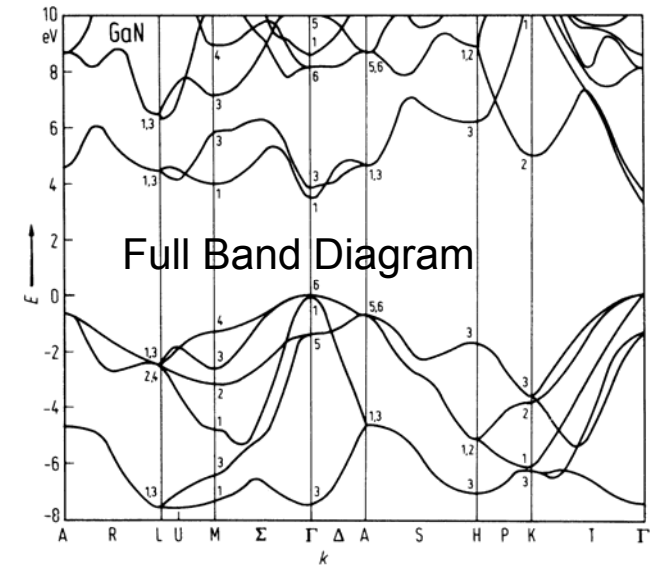
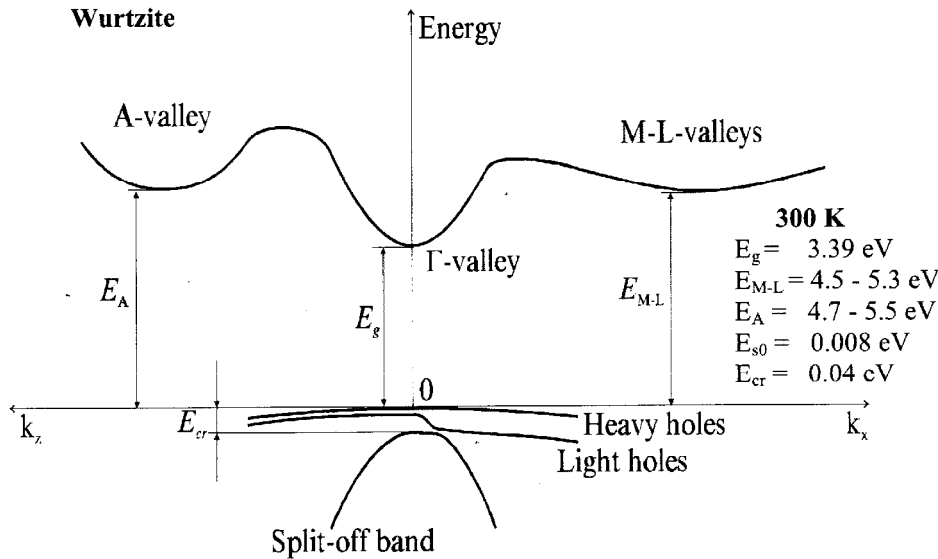
- All equivalent directions give redundant information and thus are not repeated
- Most important k-space points
  - $\Gamma$ -point is the center of crystal momentum space (k-space) at  $k=0$
  - X-point is the edge of the first Brillouin zone ( $\pi/L$  edge) of crystal momentum space (k-space) in the  $\langle 100 \rangle$  direction
  - L-point is the edge of the first Brillouin zone ( $\pi/L$  edge) of crystal momentum space (k-space) in the  $\langle 111 \rangle$  direction



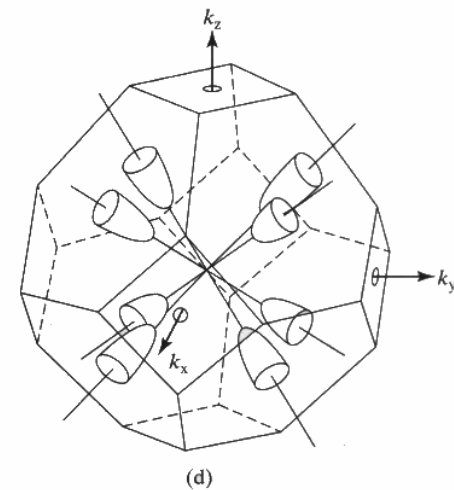
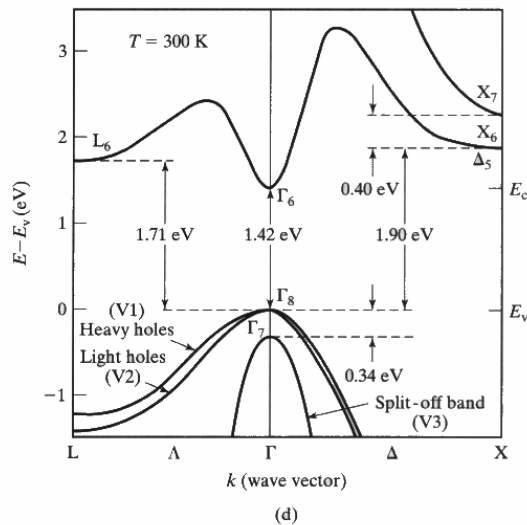
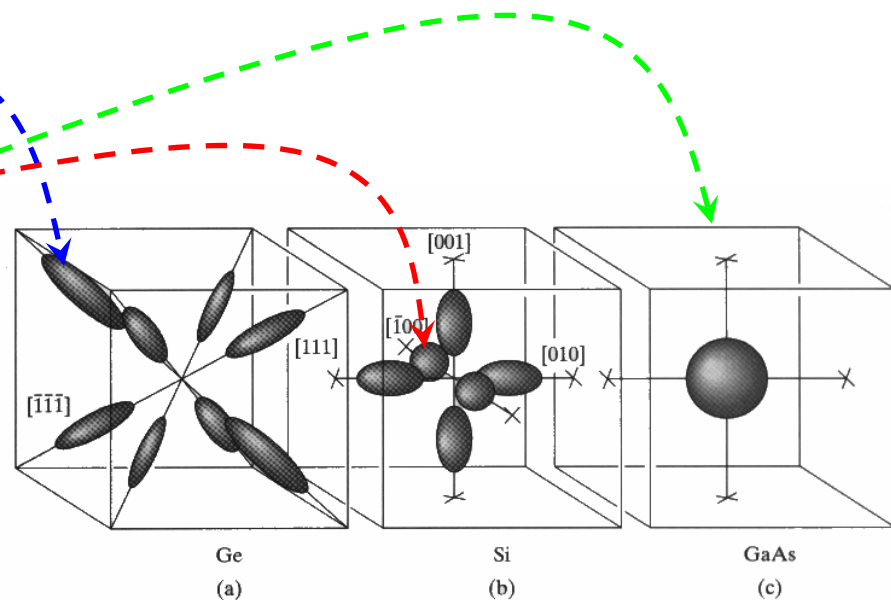
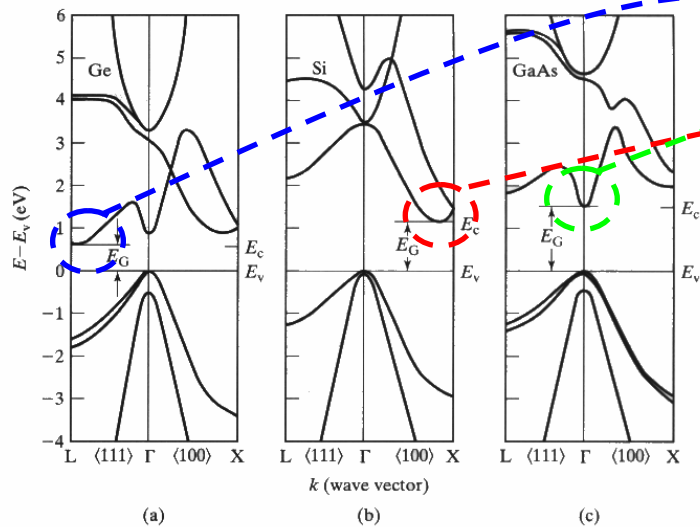
**Figure 3.13**  $\langle 100 \rangle / \langle 111 \rangle$  E-k diagrams characterizing the conduction and valence bands of (a) Ge, (b) Si, and (c, d) GaAs. [(a-c) after Sze<sup>[2]</sup>; (d) from Blakemore.<sup>[1]</sup> Reprinted with permission.]

Neudeck and Peirret Fig 3.13

# Now consider the 3D periodic potential in a hexagonal crystal



# Where are the electron trajectories/momentum vectors in the crystal?



**Figure 3.13**  $\langle 100 \rangle / \langle 111 \rangle$   $E$ - $k$  diagrams characterizing the conduction and valence bands of (a) Ge, (b) Si, and (c, d) GaAs. [(a-c) after Sze<sup>[2]</sup>; (d) from Blakemore.<sup>[1]</sup> Reprinted with permission.]  
Neudeck and Peirret Fig 3.13

Constant-energy surfaces characterizing the conduction-band structure in (a, d) Ge, (b) Si, and (c) GaAs. (d) Shows the truncation of the Ge surfaces at the Brillouin-zone boundaries. [(a-c) after Sze<sup>[2]</sup> and Ziman<sup>[3]</sup>; (d) from McKelvey.<sup>[4]</sup> Reprinted with permission; the latter from Robert E. Krieger Publishing Co., Malabar, FL.]  
Neudeck and Peirret Fig 3.14