

## **Lecture 3**

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

### **Reading:**

**Notes and Anderson<sup>2</sup> sections 1.4-1.6, 2.1-2.3, 2.6,  
Supplement 1A**

## 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

People RARELY get quantum mechanics on 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

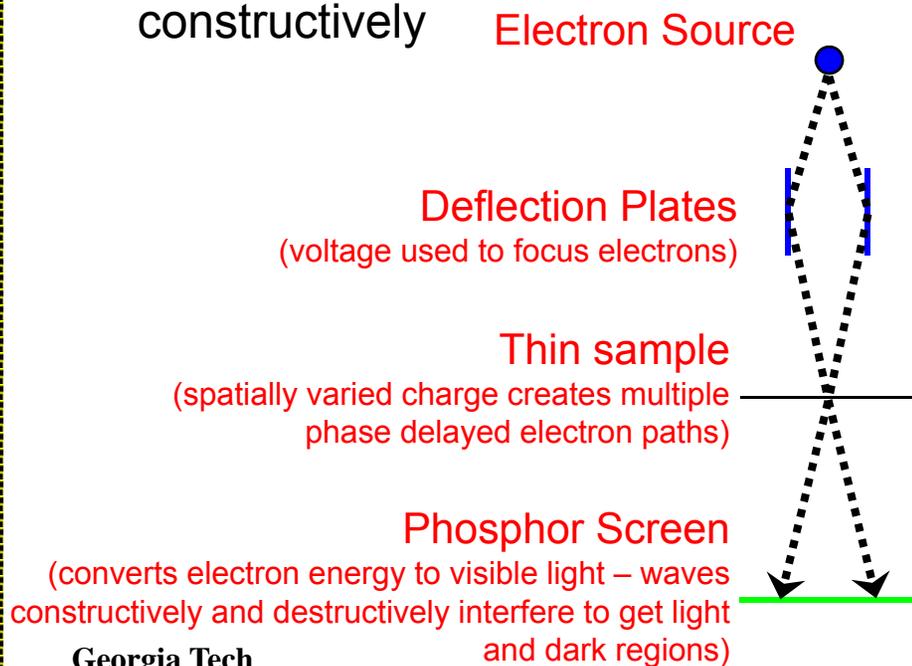
Mayer and Lau – Electronic Materials Science

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

Tipler – Physics for scientists and engineers V4.

# Introduction to Quantum Mechanics

- 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



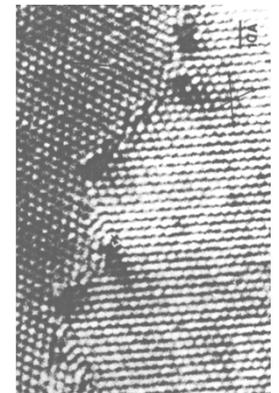
$$v = \frac{h}{m\lambda}$$

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

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

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

15KV gives sub atomic resolution!



# Introduction to Quantum Mechanics

- 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?

**Describe particles by a wave equation → Later...**

- 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

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



In Quantum mechanics, the particle is described by a wavefunction,  $\Psi(x,y,z,t)$

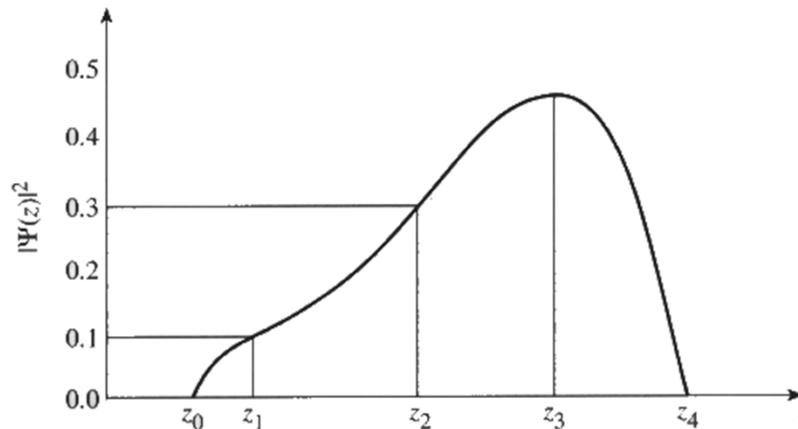
It is related to the probability of finding an electron at time  $t$  in a volume  $dxdydz$ . Specifically, this probability is:

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

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 – Operators and Observables

In Quantum Mechanics, physical observables are determined by applying an “operator” to the wavefunction,  $\Psi$ . Operators “operate” on the wavefunction to determine what the physical quantity is.

Since the Wavefunction is normalized, one can use the operator acting on the wavefunction to determine the “most likely” or “expected” value of a variable.

<u>Variable</u>		<u>Operator to be Applied</u>		<u>Expectation Value</u>
<i>position</i> $x$	$\leftrightarrow$	$x$	$\leftrightarrow$	$\langle x \rangle = \int_V \Psi^* x \Psi dV$
<i>momentum</i> $p_x p_y p_z$	$\leftrightarrow$	$\left(\frac{\hbar}{i}\right)\frac{\partial}{\partial x}, \left(\frac{\hbar}{i}\right)\frac{\partial}{\partial y}, \left(\frac{\hbar}{i}\right)\frac{\partial}{\partial z}$	$\leftrightarrow$	$\langle p_x \rangle = \int_V \Psi^* \left(\frac{\hbar}{i}\right)\frac{\partial}{\partial x} \Psi dV$
<i>Total Energy</i> $E$	$\leftrightarrow$	$-\left(\frac{\hbar}{i}\right)\frac{\partial}{\partial t}$	$\leftrightarrow$	
<i>Random function</i> $f(x, y, z)$	$\leftrightarrow$	$f(x, y, z)$	$\leftrightarrow$	$\langle f(x, y, z) \rangle = \int_V \Psi^* f(x, y, z) \Psi dV$

Note that the normalization condition is :  $1 = \int_V \Psi^* \Psi dV$

# Introduction to Quantum Mechanics - The Schrödinger equation

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

Schrödinger Equation:

• ***There are NO physical assumptions available to “derive” the Schrödinger Equation!***  
It just happens to work as a model.

• 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

# Introduction to Quantum Mechanics - solve the Schrödinger equation

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:

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

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:

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

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

# Introduction to Quantum Mechanics – Time variable solution

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 – Real Space Solution

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 – Free Space Particle

Consider a specific solution for 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,  $B=0$ .

**Important: An electron in free space turns out to be well described by a plane wave. As we move forward, to electrons in other mediums, we will use “groups of” plane waves (Fourier sums) and “modified plane waves” to describe the electrons in other mediums.**

# Introduction to Quantum Mechanics - Uncertainty

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

## Momentum-Position Space and Transformations

There exists a set of equivalent wave functions, one in real space and one in momentum space that can be used to describe the electron. They are related by Fourier transforms.



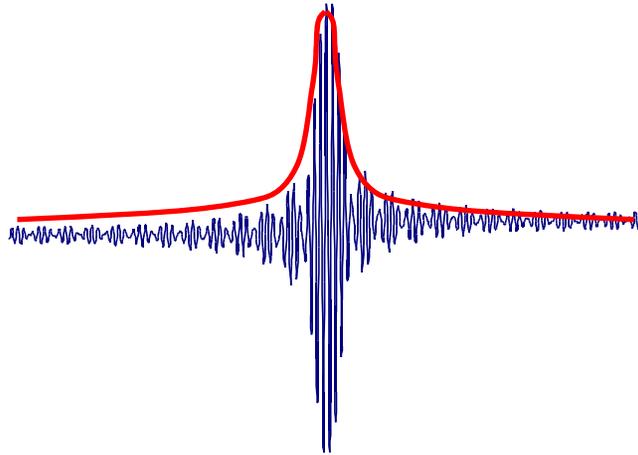
$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp \quad \Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{-ipx/\hbar} dx$$

If  $\Psi(x)$  is normalized then so is  $\Phi(p)$

$$\int_{-\infty}^{\infty} \Psi^*(x) \Psi(x) dx = \int_{-\infty}^{\infty} \Phi^*(p) \Phi(p) dp = 1$$

If a state is localized in position,  $x$ , it is delocalized in momentum,  $p$ . This leads us to a fundamental quantum mechanical principle: You can not have infinite precision measurement of position and momentum simultaneously. If the momentum (and thus wavelength from  $p=h/\lambda$ ) is known, the position of the particle is unknown and vice versa.

# Momentum-Position Space and Transformations



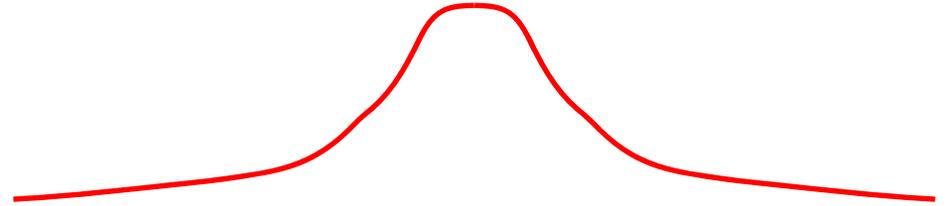
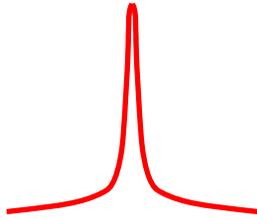
$$\Psi(x) = e^{\frac{-x^2}{2b^2}}$$



$$\phi(p) = be^{\frac{-b^2 p^2}{2\hbar^2}}$$

The above wave function is a superposition of 27 simple plane waves and creates a net wave function that is localized in space. The red line is the approximate amplitude envelope (related to  $\Psi^*\Psi$  – a smoothed version). These types of wave functions are useful in describing particles such as electrons. The wave function envelope can be approximated with a Gaussian function in space. Using the Fourier relationship between space and momentum, this can be transformed into a Gaussian in momentum. The widths of the two Gaussians are inversely related as shown on the next slide.

# Momentum-Position Space and Transformations



$$\Psi(x) = e^{\frac{-x^2}{2b^2}}$$



$$\phi(p) = be^{\frac{-b^2 p^2}{2\hbar^2}}$$

The widths of the two Gaussians are inversely related (see variance with  $b^2$  in each equations). Thus, accurate knowledge of position leads to inaccurate knowledge of momentum.

# Introduction to Quantum Mechanics – Parabolic Energy-Momentum Relationship

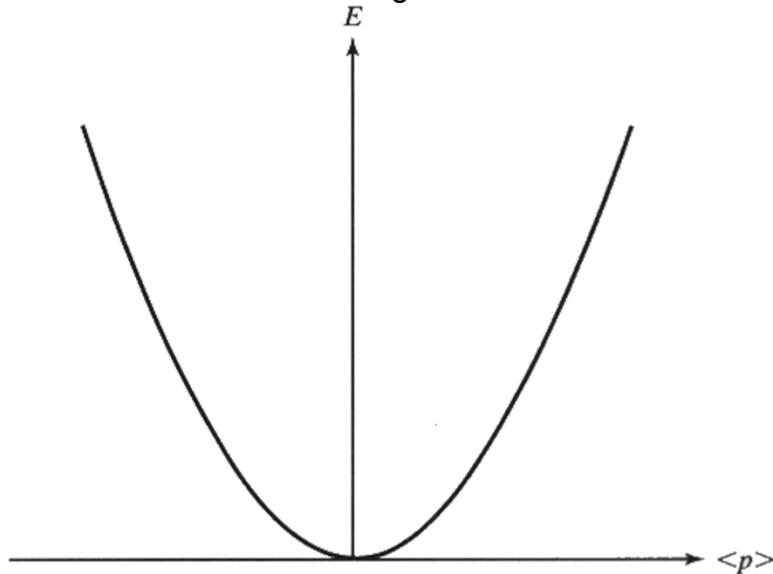
The solution to this free particle example brings out several important observations about the dual wave-particle nature of our universe:

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

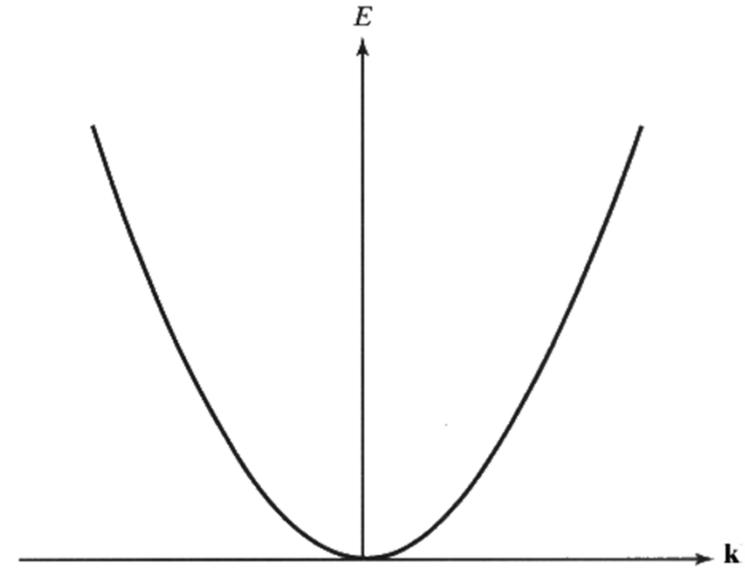
- While particles act as waves, their charge is carried as a particle. I.e. you can only say that there is a “probability” of finding an electron in a particular region of space, but if you find it there, it will have all of its charge there, not just a fraction.
- Energy of moving particles follows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



Energy-momentum relationship for a free particle.

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

Georgia Tech

ECE 3080 - Dr. Alan Doolittle

# Introduction to Quantum Mechanics

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:

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

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

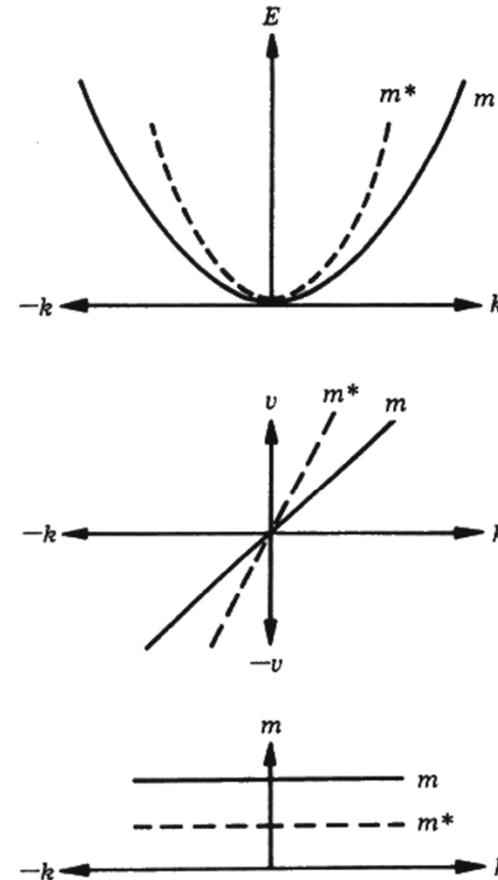


FIGURE 12.2 E-k diagram for a free electron with mass  $m$  (solid line) and a smaller mass,  $m^*$ . The parabolic E-k diagram leads to a linear  $v$  versus  $k$  relation and a constant mass.

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

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

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

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

$$\Psi(x) = A e^{ikx} + B e^{-ikx}$$

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

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

$$\Psi = \Psi(x) w(t) = A e^{-i(\omega t - kx)} + B e^{-i(\omega t + kx)}$$

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.***

# Localized Particles Result in Quantized Energy/Momentum: Infinite Square Well

First a needed tool: Consider an electron trapped in an energy well with infinite potential barriers. The reflection coefficient for an infinite potential is 1 so the electron cannot penetrate the barrier.

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

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

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

General Solution :  $\Psi(x) = A \sin(kx) + B \cos(kx)$

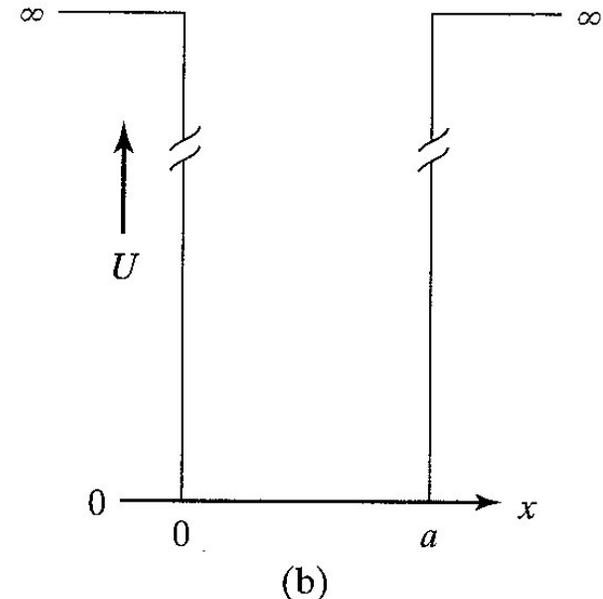
$$\text{where } k = \frac{2\pi}{\lambda} = \sqrt{\frac{2mE}{\hbar^2}} \text{ or } E = \frac{\hbar^2 k^2}{2m}$$

Boundary Conditions :

$$\Psi(0) = 0 \Rightarrow B = 0$$

$$\Psi(a) = 0 \Rightarrow A \sin(ka) = 0 \Rightarrow k = \frac{n\pi}{a} \text{ for } n = \pm 1, \pm 2, \pm 3 \dots$$

$$\Psi_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right) \text{ and } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$



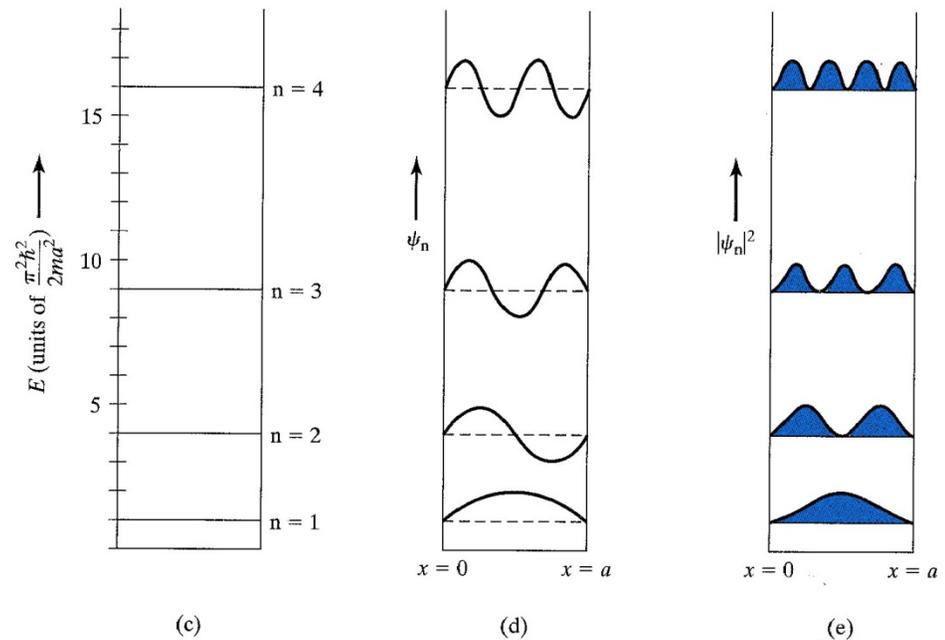
After Neudeck and Pierret Figure 2.4a

# Localized Particles Result in Quantized Energy/Momentum: Infinite Square Well

What does it mean?

$$\Psi_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right) \text{ and } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

A standing wave results from the requirement that there be a node at the barrier edges (i.e. BC's:  $\Psi(0)=\Psi(a)=0$  ). The wavelength determines the energy. Many different possible "states" can be occupied by the electron, each with different energies and wavelengths.



**Figure 2.4** Particle in an infinitely deep one-dimensional potential well. (a) Spatial visualization of the particle confinement. (b) The assumed potential energy versus position dependence. (c) First four allowed energy levels. (d) Wavefunctions and (e)  $|\psi|^2$  associated with the first four energy levels.  $|\psi|^2$  is proportional to the probability of finding the particle at a given point in the potential well.

# Localized Particles Result in Quantized Energy/Momentum: Infinite Square Well

What does it mean?

$$\Psi_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right) \text{ and } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Solution for much larger “a”. Note:  
offset vertically for clarity.

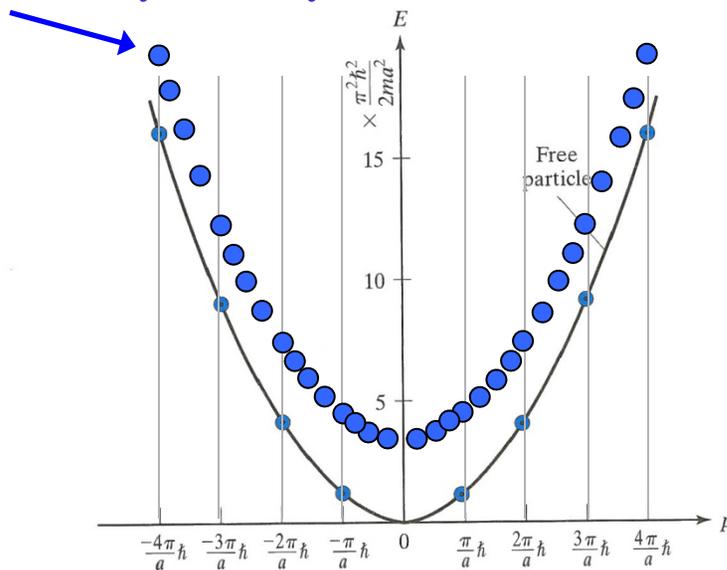


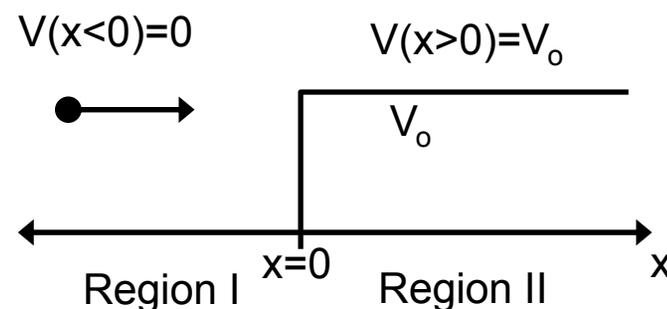
Figure 2.5 Allowed infinite-well particle energy versus counterpropagating wave momentum (discrete points) referenced against the free particle  $E-(p)$  relationship.

Recall, a free particle has  $E \sim k^2$ . Instead of being continuous in  $k^2$ ,  $E$  is discrete in  $n^2$ ! I.e. the energy values (and thus, wavelengths/ $k$ ) of a confined electron are quantized (take on only certain values). Note that as the dimension of the “energy well” increases, the spacing between discrete energy levels (and discrete  $k$  values) reduces. In the infinite crystal, a continuum the same as our free particle solution is obtained.

After Neudeck and Pierret Figure 2.5

## What about an electrostatic potential step?

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



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

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

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

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

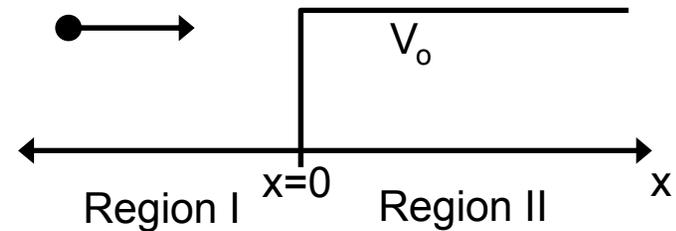
# Warning!

**The following is commonly taught in most undergraduate Quantum Mechanics Courses but, strictly speaking is WRONG!!!!**

**Specifically, the boundary conditions used in the following analysis are incomplete and one must apply the “probability density current” concept, a more complex analysis to arrive at a complete solution for the reflection and transmission coefficients. Due to the added complexity, we will chose to teach you the less complex but not exactly correct approach – a common practice for undergraduate classes as it teaches the concepts without the math complications. This neglects differing masses in regions as well as some other subtle features. If you would like to learn the exact approach, see lecture 6 from Dr. Doolittle’s ECE 6451 graduate level Quantum Mechanics class. The corrected values will be stated but not derived in this class.**

## What about an electrostatic potential step?

cont'd...



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

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

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

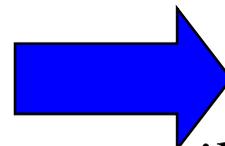
**When the “wave” is incident on the barrier, some of it is reflected, some of it is transmitted. However, since there is nothing at  $x=+\infty$  to reflect the wave back,  $B_{II}=0$ .**

**Since  $\psi$  is a wave, both  $\psi$  and it's 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

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

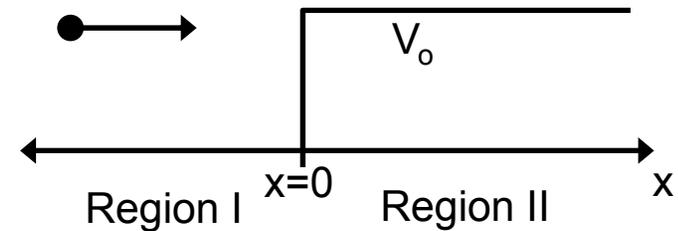
## What about an electrostatic potential step?

cont'd...

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

and

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



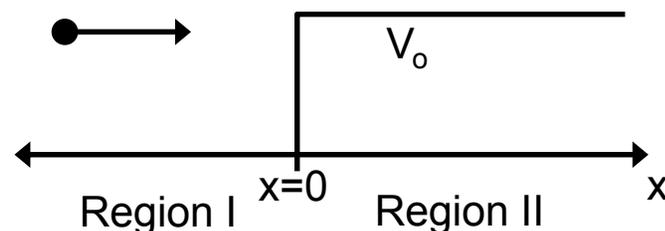
$$\Psi_I = \Psi_I(x)w_I(t) = A_I e^{-i(\omega t - k_I x)} + B_I e^{-i(\omega t + k_I x)}$$

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

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

## 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,**

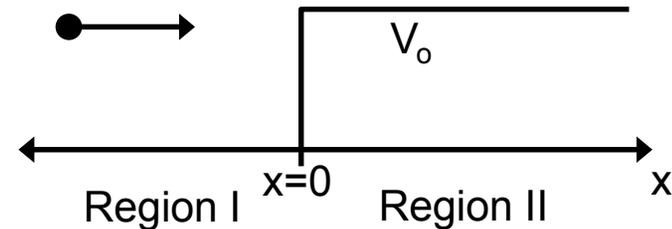
$$T \equiv \frac{A_{II}}{A_I} = \frac{2k_I}{k_I + k_{II}}$$

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

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

## What about an electrostatic potential step?

Not deriving but using the more accurate boundary condition described in the “warning”,....



**We can define a “reflection probability” as**

$$R^* R = \frac{k_I (B_I B_I^*)}{k_I (A_I A_I^*)} = \frac{(B_I B_I^*)}{(A_I A_I^*)}$$

**And likewise, we can define a transmission probability as**

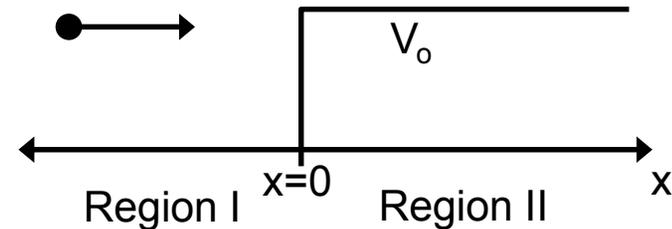
$$T^* T = \left| \frac{k_{II} (A_{II} A_{II}^*)}{k_I (A_I A_I^*)} \right|$$

**Note that the  $R^*R$  is the same but  $T^*T$  is different.**

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

# What about an electrostatic potential step?

cont'd...



**Final details:**

$$T^*T = \frac{k_{II} (A_{II} A_{II}^*)}{k_I (A_I A_I^*)} \quad \text{and} \quad R^*R = \frac{(B_I B_I^*)}{(A_I A_I^*)}$$

Since  $\frac{A_{II}}{A_I} = \frac{2k_I}{k_I + k_{II}}$  and  $T^*T = \left| \frac{k_{II}}{k_I} \left( \frac{2k_I^*}{k_I^* + k_{II}^*} \right) \left( \frac{2k_I}{k_I + k_{II}} \right) \right|$

$$T^*T = \frac{4k_{II}}{k_I} \left( \frac{1}{\left| 1 + \frac{k_{II}}{k_I} \right|^2} \right)$$

$$R^*R = \left| \frac{k_I - k_{II}}{k_I + k_{II}} \right|^2$$

$$T^*T + R^*R = 1$$

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

# What about an electrostatic potential step?

cont'd...

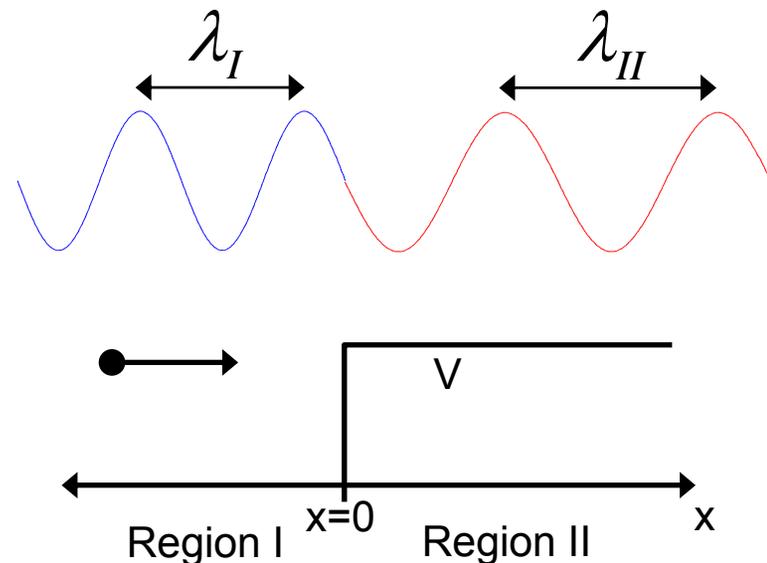
Consider 2 cases: Case 1:  $E > V$

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

However,  $R^*R$  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  $\sim 0$  ( $k_I \rightarrow k_{II}$ )

$$R^*R \equiv \left| \frac{B_I}{A_I} \right|^2 = \left| \frac{k_I - k_{II}}{k_I + k_{II}} \right|^2$$
$$T^*T = \frac{4k_{II}}{k_I} \left( \frac{1}{\left| 1 + \frac{k_{II}}{k_I} \right|^2} \right)$$



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

# 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,  $e^{(ik_{II}x)}$ , a decaying function of the form,  $e^{(-ax)}$  results in region II.

**Transmitted Wave**

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

$A_{II}$  can be complex

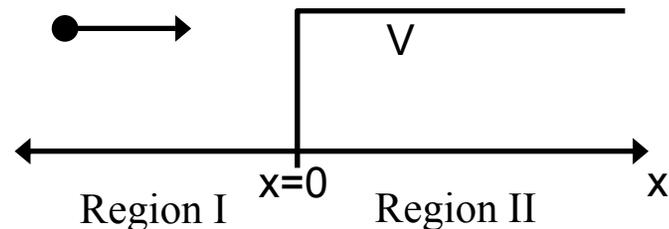
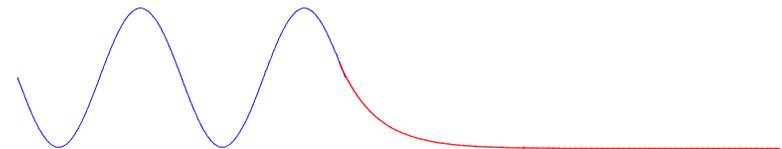
However,  $T^*T$  is now finite but evanescent. Evanescent waves carry no current (see homework). So even though the electron has an energy,  $E$ , less than  $V$  it will have a finite probability of being found within the potential barrier. The probability of finding the electron deep inside the potential barrier is  $\sim 0$  due to the rapid decay of  $\psi$ .

$$R^*R \equiv \left| \frac{B_I}{A_I} \right|^2 = \left| \frac{k_I - i|k_{II}|}{k_I + i|k_{II}|} \right|^2 = \frac{z^*}{z} = 1$$

$T^*T = 0$

↑

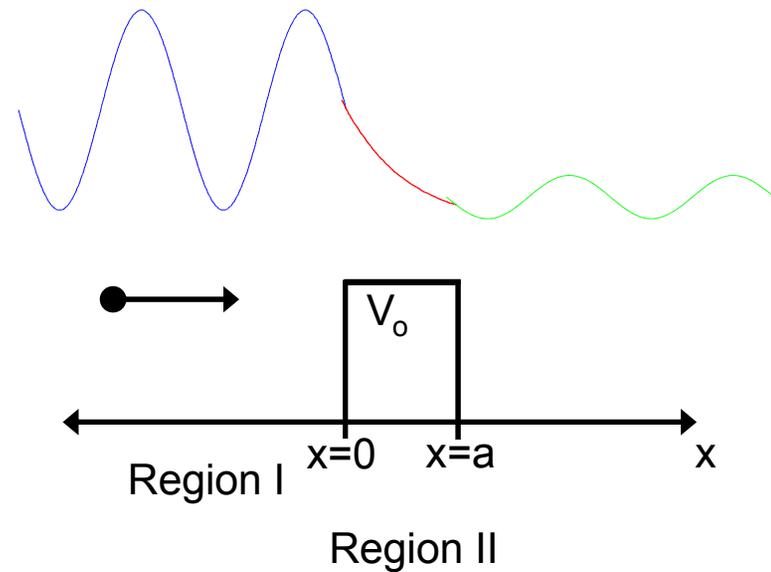
Due to  $J_{\text{Transmitted}} = 0$



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

## What about an electrostatic potential step?

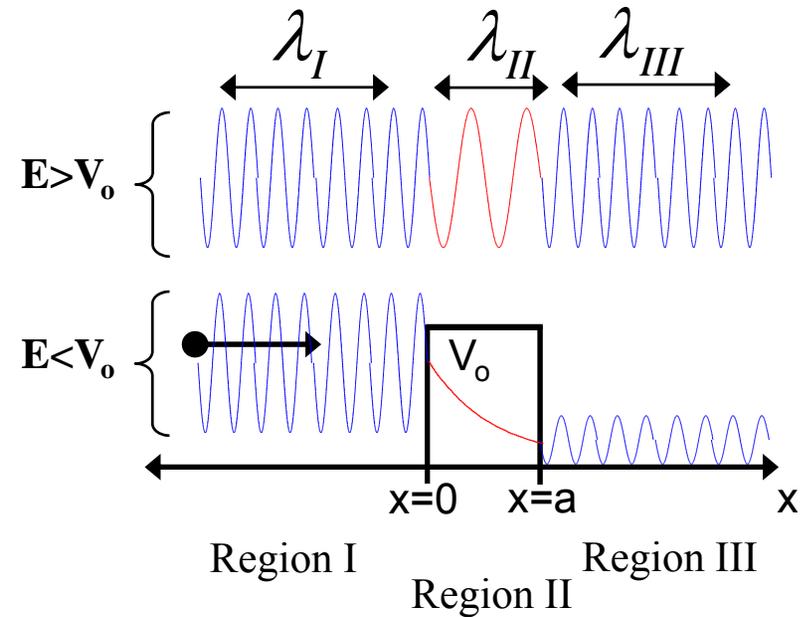
Without proof, consider the following potential profile with an electron of energy  $E < V_0$ .



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.

## What about an electrostatic potential step?

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 its way.

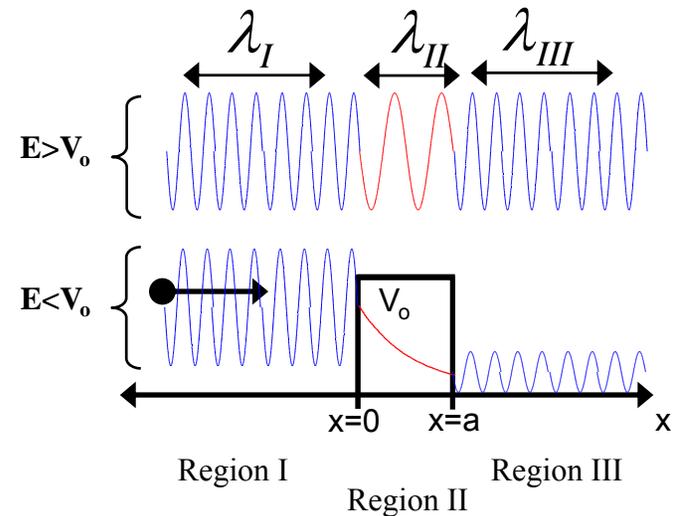
# What about an electrostatic potential step?

Consider the following potential profile with an electron of energy  $E < V_0$ .

$$\Psi_I = \underbrace{Ae^{-i(\omega t - k_1 x)}}_{\text{Incident Wave}} + \underbrace{Be^{-i(\omega t + k_1 x)}}_{\text{Reflected Wave from } x=0}$$

$$\Psi_{II} = \underbrace{Ce^{-i(\omega t - k_2 x)}}_{\text{+x Wave Region II}} + \underbrace{De^{-i(\omega t + k_2 x)}}_{\text{Reflected Wave from } x=+a}$$

$$\Psi_{III} = \underbrace{Fe^{-i(\omega t - k_1 x)}}_{\text{Transmitted Wave}}$$



**Energy is conserved across the boundary so,**

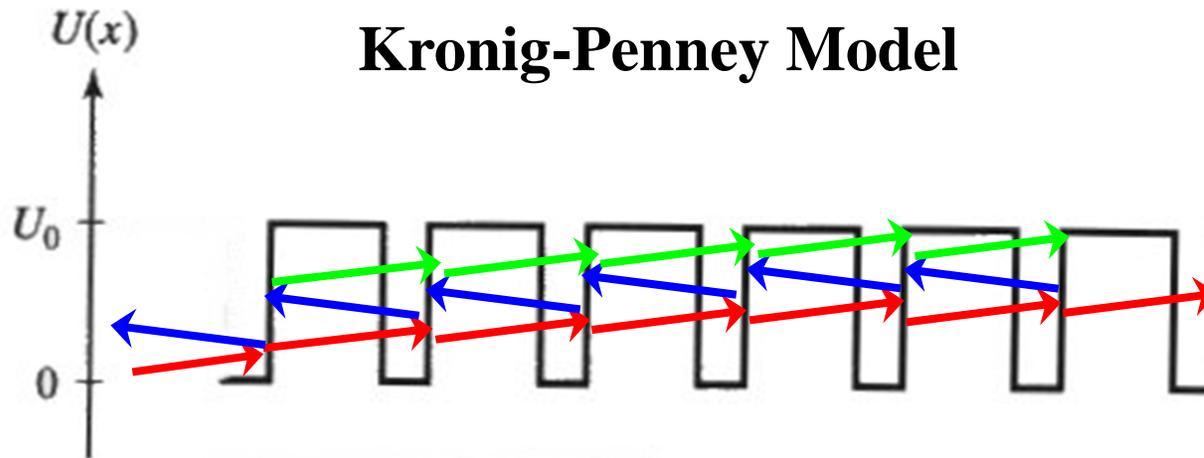
$$\frac{\hbar^2 k_1^2}{2m} = E$$

$$\frac{\hbar^2 k_2^2}{2m} = E - V_0$$

$$\frac{\hbar^2 k_1^2}{2m} = E$$

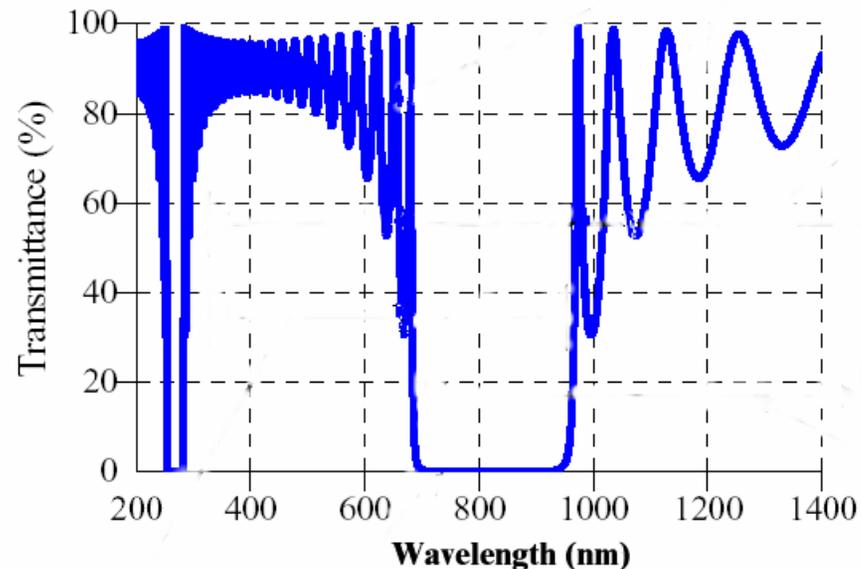
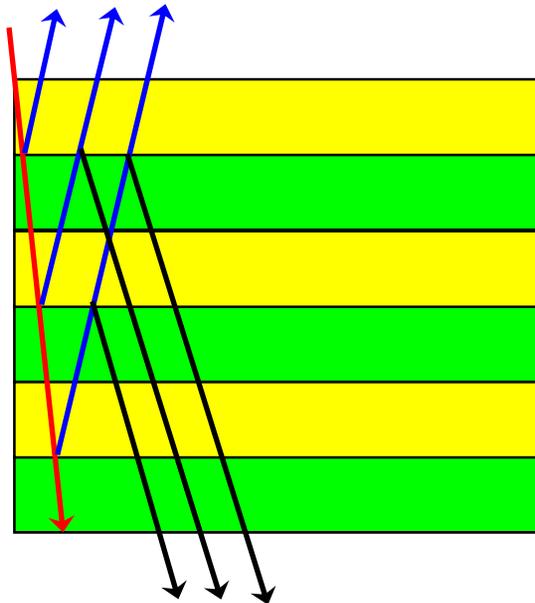
$$k_1 = \frac{2\pi}{\lambda_1} = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k_2 = \frac{2\pi}{\lambda_2} = \sqrt{\frac{2m(E - V)}{\hbar^2}}$$

# Kronig-Penney Model



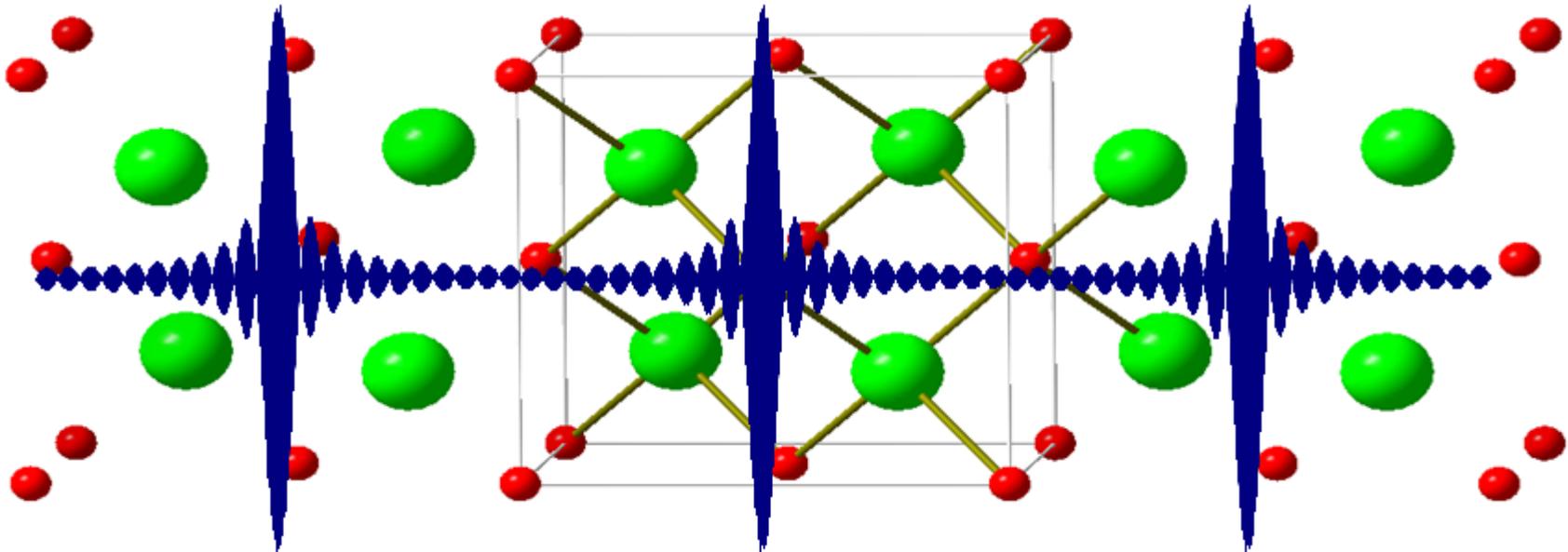
Resonant reflectance/transmission creates “standing waves” in the crystal. Only certain wavelengths (energies) can pass through the 1D crystal.

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”.



# Now consider an periodic potential in 1D

## Kronig-Penney Model: Bloch Functions Explained

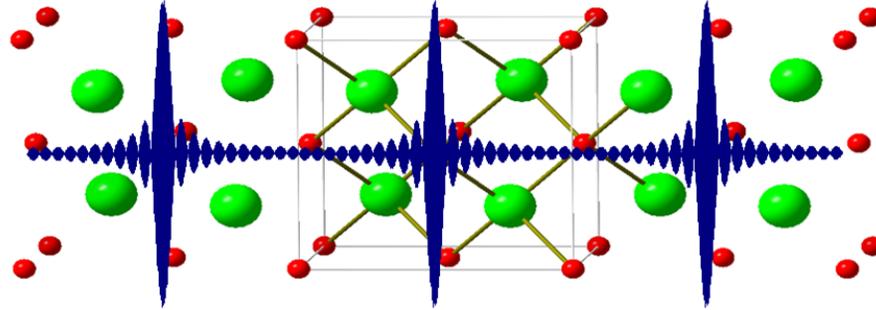


Since each unit cell is indistinguishable from the next, the probability of finding an electron in one unit cell is identical to that of finding it in an adjacent unit cell.

The Bloch theorem states that since the potential repeats every “ $a$ ” lengths, the magnitude of the wavefunction (but not necessarily the phase) must also repeat every “ $a$ ” 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.

# Now consider an periodic potential in 1D

## Kronig-Penney Model: Bloch Functions Explained



To achieve this property, the **MAGNITUDE** of the wavefunction (but not necessarily the wavefunction) must have the same periodicity as the lattice. Thus, we choose a wavefunction that is modulated by the periodicity of the lattice.

Since  $V(r + a) = V(r)$

we choose plane waves modulated by a periodic function,

$$\Psi(r) = e^{ikr} u_{nk}(r) \text{ where } u_{nk}(r) = u_{nk}(r + a)$$

Thus,

$$\Psi(r + a) = u_{nk}(r + a) e^{ik(r+a)}$$

$$\Psi(r + a) = e^{ika} [u_{nk}(r) e^{ikr}] = e^{ika} \Psi(r) \text{ or merely a phase shifted version of } \Psi(r)$$

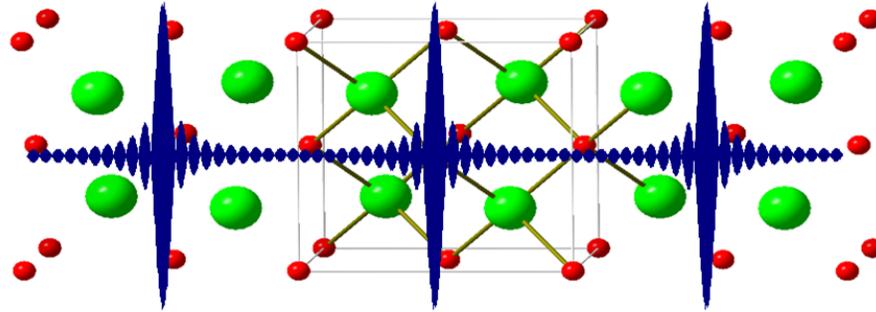
The wavefunction in one unit cell is merely a phase shifted version of the wavefunction in an adjacent unit cell.

Thus,

$$\Psi^*(r + a) \Psi(r + a) = e^{-ika} \Psi^*(r) e^{ika} \Psi(r) = \Psi^*(r) \Psi(r)$$

**Thus, by using this Bloch Function choice for the wave function, the probability of finding an electron in one unit cell is identical to that of finding it in an adjacent unit cell – as expected.**

## An Important Aside: Effect of Bloch Functions



Assuming a large number of unit cells in a material,  $N$ , the boundary condition for the system is  $Na$  translations must result in the wavefunction being translated to return to itself? (The probability at the material edges must be symmetric and equal).

$$\Psi(x + Na) = e^{ikNa} \Psi(x) = \Psi(x)$$

Thus,

$$e^{ikNa} = 1 \text{ so taking the } N\text{th root,}$$

$$e^{ika} = 1^{(1/N)} = (e^{in2\pi})^{(1/N)} = e^{(in2\pi/N)}$$

$$ka = \left( n2\pi/N \right)$$

So the allowed states of  $k$  are :

$$k = \frac{2\pi n}{Na}$$

Thus, if  $N$  (the number of unit cells available) is very large, like in a semiconductor, the spacing between the allowed  $k$ -values ( $kn=2-kn=1$  etc... are almost continuous, justifying the treatment of the  $k$ -states as a continuum.

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

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

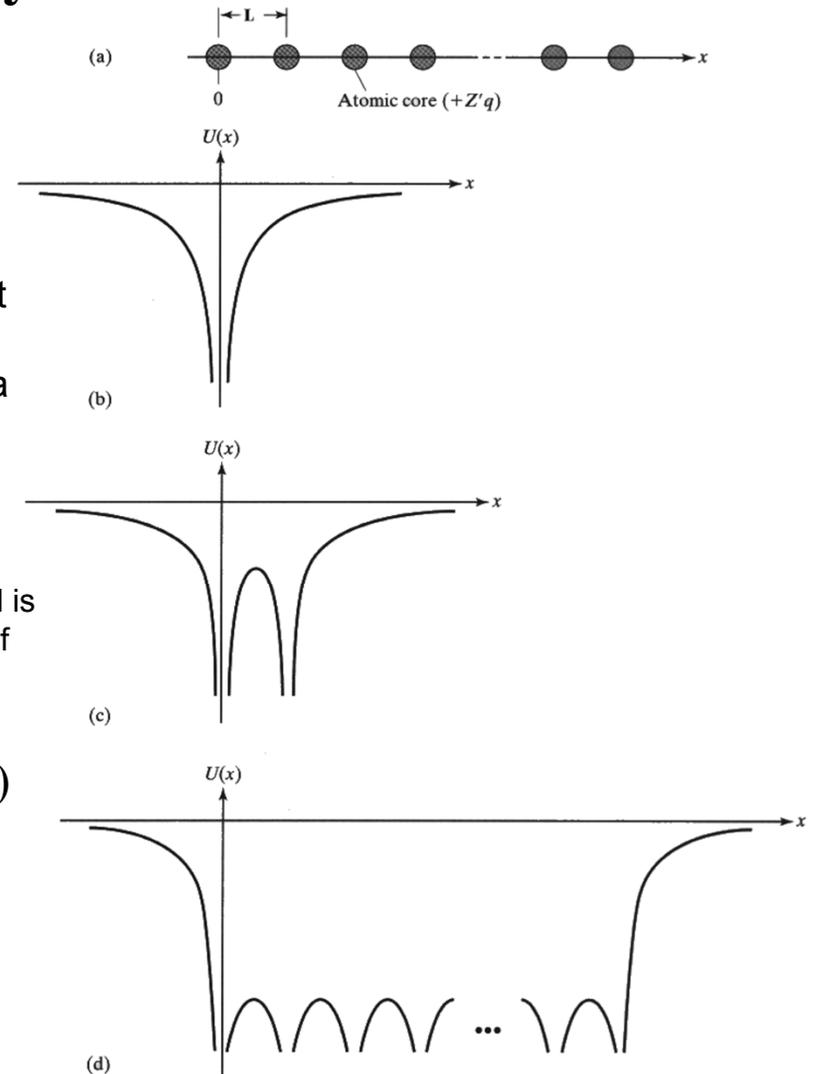
← The wavefunction in one unit cell is merely a phase shifted version of the wavefunction in an adjacent unit cell.

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

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  $(2\pi/\lambda)a \leq 1$ )

Georgia Tech



After Neudeck and Peirret Fig 3.1 ECE 3080 - Dr. Alan Doolittle

# 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,

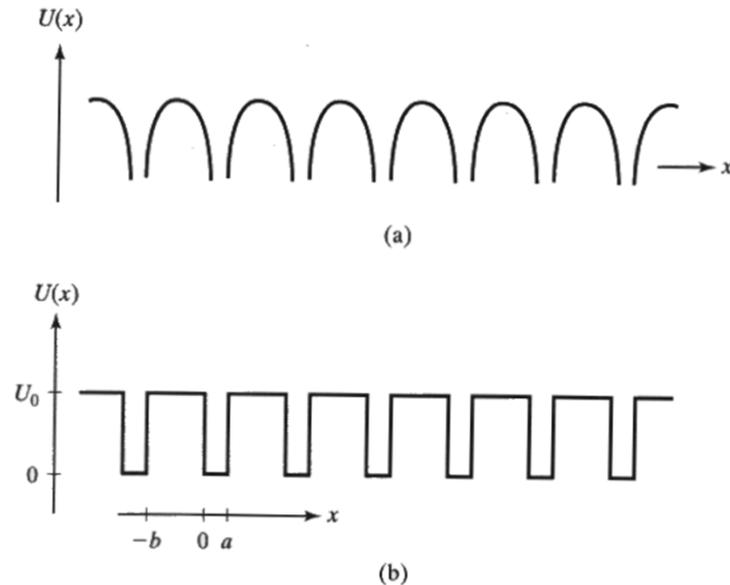
$$e^{ikx}$$

...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.

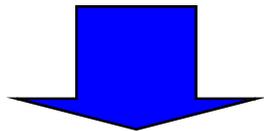
# Kronig-Penney Model

For  $0 < x < a$ :

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

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

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



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

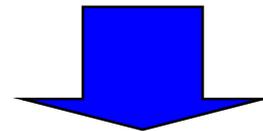
For  $-b < x < 0$ :

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

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

$$\beta = i \sqrt{\frac{2m(E - U_0)}{\hbar^2}} \text{ for } E > U_0$$

$$\beta = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \text{ for } 0 < E < U_0$$



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

# 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:

$$\left. \begin{aligned} \Psi_a(x) &= \Psi_b(x) \\ \frac{d\Psi_a(x)}{dx} \Big|_{x=0} &= \frac{d\Psi_b(x)}{dx} \Big|_{x=0} \end{aligned} \right\} \text{BC for continuous wave function at the boundary}$$

$$\left. \begin{aligned} \Psi_a(x=a) &= e^{ik(a+b)} \Psi_b(x=-b) \\ \frac{d\Psi_a(x)}{dx} \Big|_{x=a} &= e^{ik(a+b)} \frac{d\Psi_b(x)}{dx} \Big|_{x=-b} \end{aligned} \right\} \text{BC for periodic wave function at the boundary}$$

# 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:

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

**Function of Energy and not constrained.**

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

**Function of k and constrained to <+/- 1**

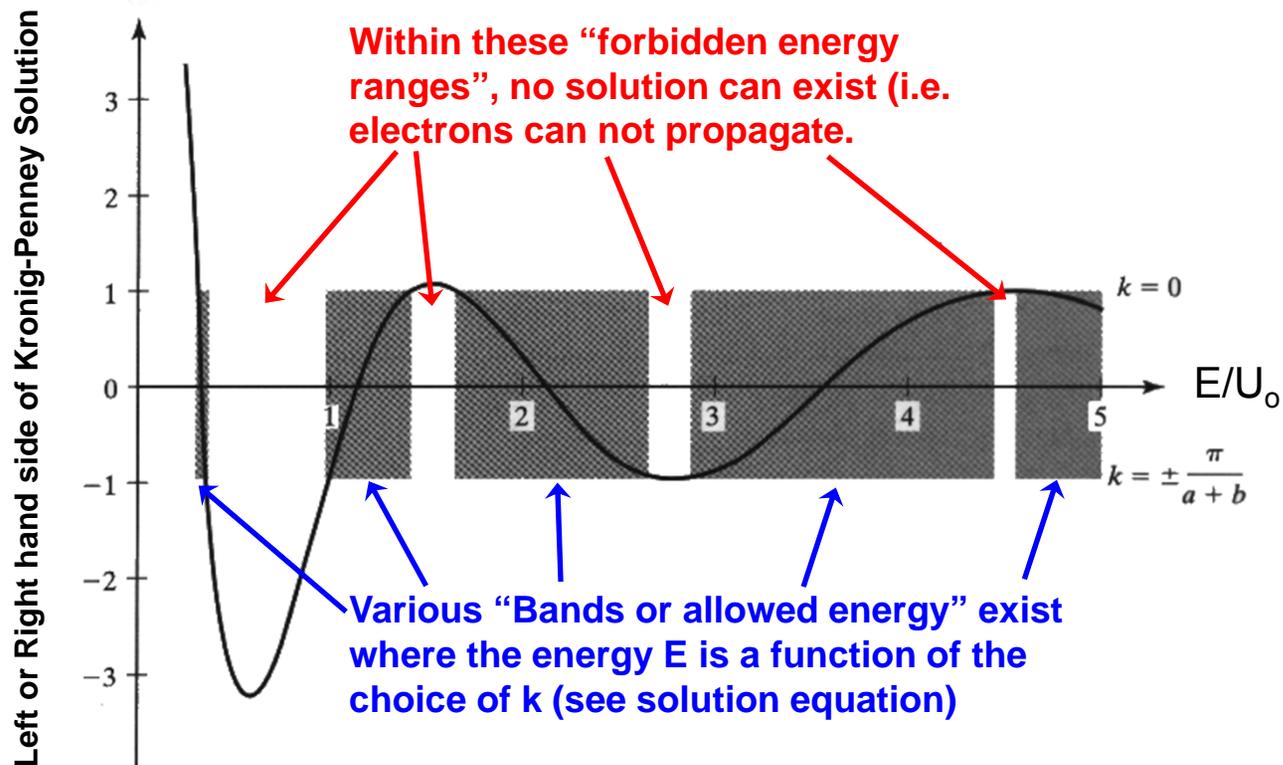
The right hand side is constrained to a range of +/- 1 and is a function of k only. The limits of the right hand side (+/- 1) occurs at  **$k=0$  and  $\pm \pi/(a+b)$**  where  $a+b$  is the period of the crystal potential. In other words, the min and maximum occur at k values corresponding to the center and edge of the “reciprocal lattice” (k-space version of real lattice).

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

The left hand side is NOT constrained to +/- 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,

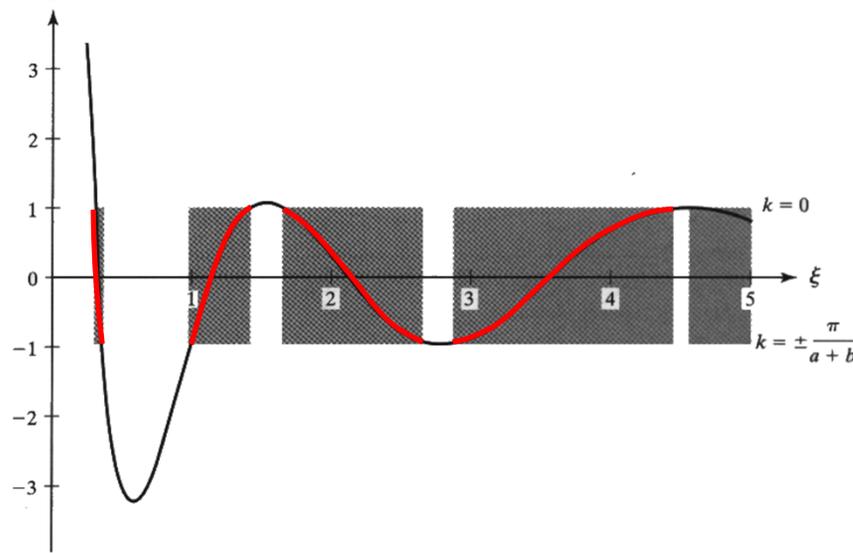
$$a\sqrt{\frac{2mU_0}{\hbar^2}} = b\sqrt{\frac{2mU_0}{\hbar^2}} = \pi$$

# Kronig-Penney Model

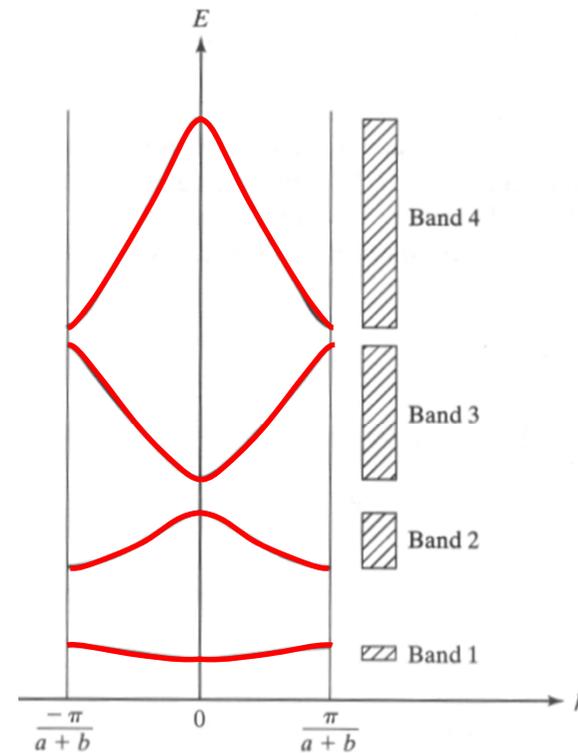
Replotting the previous result in another form recognizing the lower k limit is shared by + and  $-\pi/(a+b)$  while the upper limit is for  $k=0$ .

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.



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 ( $\alpha_0 a = \alpha_0 b = \pi$ ).

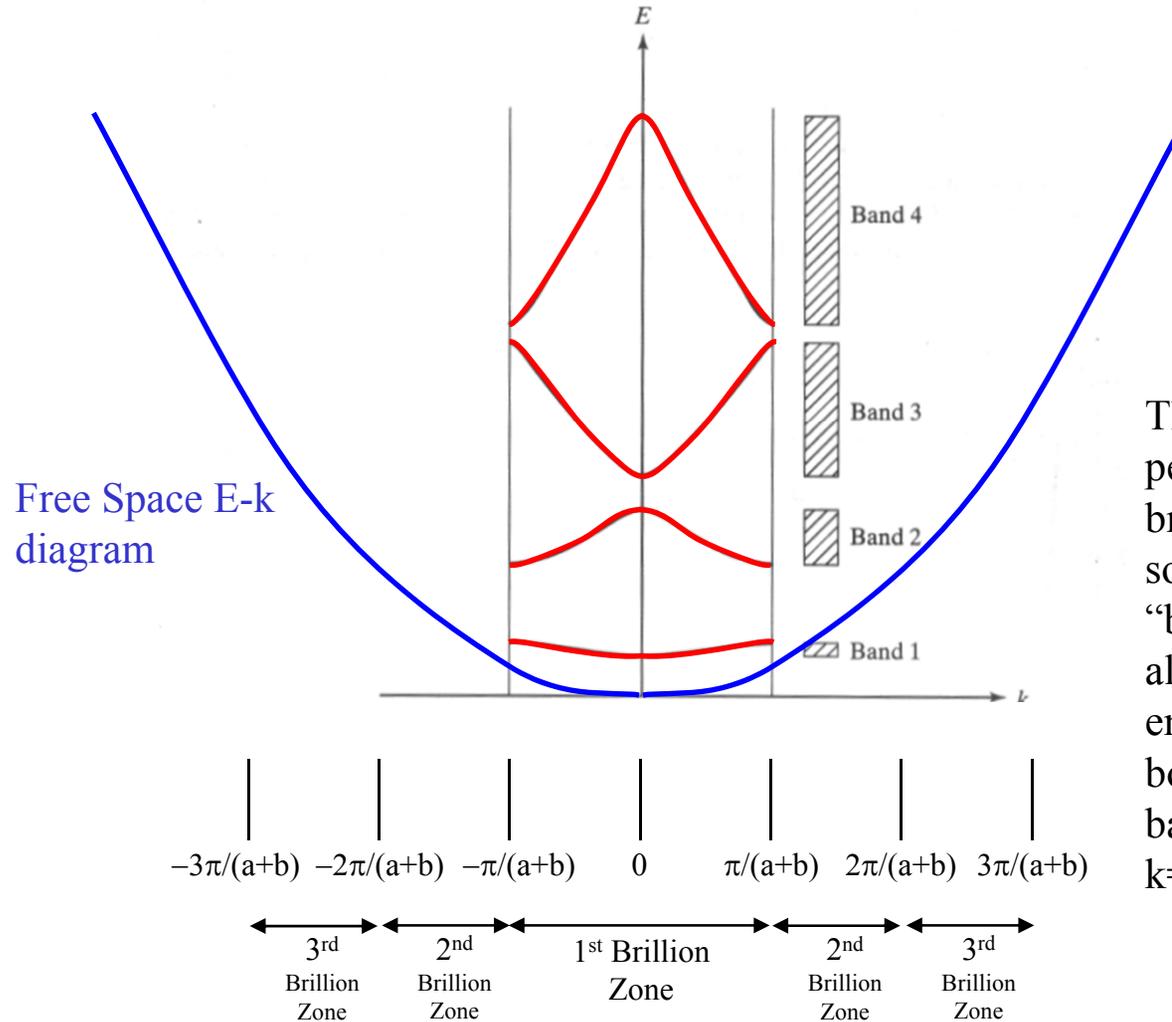


**Figure 3.5** Reduced-zone representation of allowed  $E-k$  states in a one-dimensional crystal

Note: k-value solutions differing by  $2\pi/(a+b)$  are indistinguishable

# Kronig-Penney Model

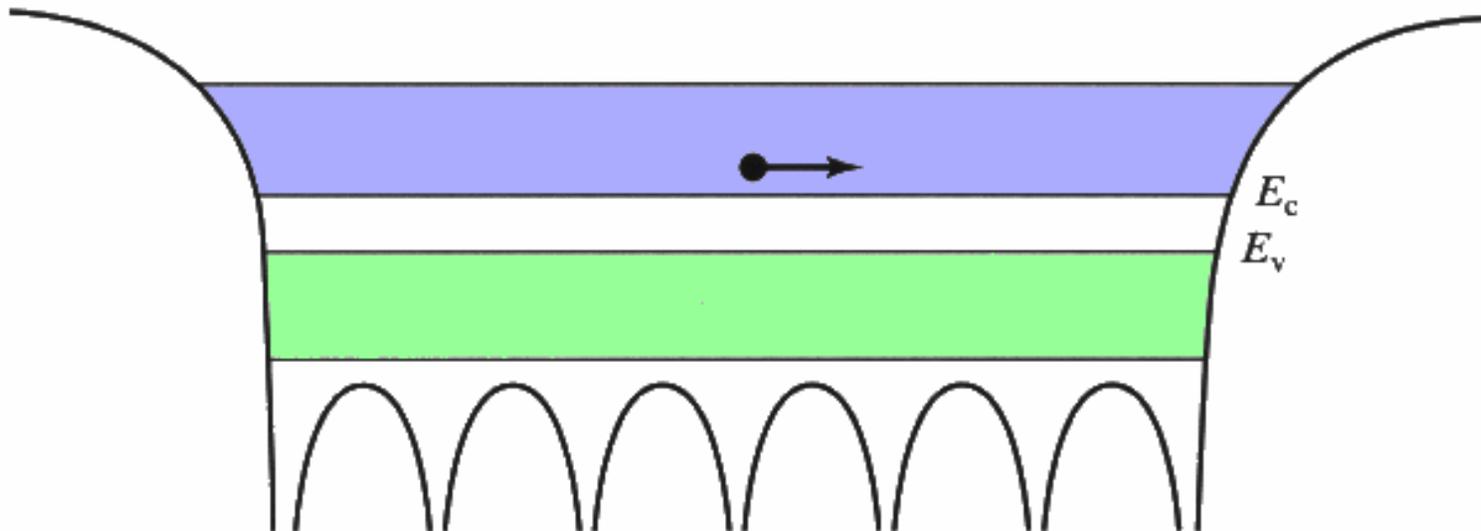
Replotting the previous result in another form ...



The presence of the periodic potential breaks the “free space solution” up into “bands” of allowed/disallowed energies. The boundaries of these bands occurs at  $k=\pm\pi/(a+b)$

Note: k-value solutions differing by  $2\pi/(a+b)$  are indistinguishable. Also due to animations printed version does not reflect same information.

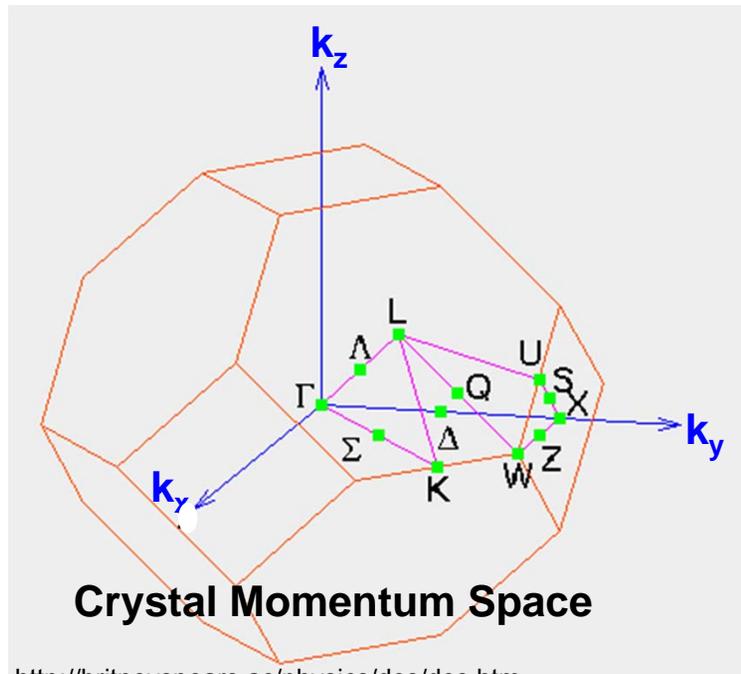
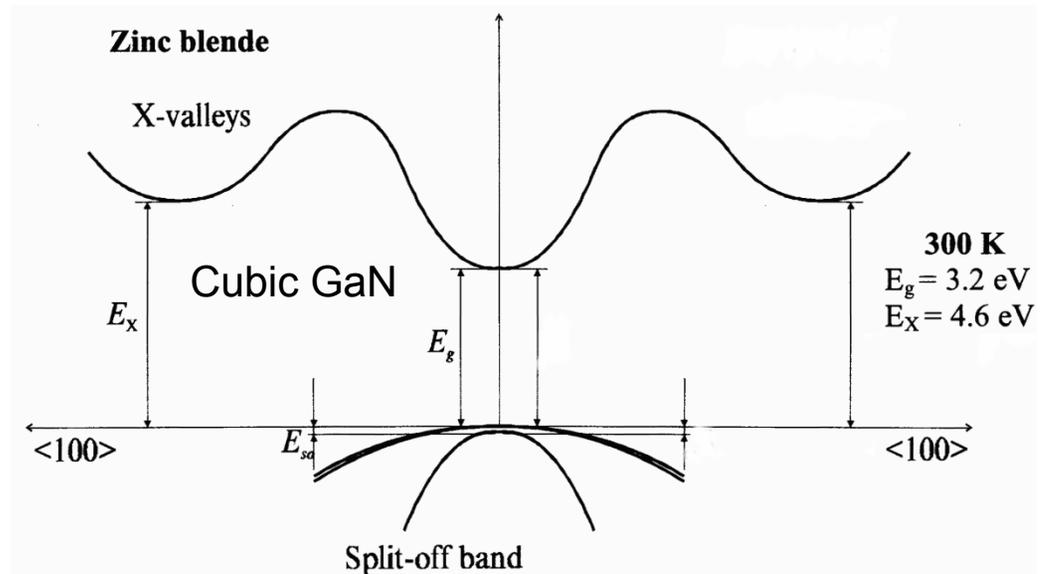
# Now consider an periodic potential in 1D Kronig-Penney Model



Visualization of a conduction band electron moving in a crystal.

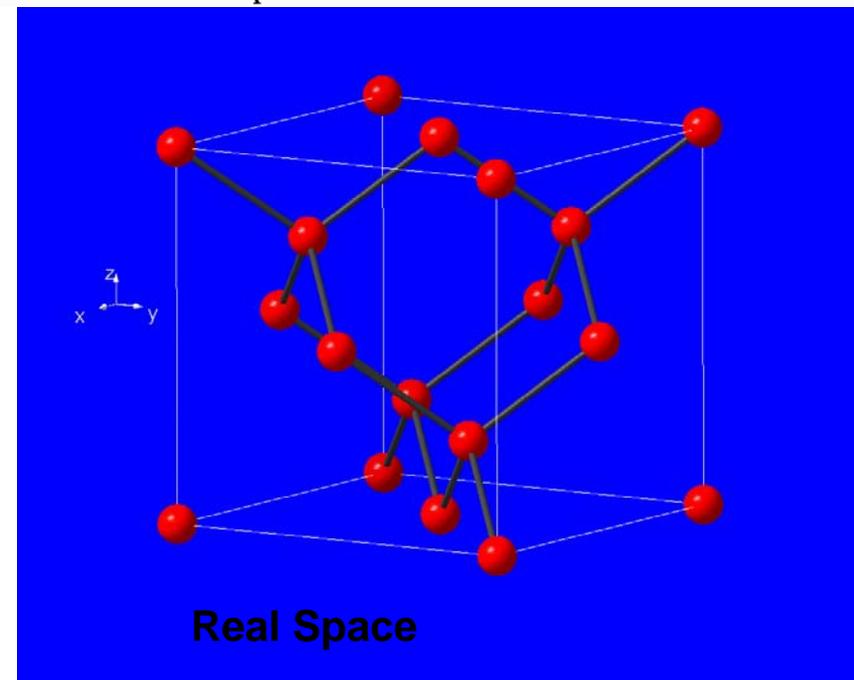
# Now consider the 3D periodic potential in a cubic crystal

- 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



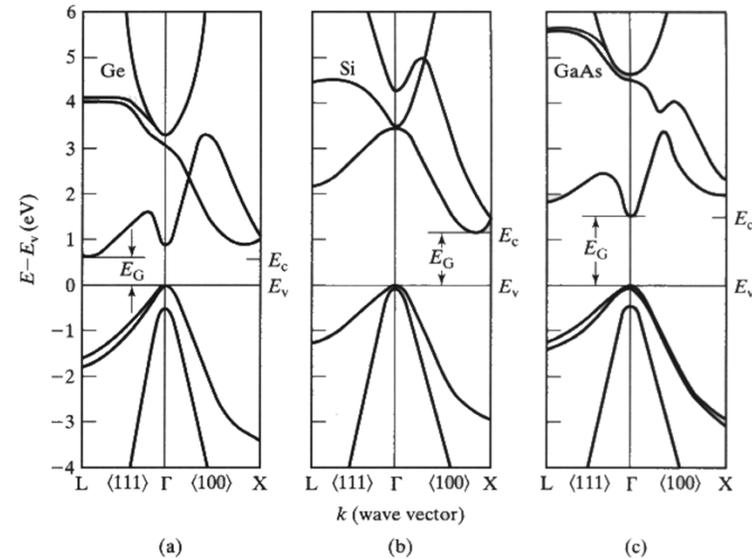
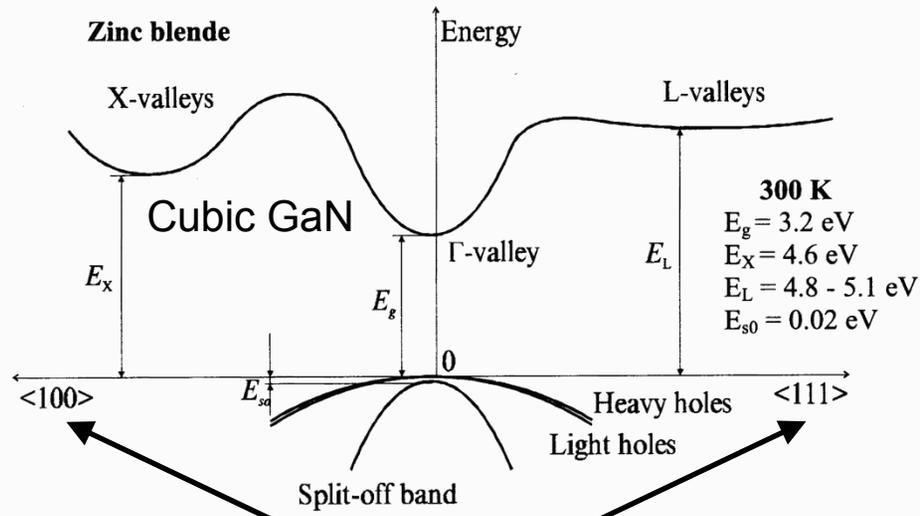
<http://britneyspears.ac/physics/dos/dos.htm>

Georgia Tech



ECE 3080 - Dr. Alan Doolittle

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



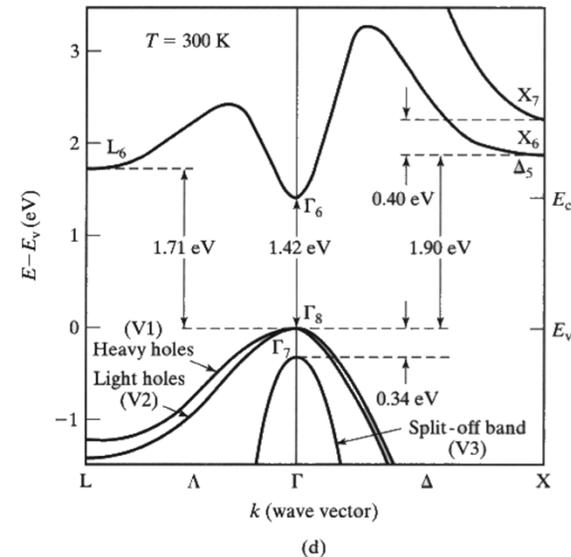
- All equivalent directions give redundant information and thus are not repeated

- 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

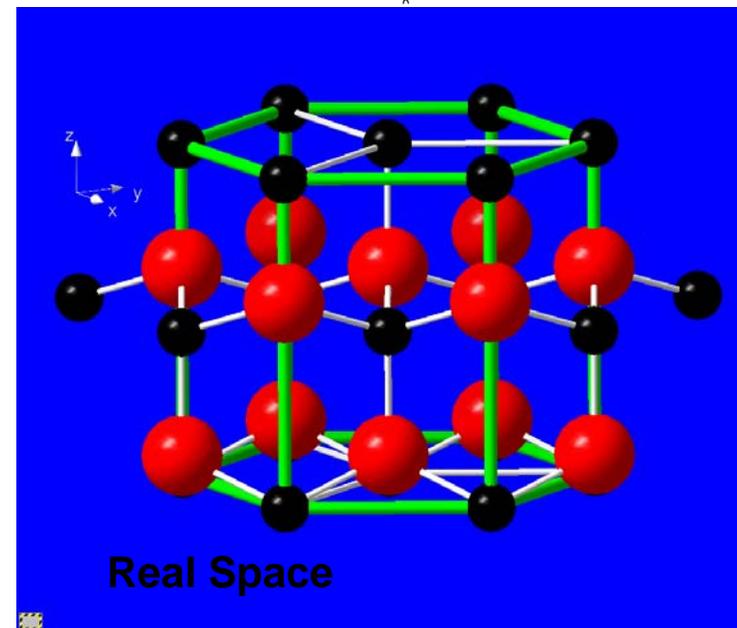
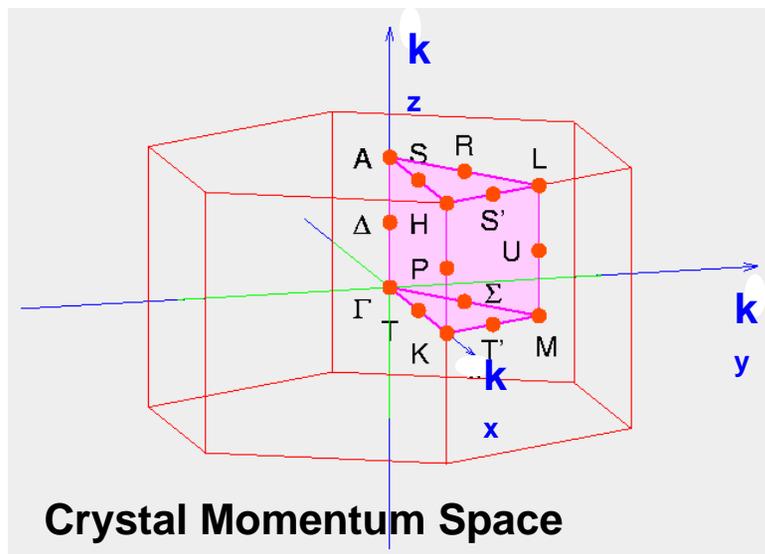
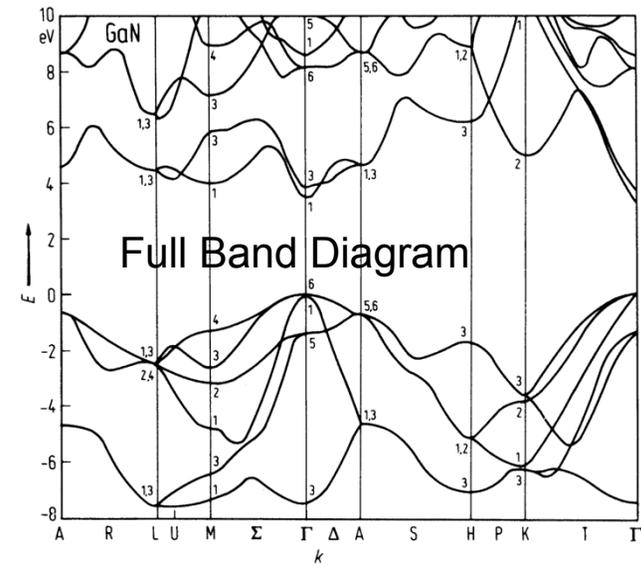
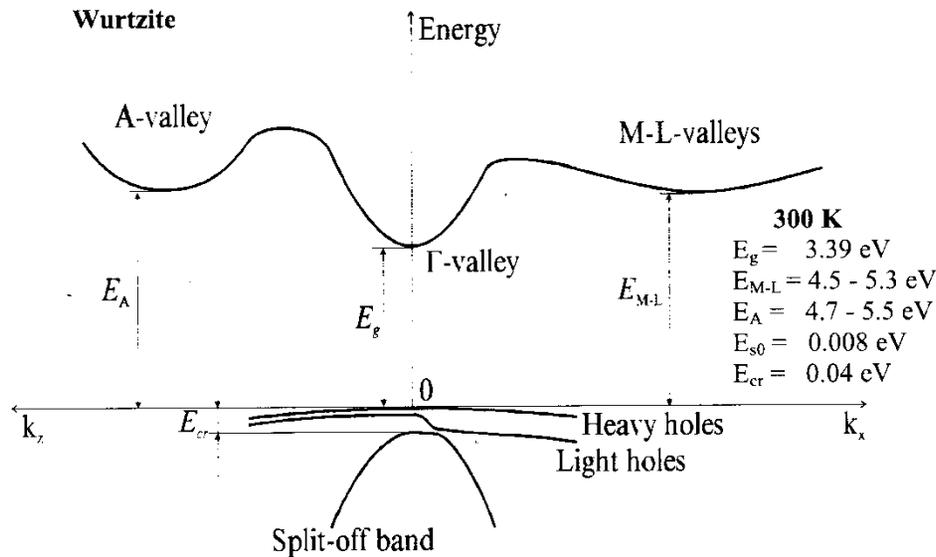
- L-point is the edge of the first Brillouin zone ( $\pi/L$  edge) of crystal momentum space (k-space) in the  $\langle 111 \rangle$  direction



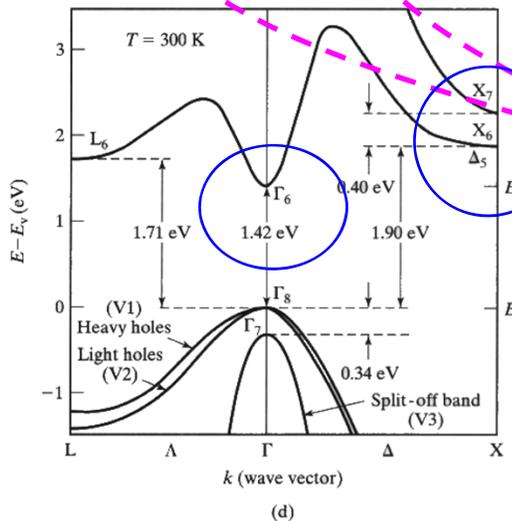
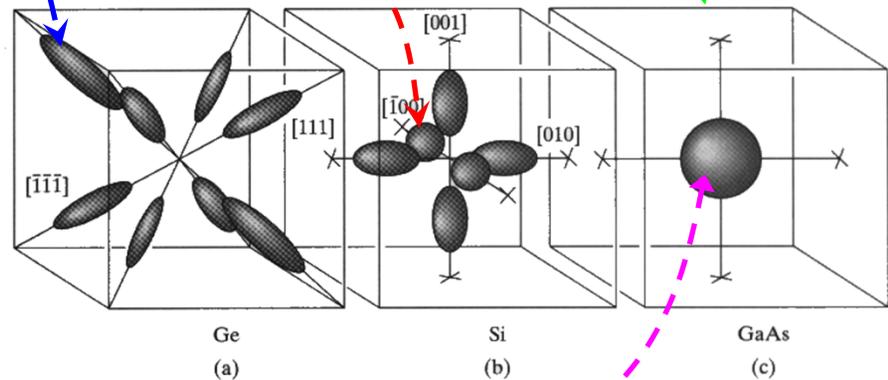
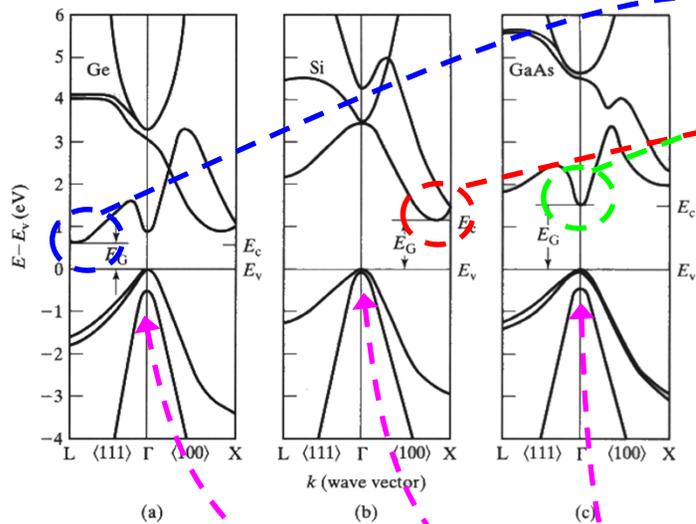
**Figure 3.13**  $\langle 100 \rangle / \langle 111 \rangle$   $E$ - $k$  diagrams characterizing the conduction and valence bands of (a) Ge, (b) Si, and (c, d) GaAs. [(a-c) after Sze<sup>[2]</sup>; (d) from Blakemore.<sup>[1]</sup> Reprinted with permission.]

Neudeck and Peirret Fig 3.13

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

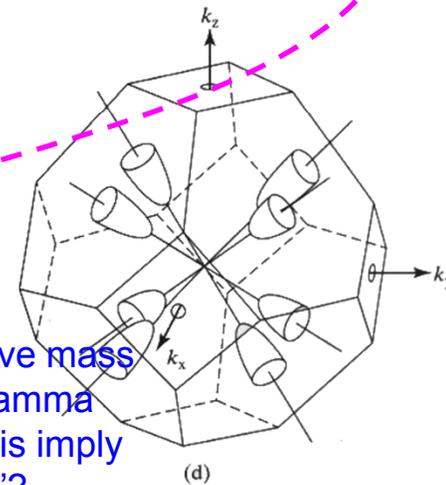


# Where are the electron trajectories/momentum vectors in the crystal?



Valence Band E-k and constant energy surfaces all look similar

An Aside: What is the effective mass of electrons in GaAs in the gamma and x valleys? What does this imply for "electron transfer devices"?



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

Figure 3.13 (100)/(111) 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

**Appendix to Lecture**  
**A Review of the Properties of Waves**

## Properties of Waves

**Classical Mechanics describes the dynamical\* state variables of a particle as  $x, y, z, p,$  etc...**

**Quantum Mechanics takes a different approach. QM describes the state of any particle by an abstract “Wave Function”,  $\Psi(x, y, z, t)$ , we will describe in more detail later.**

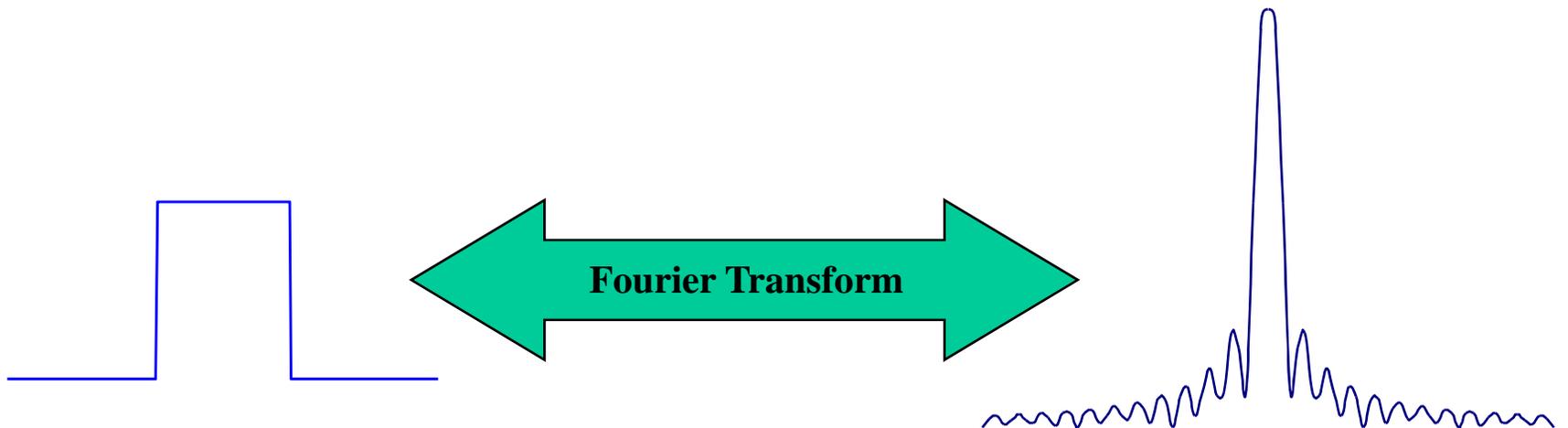
**Thus, we will review some properties of waves.**

**\*There are also classical static variable such as mass, electronic charge, etc... that do not change during physical processes.**

# Properties of Waves

As waves are important in Quantum Mechanics, it is worth re-examining some properties of waves.

- 1) **Generality of Waves and Superposition:** Any complex wave or shape of any kind can be decomposed into a set of orthogonal plane waves using a Fourier Series. (Same as in signal processing).



## Properties of Waves

2) Phase Velocity: Given a wave of the form,

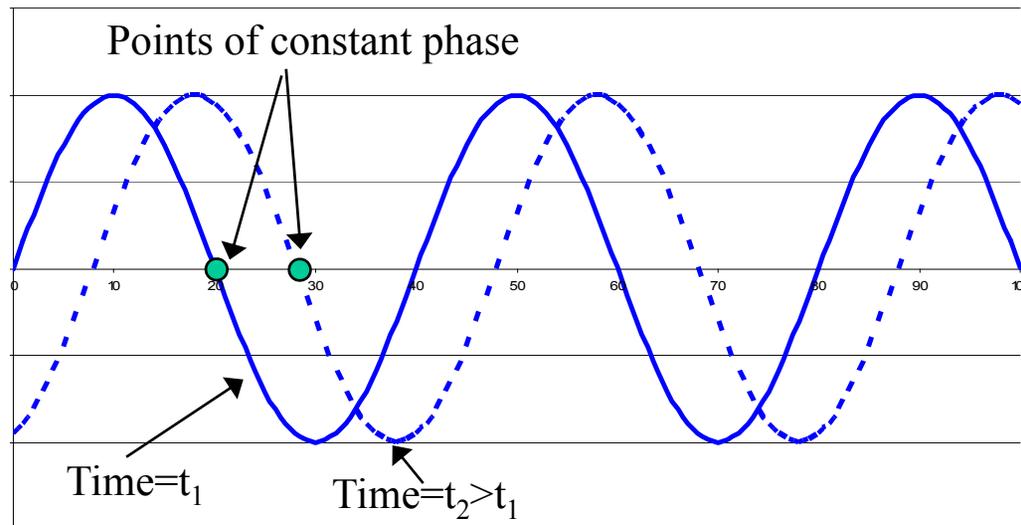
$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

Points of constant phase can be found by the following relationship:

$$kx - \omega t = \text{constant} \quad \text{or} \quad x = \left(\frac{\omega}{k}\right)t$$

Thus, we can differentiate this equation to find the phase velocity (speed of propagation) of the wave

$$v_{\text{phase}} = \frac{dx}{dt} = \frac{\omega}{k}$$



## Properties of Waves

- 3) **Group Velocity:** Any combination of waves can result in a complex wave through superposition. This complex wave moves in space.

$$\Psi(x, t) = A \int_{-\infty}^{\infty} g(k) e^{i(kx - \omega t)} dk$$

Consider a simple sum of two cosine functions:

$$\Psi(x, t) = A \cos(k_1 x - \omega_1 t) + B \cos(k_2 x - \omega_2 t)$$

Defining  $\omega$  as the average of  $\omega_1$  and  $\omega_2$

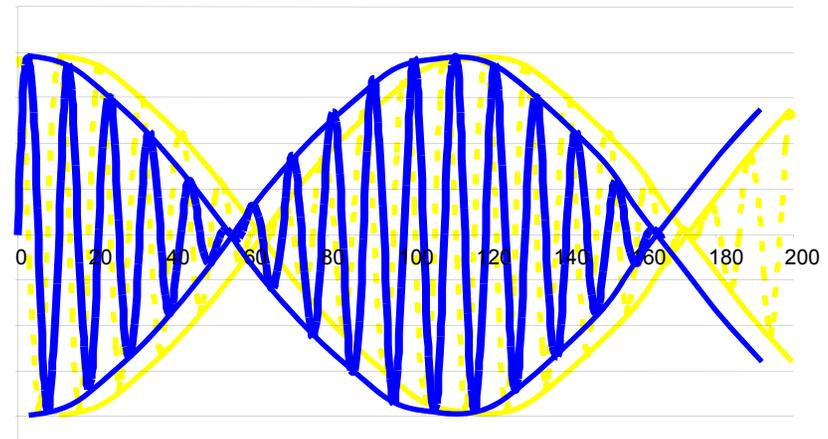
and  $k$  as the average of  $k_1$  and  $k_2$ ,

$$\omega_1 = \omega - \Delta\omega \quad \text{and} \quad \omega_2 = \omega + \Delta\omega$$

$$k_1 = k - \Delta k \quad \text{and} \quad k_2 = k + \Delta k$$

$$\Psi(x, t) = 2A \cos(\underbrace{\omega t - kx}_{\text{High Frequency}}) \cos(\underbrace{(\Delta\omega)t - (\Delta k)x}_{\text{Low Frequency}})$$

High Frequency      Low Frequency  
"Carrier"                  "Signal"



Addition of two waves of slightly different frequency

If  $\omega_1$  and  $\omega_2$  are similar,  $\Delta\omega \ll \omega$  and thus the slowly varying group (relative to the quickly varying "carrier") has a "group velocity" of:

$$v_{\text{Group}} = \frac{\Delta\omega}{\Delta k} \Rightarrow \text{and in the infinitesimal limit} \Rightarrow v_{\text{Group}} = \frac{d\omega}{dk}$$

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