Network for Computational Nanotechnology (NCN)

Purdue, Norfolk State, Northwestern, UC Berkeley, Univ. of Illinois, UTEP

ECE606: Solid State Devices
Lecture 2

Gerhard Klimeck
gekco@purdue.edu

PURDUE UNIVERSITY

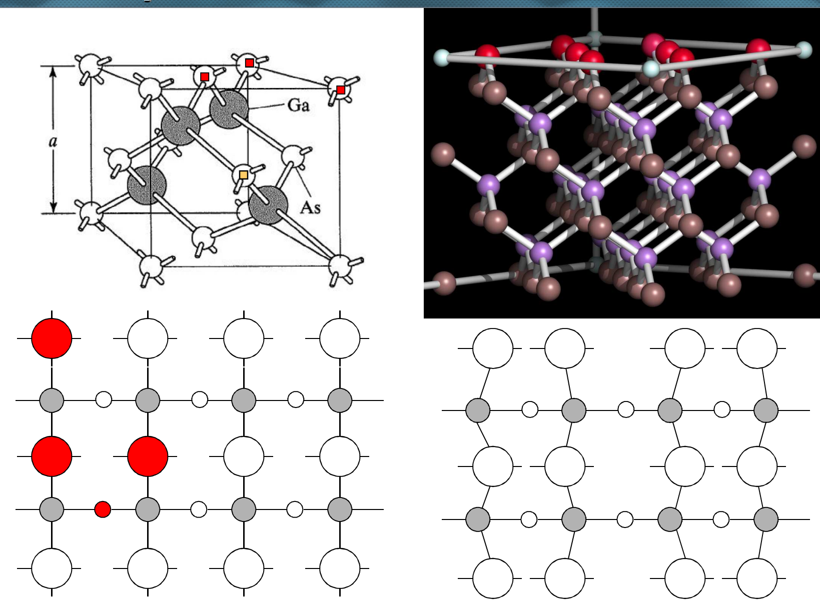
Outline - first lecture

- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - » Bravais Lattices
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces ←===== start here agains

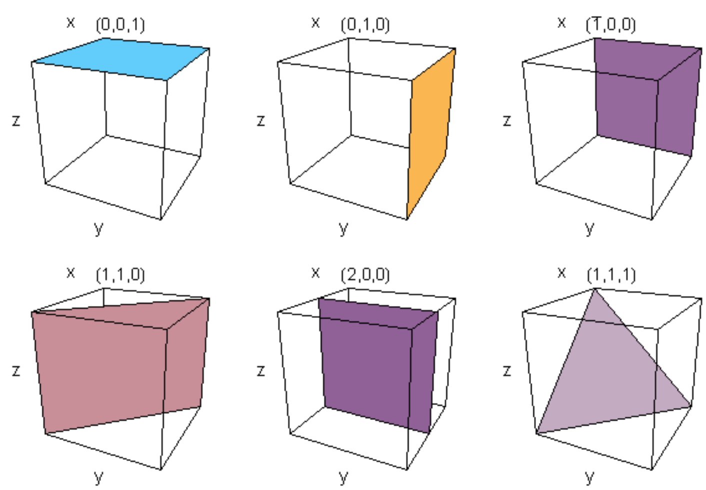
Pain Pointer

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

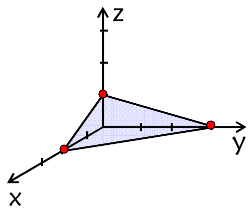
Surface Reconstruction



Miller-Indices and Definition of Planes



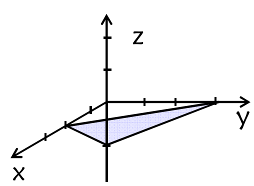
Miller Indices: Rules



1. Set up axes along the edges of unit cell
2. Normalize intercepts …. 2, 3, 1
3. Invert/rationalize intercepts … 1/2, 1/3, 1
   3/6, 2/6, 6/6
4. Enclose the numbers in curvilinear brackets
   (326)

Few more rules …

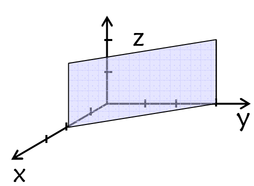
Negative Intercept



2,	3,	-2
1/2,	1/3,	-1/2
3,	2,	-3

$(3\ 2\ \bar{3})$

Intercept at infinity

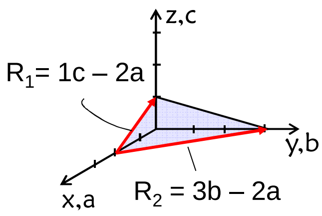


2,	3,	∝
1/2,	1/3,	0
3,	2,	0

(3 2 0)

Where does Miller Indices come from ?

Miller indices: (326)



$$\vec{R}_1 = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} \quad \vec{R}_2 = \begin{pmatrix} -2 \\ 3 \\ 0 \end{pmatrix}$$

Normal to the surface and R_1,R_2

$$R_2 x R_1 = \begin{vmatrix} a & b & c \\ -2 & 3 & 0 \\ -2 & 0 & 1 \end{vmatrix} = 3a + 2b + 6c$$

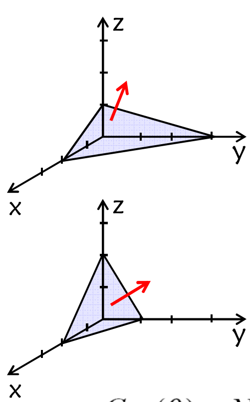
Vector indices same as Miller indices !

(326) vs. [326]

Specification of vectors normal to a particular plane!

Angle between Two Planes

⇒Angle between two vectors
⇒Dot product / inner product between two vectors



Unit vector normal to plane 1:

$$N_1 = (h_1\vec{a} + k_1\vec{b} + l_1\vec{c})/(h_1^2 + k_1^2 + l_1^2)^{1/2}$$

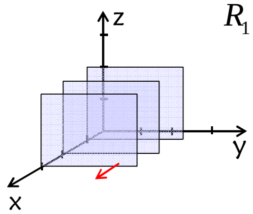
Unit vector normal to plane 2:

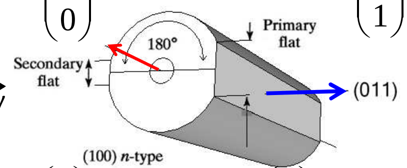
$$N_2 = (h_2\vec{a} + k_2\vec{b} + l_2\vec{c})/(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

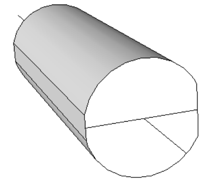
$$Cos(\theta) = N_1 \bullet N_2$$
$$= (h_2 h_1 + k_2 k_1 + l_2 l_1)/(h_2^2 + k_2^2 + l_2^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

Examples …

$$\vec{R}_1 = \begin{pmatrix}1\\0\\0\end{pmatrix} \qquad \vec{R}_2 = \begin{pmatrix}0\\1\\1\end{pmatrix}$$







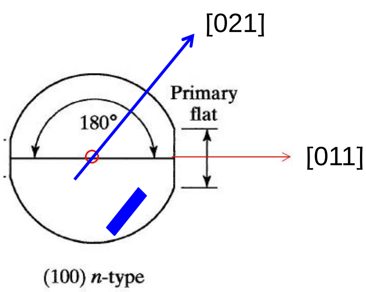
$$\vec{N}_1 = \begin{pmatrix}1\\0\\0\end{pmatrix} / \sqrt{1} \qquad \vec{N}_2 = \begin{pmatrix}0\\1\\1\end{pmatrix} / \sqrt{2}$$

cos(θ)=(1x0+0x1+0x1)/(√1x√2) = 0

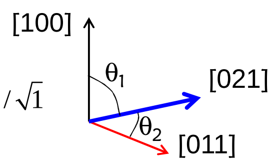
so θ=90 degrees

(011) surface is normal to (100) surface

Example: Find the [021] direction



$$\vec{N}_1 = \begin{pmatrix}1\\0\\0\end{pmatrix} / \sqrt{1}$$

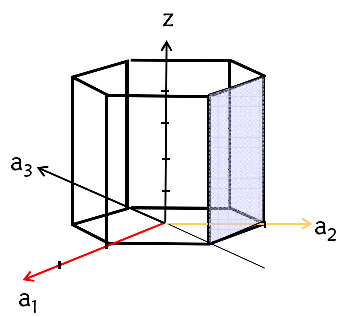


$$\vec{T} = \begin{pmatrix}0\\2\\1\end{pmatrix} / \sqrt{1} \qquad \vec{N}_2 = \begin{pmatrix}0\\1\\1\end{pmatrix} / \sqrt{2}$$

N_1•T =cos(θ_1)=(1x0+0x2+0x1)/(1x√5) = 0, so θ=90 degrees
[021] vector lies on (100) plane.

N_2•T =cos(θ_2)=(0x0+2x1+1x1)/(√5 √2) = 3/ √10, so θ=18.43 degrees with respect to [011] direction.

Bravais-Miller Indices



∝,	1,	-1,	∝
0,	1,	-1,	0
0,	1,	-1,	0

$(0\ 1\ \bar{1}\ 0)$

First three indices sum to zero.

Outline - lecture 1

- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - » Bravais Lattices
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

Summary - Lecture 1 - Crystals

1. To understand transport in semiconductors, we need to know carrier density (n) and carrier velocity (v). In order to find these quantities, we need to understand the chemical composition and atomic arrangements.

2. Crystalline material can be built by repeating the basic building blocks. This simplifies the quantum solution of the material, which will allow us to compute n and v for these systems easily.

3. Silicon, GaAs, PbS do not have simple Bravais lattice; but they have Bravais lattice with basis.

4. Often we need to calculate the direction of crystal planes because material properties differ along different planes. Miller indices are one useful way of characterizing crystal planes. In is useful to to review some identities of vector calculus to such calculations involving crystal planes.

ECE606: Solid State Devices
Lecture 2
Quantum ~~Mechanics~~ WHAT?

Gerhard Klimeck

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography
- Strange Experimental Results => The Advent of Quantum Mechanics
  - » Discrete Optical Spectra
  - » Photoelectric Effect
  - » Particle-Wave Duality
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

Classical Macroscopic Particles

Properties:

- Have a finite extent • continuous (ignoring atomic granularity)
- Have a finite weight • continuous (ignoring atomic granularity)
- Are countable with integers • discrete

Laws of Motion

- Classical Newtonian Mechanics

Interactions with other particles

- Energy continuity
- Momentum continuity

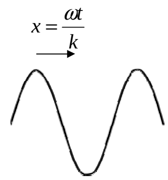
Example

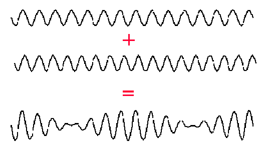
- Billiard balls

Propagating Plane Waves

Properties:
- Have infinite extent
- Have finite wavelength
- Have a finite frequency

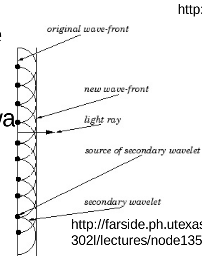
Laws of Motion
- Wave equation $\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$
- One solution $u = u_0 \sin(kx - \omega t) \quad c = \pm \omega / k = \pm \lambda f$





http://www.qmw.ac.uk/~zgap118/5/

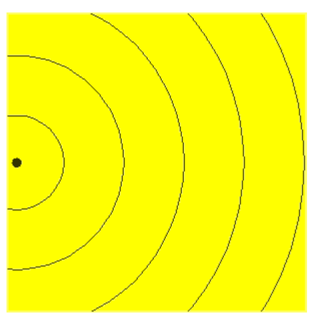
Interactions with other waves / environment
- Coherent superposition
  => interference, constructive and destructive
  => one wave can cancel out another
- Huygens principle:
  one plane wave made up by many circular wa
  => diffraction
  => waves go around corners



http://farside.ph.utexas.edu/teaching/302l/lectures/node135.html

Huygens' Principle

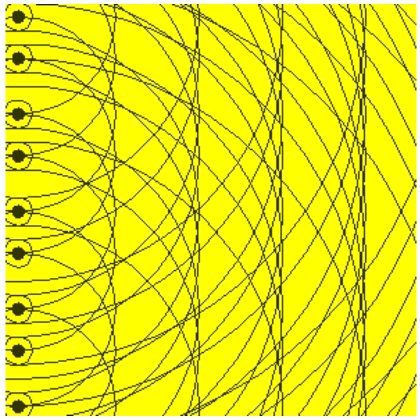
- All waves can be represented by point sources
- This animation shows an example of a single point source



http://id.mind.net/~zona/mstm/physics/waves/propagatio

Huygens' Principle

- All waves can be represented by point sources
- This animation shows an example of multiple single point sources creating a wavefront.



http://id.mind.net/~zona/mstm/physics/waves/propagatio

Propagating Plane Waves
Light is an Electromagnetic Wave

Properties:

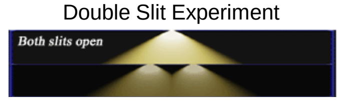
- Have infinite extent
- Have finite wavelength
- Have a finite frequency

- Not countable
- Continuous
- Continuous

Laws of Motion

- Wave equation $$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$$
- One solution $$u = u_0 \sin(kx - \omega t) \quad c = \pm \omega/k = \pm \lambda f$$

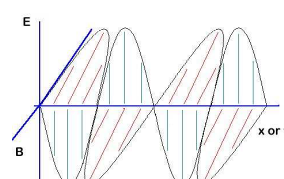
Double Slit Experiment



http://en.wikipedia.org/wiki/Double-slit_experiment

Interactions with other waves / environment

- Coherent superposition
  => interference, constructive and destructive
  => one wave can cancel out another
- Huygens principle:
  one plane wave made up by many circular waves
  => diffraction
  => light goes around corners



http://www.qmw.ac.uk/~zgap118/2/

Accepted Proof:

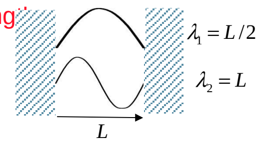
- Light is an electromagnetic wave

Standing Waves

Properties:

- Have finite extent
- Have discrete wavelengths
- Have discrete frequencies

- Countable in 1/2 waveleng…
- Integer multiples
- Integer fractions



Laws of Motion

- Wave equation $$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$$
- One solution $$u = \begin{cases} u_0 \sin(kx - \omega t); & 0 \le x \le L \\ 0; & x < 0; x > L \end{cases}$$

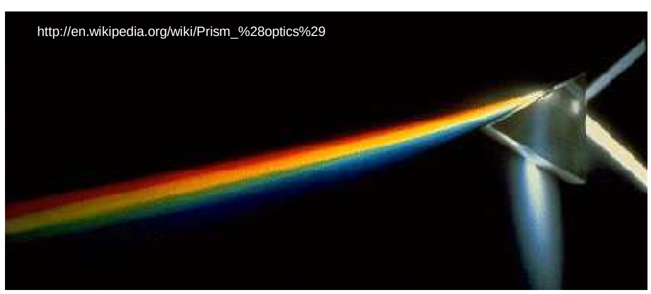
$$k_j = j\frac{\pi}{L}$$

- Quantized momentum k_j

Interactions with other waves / environment

- Coherent superposition
  => e.g. sounds add in an instrument
- A standing wave is a resonator
- one resonator can couple to another
  => e.g. string <=> guitar
  => energy is transferred between resonators
  => energy conservation
- resonators must be "in-tune"
  => momentum conservation

Frequency Content of Light

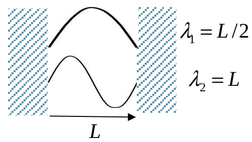


- "White" light consists of a broad spectrum of colors
- Each individual color is associated with a particular frequency of wave
- A prism can dissect white light into its frequency components

- Is there some information in this kind of frequency spectrum?
  => chromatography

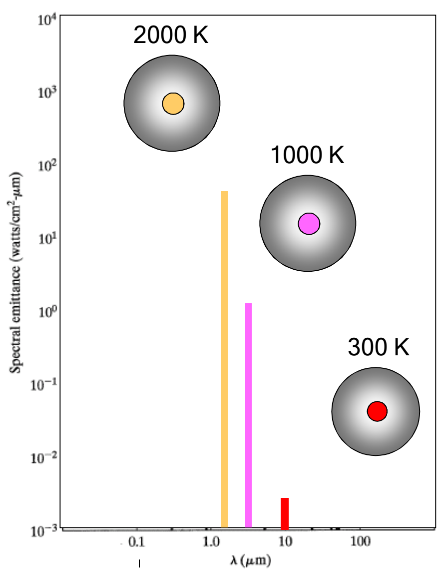
Presentation Outline

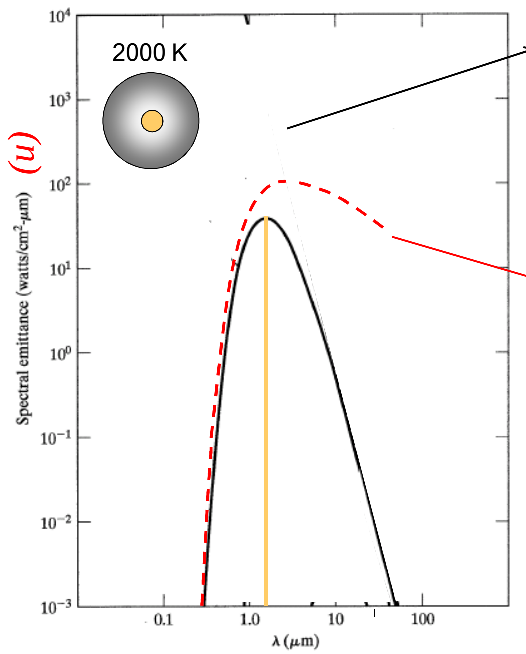
- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography



- Strange Experimental Results => The Advent of Quantum Mechanics
  - » Black Body Radiation
  - » Discrete Optical Spectra
  - » Photoelectric Effect
  - » Particle-Wave Duality

(1) black-body radiation





Rayleigh-Jeans Formula

$$u(\lambda,T) \propto k_B T / \lambda^4$$

$$\log(u) = -4\log(\lambda) + \log(T)$$

Wein's Formula

$$u \propto \frac{e^{-\beta/\lambda T}}{\lambda^5}$$

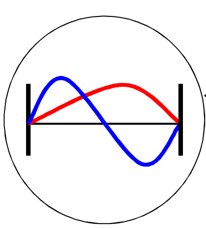
Plank's fitting formula

$$u(\lambda,T) \propto \frac{1}{\lambda^5}\left[\frac{1}{e^{\beta/\lambda T}-1}\right]$$

Interpretation of Plank's Formula

$$u(f,T) = u(\lambda,T)\frac{d\lambda}{df} \sim \frac{1}{\lambda^5}\left[\frac{1}{e^{\beta/\lambda T}-1}\right]\frac{d\lambda}{df} \qquad \lambda = \frac{c}{f}$$

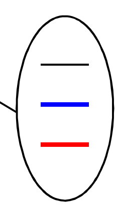
$$\sim f^2 \times hf \times \left(\frac{1}{e^{hf/kT}-1}\right)$$



nos. of modes

Energy of mode

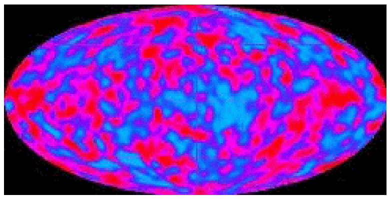
Occupation Probability

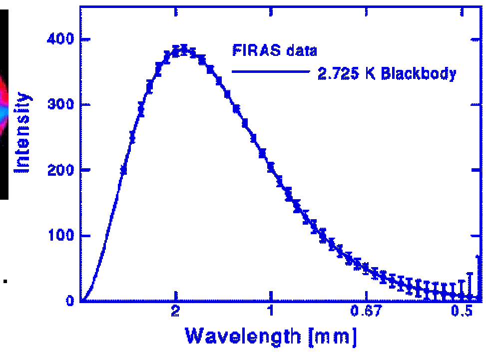


EM emission occurs in discrete quanta of

$E = hf$ n=1,2, …….. N

Recent Example: COBE Data



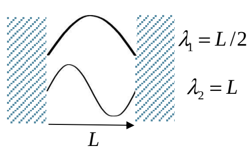


J.C. Mather, Astrophysics J., 1990.

Show that the cosmic background temperature is approximately 3K. Can you "see" this radiation?

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography



- Strange Experimental Results => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra
  - » Photoelectric Effect
  - » Particle-Wave Duality
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

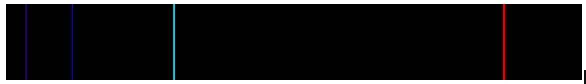
Strange Experimental Observations The Advent of Quantum Mechanics

Discrete light spectrum:

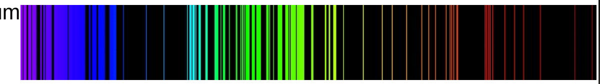
- Light emitted from hot elemental materials has a discrete spectrum
- The spectrum is characteristic for the material (fingerprint)

Images from: http://en.wikipedia.org

- E.g.: H spectrum



- E.g.: Iron spectrum

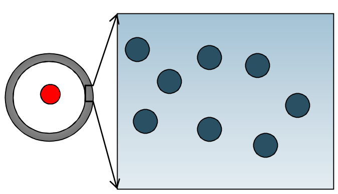


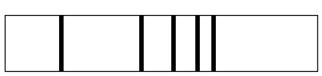
- E.g. application - bright yellow Na lamps
  => lot of excitation energy converted into single frequency

Development of atomic models

- Bohr atom model - electrons in looping orbits
-
-

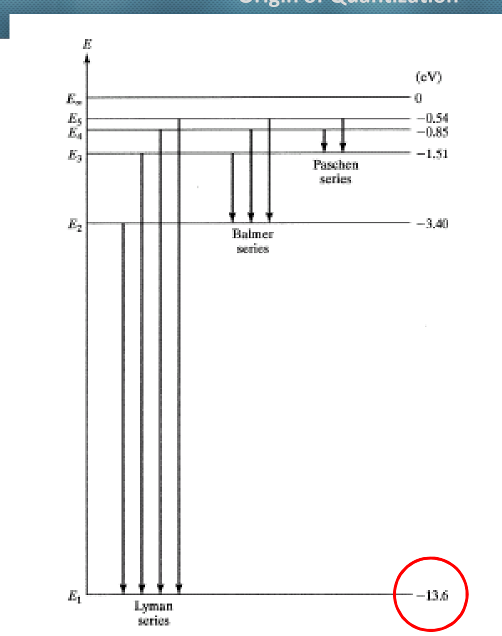
Origin of Quantization





frequency

$$E_{m,n} = const \times \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$



(3) Bohr Atom ..

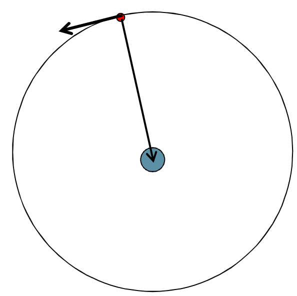
Assume that angular momentum is quantized:

$$L_{\mathbf{n}} = m_0 v r_{\mathbf{n}} = \mathbf{n}\hbar \qquad \mathbf{n} = 1, 2, 3, \ldots$$

$$\upsilon = n\hbar / m_0 r_n$$

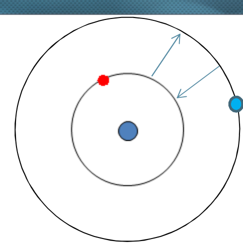
$$\frac{m_0 v^2}{r_{\mathbf{n}}} = \frac{q^2}{4\pi\varepsilon_0 r_{\mathbf{n}}^2}$$

$$r_{\mathbf{n}} = \frac{4\pi\varepsilon_0 (\mathbf{n}\hbar)^2}{m_0 q^2}$$



(3) Bohr Atom (continued) ...

$$r_{\mathbf{n}} = \frac{4\pi\varepsilon_0 (\mathbf{n}\hbar)^2}{m_0 q^2}$$



$$\text{K.E.} = \frac{1}{2} m_0 v^2 = \frac{1}{2}\left(q^2/4\pi\varepsilon_0 r_{\mathbf{n}}\right)$$

$$\text{P.E.} = -q^2/4\pi\varepsilon_0 r_{\mathbf{n}} \qquad (\text{P.E. set} = 0 \text{ at } r = \infty)$$

$$E_{\mathbf{n}} = \text{K.E.} + \text{P.E.} = -\frac{1}{2}\left(q^2/4\pi\varepsilon_0 r_{\mathbf{n}}\right)$$

$$E_{\mathbf{n}} = -\frac{m_0 q^4}{2(4\pi\varepsilon_0 \mathbf{n}\hbar)^2} = -\frac{13.6}{\mathbf{n}^2}\,\text{eV}$$

$$E_{m,n} = const \times \left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

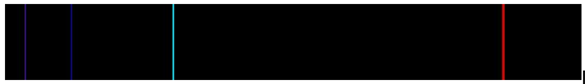
Strange Experimental Observations The Advent of Quantum Mechanics

Discrete light spectrum:

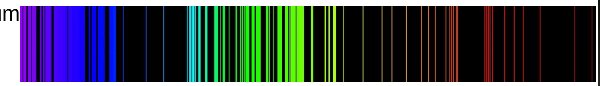
- Light emitted from hot elemental materials has a discrete spectrum
- The spectrum is characteristic for the material (fingerprint)

Images from: http://en.wikipedia.org

- E.g.: H spectrum



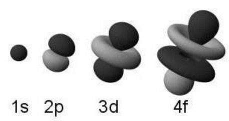
- E.g.: Iron spectrum

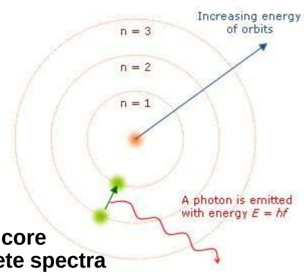


- E.g. application - bright yellow Na lamps
  => lot of excitation energy converted into single frequency

Development of atomic models

- Bohr atom model - electrons in looping orbits
- Quantum mechanical model

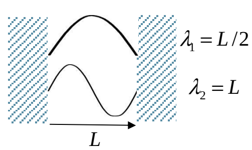




=> electrons are standing waves bound to a core
=> discrete transition energies lead to discrete spectra

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography

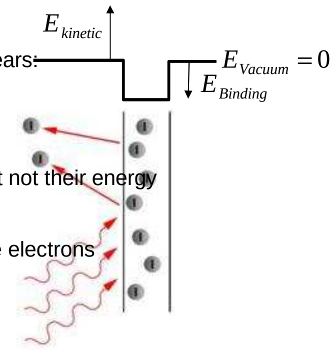


- Strange Experimental Results => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra => light emission/absorption quantized
  - » Photoelectric Effect
  - » Particle-Wave Duality
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

Strange Experimental Observations
The Advent of Quantum Mechanics

Photoelectric Effect:
- Light can eject electrons from a clean metal
- Observed by many researchers but not explained for 55 years: 1839, 1873, 1887, 1899, 1901
  see details: http://en.wikipedia.org/wiki/Photoelectric_effect

Unexplained problems:
- Electrons emitted immediately, no time lag
- Increasing light intensity increases number of electrons but not their energy
- Red light will not cause emission, no matter what intensity
- Weak violet light will eject few electrons with high energy
  => Light had to have a minimum frequency / color to excite electrons
- => Emitted electrons have light dependent energy f_m



http://en.wikipedia.org/wiki/Photoelectric_effect

The solution in 1905 (Nobel prize for Einstein in 1921)

$$\Delta E \propto (f - f_m)$$

$$E = hf$$

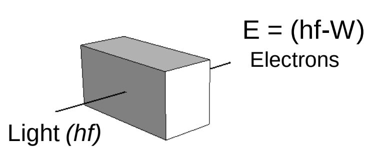
Light consists of particles

Photons

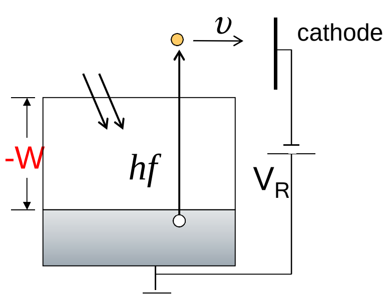
- Light can be described by discrete particles of discrete energy
- Planck's constant - h
- Light energy is not divisible
- Have to have minimum energy to kick out an electron from the bound state

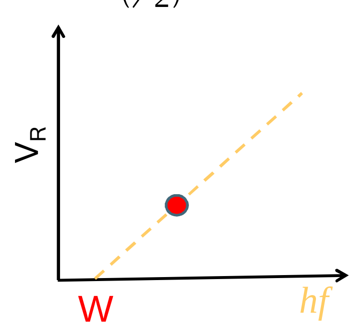
$$E_{Binding} = hf_m \qquad E_{kinetic} = E_{light} - E_{Binding} = h\left(f_{light} - f_m\right) \geq 0$$

Photoelectric Effect



$$qV_R \approx \left(\tfrac{1}{2}\right) m_0 \upsilon^2 = hf - W$$

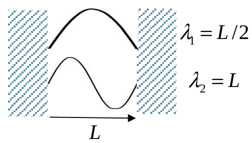




Absorption occurs in quanta as well, consistent with photons having ***E=hf***

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography



- Strange Experimental Results => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra => light emission/absorption quantized
  - » Photoelectric Effect => light is described by particles
  - » Particle-Wave Duality
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

Wave - Particle Duality

All particles have a wave property
- Can interfere
- Can diffract
- Can form standing waves

All waves have particle properties
- Have momentum
- Have an energy
- Can be created and destroyed

Typical descriptions:
- Energy E, frequency f, Momentum k
- A set of discrete quantum numbers

- Choose wave/particle description according to problem

(4) Wave-Particle Duality

Photons act both as wave and particle, what about electrons ?

$$E = \sqrt{m_0^2 c^4 + p^2 c^2}$$

$$hf = pc$$

m_0=0 (photon rest mass)

$$p = hf / c$$
$$= h/\lambda \quad \text{(because } c = \lambda f\text{)}$$
$$= \hbar k \quad \text{(because } k = 2\pi/\lambda\text{)}$$

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography
- Strange Experimental Results
  => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra => light emission/absorption quantized
  - » Photoelectric Effect => light is described by
  - » Particle-Wave Duality => true for all waves and particles
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

Pain Pointer

Which electrons contribute to device current?

Number of atoms/volume from crystal structure

Number of electrons available for conduction

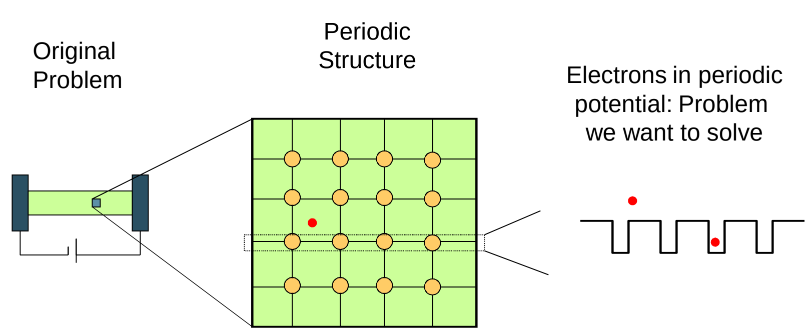
Number of electrons/atoms

$$n \neq \rho \times N$$

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 **Al**	14 **Si**	15 **P**	16 S
30 **Zn**	31 **Ga**	32 Ge	33 **As**	34 **Se**
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

All electrons may be created equally,
but they appear do not behave identically!

Do I really need Quantum Mechanics ?



If it were large objects, like a skier skiing past a set of obstacles, Newton's mechanics would work fine, but in a micro-world ……

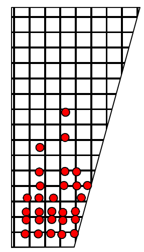
- Some electrons are closely bound to the atomic cores
- Some electrons are loosely bound
  => they can move through the structure freely
- Even free electrons need empty states to flow into
  => not only the states, but their filling is important!

Carrier Density

Carrier number = Number of states x filling factor

↑ Chapters 2-3 ↑ Chapter 4

Total number of occupants
= Number of apartments
X The fraction occupied



Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography
- Strange Experimental Results
  => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra => light emission/absorption quantized
  - » Photoelectric Effect => light is described by particles
  - » Particle-Wave Duality => true for all waves and particles
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

Schrodinger Equation for electrons

$$E = \sqrt{m_0^2 c^4 + p^2 c^2} \approx m_0 c^2 \left[1 + p^2 c^2 / 2 m_0^2 c^4 + \ldots \right]$$

$$E - m_0 c^2 \quad = \quad V \ + \ (p^2 / 2 m_0)$$

$$hf = \hbar\omega \quad = \quad V \ + \ (\hbar^2 k^2 / 2 m_0)$$

Schrodinger Equation (continued)

$$\hbar\omega \quad = \quad (\hbar^2 k^2 / 2 m_0) + V$$

Assume, $\Psi(x,t) = A \exp(-i(\omega t - kx))$

$$d\Psi / dt = -i\omega\Psi \quad \text{and} \quad d^2\Psi / dx^2 = -k^2 \Psi$$

$$i\hbar \frac{d\Psi}{dt} = \left(-\frac{\hbar^2}{2 m_0} \frac{d^2 \Psi}{dx^2} \right) + V\Psi$$

Presentation Outline

- Classical Systems
  - » Particles
  - » Propagating Waves
  - » Standing Waves
  - » Chromatography
- Strange Experimental Results
  => The Advent of Quantum Mechanics
  - » Black Body Radiation => light emission is quantized
  - » Discrete Optical Spectra => light emission/absorption quantized
  - » Photoelectric Effect => light is described by particles
  - » Particle-Wave Duality => true for all waves and particles
- Why do we need quantum mechanics?
- Formulation of Schrödinger's Eq.

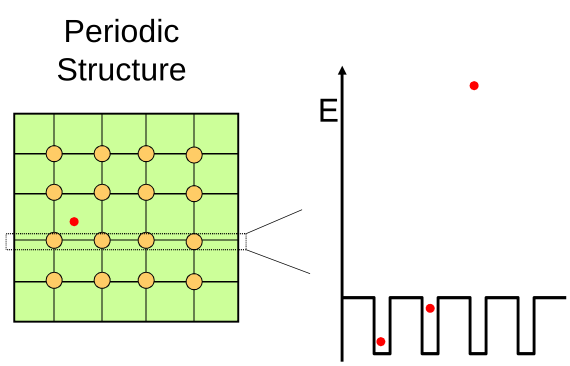
Conclusions

1. Given chemical composition and atomic arrangements, we can compute electron density by using quantum mechan
2. We discussed the origin of quantum mechanics – experiments were inconsistent with the classical theory.
3. We saw how Schrodinger equation can arise as a consequence of quantization and relativity, but *this is not a derivation*.
4. We will solve some toy problems in the next class to get a feeling of how to use quantum mechanics.

ECE606: Solid State Devices
Lecture 3

Gerhard Klimeck
gekco@purdue.edu

Motivation



Time-independent Schrodinger Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\Psi}{dx^2}+U(x)\Psi=i\hbar\frac{d\Psi}{dt}$$

Assume

$$\Psi(x,t)=\psi(x)\,e^{-iEt/\hbar}$$

$$-e^{-\frac{iEt}{\hbar}}\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+e^{-\frac{iEt}{\hbar}}U(x)\psi(x)=i\hbar\frac{-iE}{\hbar}\psi(x)e^{-\frac{iEt}{\hbar}}$$

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

Time-independent Schrodinger Equation

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

If E >U, then ….

$$k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar}\qquad \frac{d^2\psi}{dx^2}+k^2\psi=0\qquad \psi(x)=A\sin(kx)+B\cos(kx)\equiv A_+e^{ikx}+A_-e^{-ikx}$$

If U>E, then ….

$$\alpha\equiv\frac{\sqrt{2m_0[U-E]}}{\hbar}\qquad \frac{d^2\psi}{dx^2}-\alpha^2\psi=0\qquad \psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$$

A Simple Differential Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

- Obtain U(x) and the boundary conditions for a given problem.
- Solve the 2nd order equation – pretty basic
- Interpret $|\psi|^2=\psi^*\psi$ as the probability of finding an electron at x
- Compute anything else you need, e.g.,

$$p=\int_0^\infty \Psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi\,dx \qquad E=\int_0^\infty \Psi^*\left[-\frac{\hbar}{i}\frac{d}{dt}\right]\Psi\,dx$$

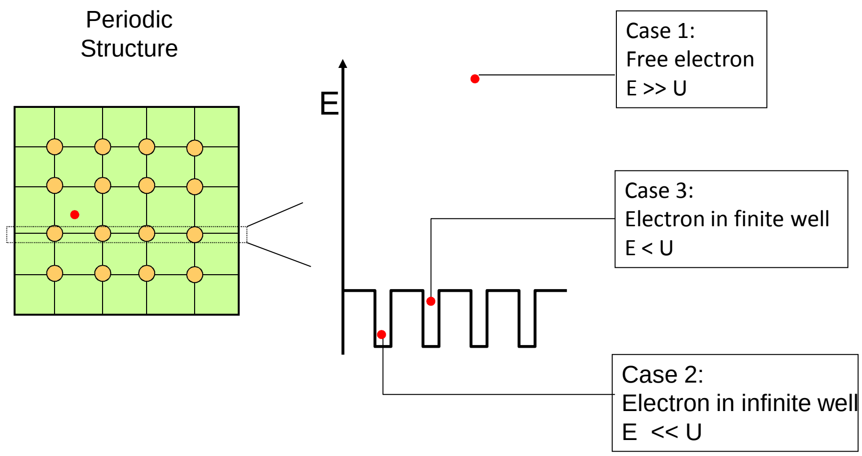
Presentation Outline

- Time Independent Schroedinger Equation
- Analytical solutions of Toy Problems
  - » (Almost) Free Electrons
  - » Tightly bound electrons – infinite potential well
  - » Electrons in a finite potential well
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers
- Additional notes
  - » Discretizing Schroedinger's equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)

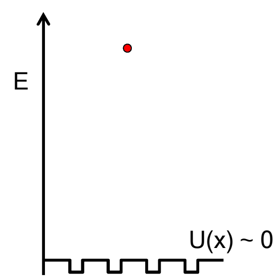
- piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt

Full Problem Difficult: Toy Problems First



Case 1: Solution for Particles with E>>U

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad k\equiv\frac{\sqrt{2m_0\left[E-U\right]}}{\hbar}$$



1) Solution $\psi(x)=A\sin(kx)+B\cos(kx)$

$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

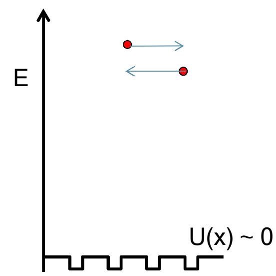
2) Boundary condition $\psi(x)=A_+e^{ikx}$ positive going wave

$=A_-e^{-ikx}$ negative going wave

Free Particle ...

$$\psi(x) = A\sin(kx) + B\cos(kx)$$
$$\equiv A_+ e^{ikx} + A_- e^{-ikx}$$

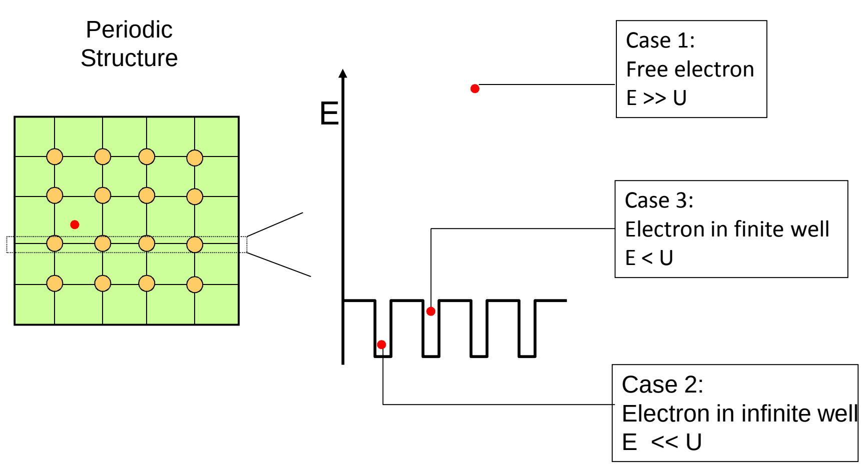
$$\psi(x) = A_+ e^{ikx} \quad \text{positive going wave}$$
$$= A_- e^{-ikx} \quad \text{negative going wave}$$



Probability: $|\psi|^2 = \psi\psi^* = |A_+|^2 \text{ or } |A_-|^2$

Momentum: $p = \int_0^\infty \Psi^* \left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi \, dx = \hbar k \text{ or } -\hbar k$

Full Problem Difficult: Toy Problems First

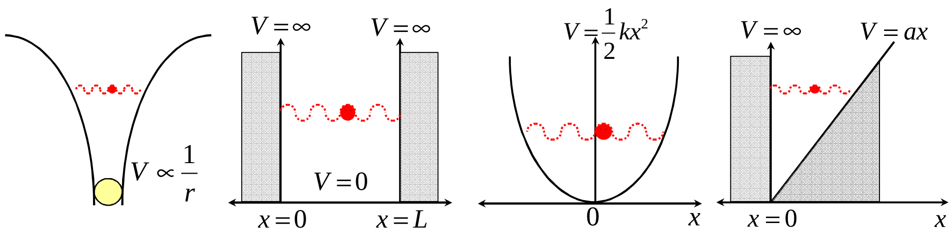


Case 2: Bound State Problems

- Mathematical interpretation of Quantum Mechanics(QM)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

  » Only a few number of problems have exact mathematical solutions
  » They involve specialized functions



Coulomb Potential by nucleus in an atom	Particle in a box	Harmonic Oscillator	Triangular Potential Well
$\Psi_n(r)=AR_n(r)Y_n(\theta,\varphi)$	$\Psi_n(x)=A\sin(k_n x)$	$\Psi_n(x)=A\frac{1}{\sqrt{2^n n!}}H_n(Bx)e^{-\frac{Cx^2}{2}}$	$\Psi_n(x)=N\text{Ai}(\xi_n)$

1-D Particle in a Box - A Solution Guess

- (Step 1) Formulate time independent Schrödinger equation

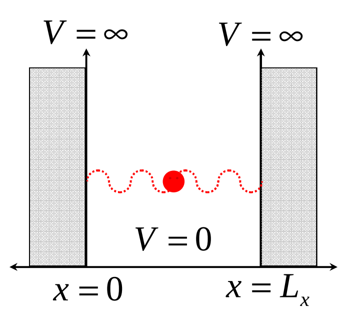
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \quad \text{where, } V(x)=\begin{cases}0 & 0<x<L_x \\ \infty & \text{elsewhere}\end{cases}$$

- (Step 2) Use your intuition that the particle will never exist outside the energy barriers to guess,

$$\psi(x)=\begin{cases}0 & 0\le x\le L_x \\ \neq 0 & \text{in the well}\end{cases}$$

- (Step 3) Think of a solution in the well as:

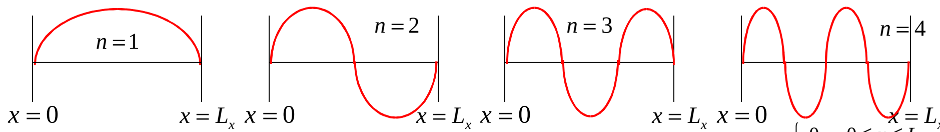
$$\psi_n(x)=A\sin\left(\frac{n\pi}{L_x}x\right),\quad n=1,2,3,\ldots$$



1-D Particle in a Box - Visualization

- (Step 4) Plot first few solutions

$$\psi_n(x) = A\sin\left(\frac{n\pi}{L_x}x\right),\ n = 1,2,3,\ldots$$

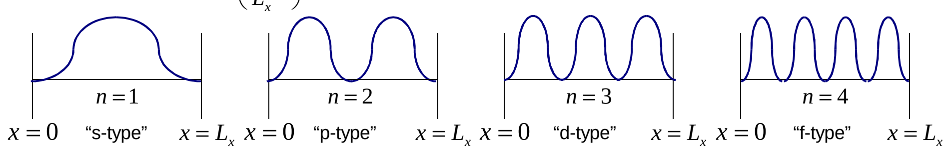


Matches the condition we guessed at step 2! $\psi(x) = \begin{cases} 0 & 0 \le x \le L_x \\ \neq 0 & \text{in the well} \end{cases}$

But what do the NEGATIVE numbers mean?

- (Step 5) Plot corresponding electron densities

$$|\psi_n(x)|^2 = A^2\sin^2\left(\frac{n\pi}{L_x}x\right),\ n = 1,2,3,\ldots$$ ➡ The distribution of SINGLE particle



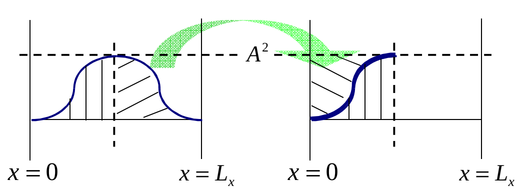
ONE particle => density is normalized to ONE

1-D Particle in a Box - Normalization to ONE particle

(Step 6) Normalization (determine the constant A)

Method 1) Use symmetry property of sinusoidal function

$$|\psi_n(x)|^2 = A^2\sin^2\left(\frac{n\pi}{L_x}x\right)$$



$$(\text{Area}) = 1 = \frac{L_x}{2} \times A^2$$

$$\therefore A = \sqrt{\frac{2}{L_x}}$$

Method 2) Integrate $|\psi_n(x)|^2$ over $0 \sim L_x$

$$1 = \int_0^{L_x} |\psi_n(x)|^2 dx = \int_0^{L_x} A^2\sin^2\left(\frac{n\pi}{L_x}x\right)dx = A^2\int_0^{L_x}\frac{1-\cos\left(\frac{2n\pi x}{L_x}\right)}{2}dx = A^2\frac{L_x}{2}$$

$$\therefore \psi_n(x) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right),\quad n = 1,2,3,\ldots \quad 0 < x < L_x$$

1-D Particle in a Box - The Solution

(Step 7) Plug the wave function back into the Schrödinger equation

$$\psi_n(x) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right) \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

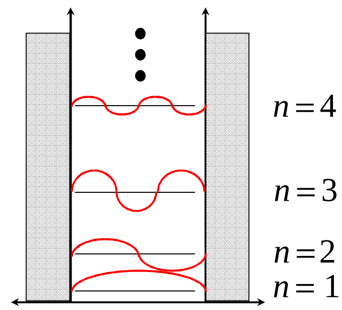
$$\frac{\hbar^2}{2m}\frac{n^2\pi^2}{L_x^2} = E_n$$

$$\psi_n(x) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right)$$

$$E_n = \frac{\hbar^2\pi^2}{2mL_x^2}n^2$$

$$n = 1, 2, 3, \ldots, \quad 0 < x < L_x$$

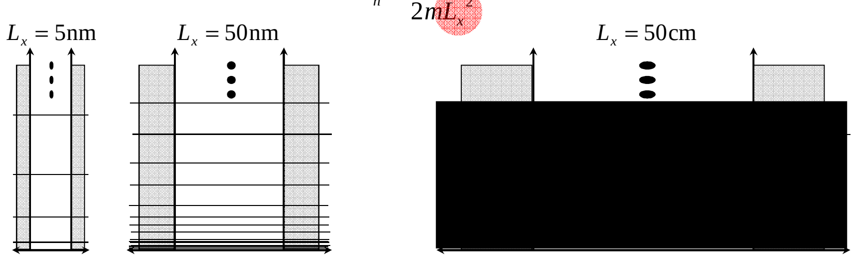
Discrete Energy Levels!



1-D Particle in a Box - Quantum vs. Macroscopic

- Quantum world → Macroscopic world
  - » What will happen with the discretized energy levels if we increase the length of the box?

$$E_n = \frac{\hbar^2\pi^2}{2mL_x^2}n^2$$



- Energy level spacing goes smaller and smaller as physical dimension increases.
- In macroscopic world, where the energy spacing is too small to resolve, we see continuum of energy values.
- Therefore, the quantum phenomena is only observed in nanoscale environment.

Presentation Outline

- Time Independent Schroedinger Equation
- Analytical solutions of Toy Problems
  - » (Almost) Free Electrons
  - » Tightly bound electrons – infinite potential well
  - » Electrons in a finite potential well
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers
- Additional notes
  - » Discretizing Schroedinger's equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)

- piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt