ECE606: Solid State Devices
Lecture 2

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

Miller-Indices and Definition of Planes
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 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:** \((326)\)

\[
\begin{pmatrix}
-2 \\
0 \\
1
\end{pmatrix}
\quad \begin{pmatrix}
-2 \\
3 \\
0
\end{pmatrix}
\]

Normal to the surface and \(R_1, R_2\)

\[
\begin{pmatrix}
a & b & c \\
-2 & 3 & 0 \\
-2 & 0 & 1
\end{pmatrix} = 3a + 2b + 6c
\]

Vector indices same as Miller indices!

\((326)\) vs. \([326]\)

**Specify of vectors normal to a particular plane!**

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**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:**

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

\[
\cos(\theta) = N_1 \cdot N_2
= (h_2 h_1 + k_2 k_1 + l_2 l_1)/(h_2^2 + k_2^2 + l_2^2)^{1/2} (h_1^2 + k_1^2 + l_1^2)^{1/2}
\]
cos(θ) = \frac{(1x0 + 0x1 + 0x1)}{\sqrt{1x\sqrt{2}}} = 0
so θ = 90 degrees

(011) surface is normal to (100) surface

Example: Find the [021] direction

N_1 \cdot T = \cos(θ_1) = \frac{(1x0 + 0x2 + 0x1)}{1x\sqrt{5}} = 0, so θ = 90 degrees
[021] vector lies on (100) plane.

N_2 \cdot T = \cos(θ_2) = \frac{(0x0 + 2x1 + 1x1)}{\sqrt{5} \sqrt{2}} = 3/\sqrt{10}, so θ = 18.43 degrees with respect to [011] direction.
Bravais-Miller Indices

First three indices sum to zero.

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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. It is useful to review some identities of vector calculus to such calculations involving crystal planes.

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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
\[ \frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0 \]
• Wave equation
• One solution

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
  => waves go around corners

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/propagation

Propagating Plane Waves

Light is an Electromagnetic Wave

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

Laws of Motion:
• Wave equation: $u = u_0 \sin(kx - \omega t)$
• One solution

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

Accepted Proof:
• Light is an electromagnetic wave

Double Slit Experiment


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

**Properties:**
- Have finite extent
- Have discrete wavelengths
- Have discrete frequencies

**Laws of Motion:**
- Wave equation
- One solution

**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

```
\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0
```

```
u(x, 0) = \sin(kx)\ e^{-\alpha x}, \quad \frac{\partial u}{\partial t}(x, 0) = 0
```

- Countable in 1/2 wavelength
- Integer multiples
- Integer fractions
- Quantized momentum $k_j$

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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
Presented Outline

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

1 = L / 2

2 = L / 2

(1) black-body radiation
Rayleigh-Jeans Formula

\[ u(\lambda, T) \propto \frac{k_B T}{\lambda^3} \]

\[ \log(u) = -4 \log(\lambda) + \log(T) \]

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

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

\[ \lambda = \frac{c}{f} \]

\[ \sim f^2 \times hf \times \left( \frac{1}{e^{\beta / \lambda T} - 1} \right) \]

- nos. of modes
- Energy of mode
- Occupation Probability

EM emission occurs in discrete quanta of

\[ E = hf \quad n=1,2, \ldots \mid N \]
Show that the cosmic background temperature is approximately 3K. Can you “see” this radiation?
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)
• 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

\[ E_{m,n} = \text{const} \times \left( \frac{1}{m^2} - \frac{1}{n^2} \right) \]
Assume that angular momentum is quantized:

\[ L_n = m_0 v_n r_n = n \hbar \]

\[ v = n \hbar / m_0 r_n \]

\[ \frac{m_0 v^2}{r_n} = \frac{q^2}{4 \pi \epsilon_0 r_n^2} \]

\[ r_n = \frac{4 \pi \epsilon_0 (n \hbar)^2}{m_0 q^2} \]

K.E. = \( \frac{1}{2} m_0 v^2 = \frac{1}{2} \left( \frac{q^2}{4 \pi \epsilon_0 r_n} \right) \)

P.E. = \( -\frac{q^2}{4 \pi \epsilon_0 r_n} \) \( (\text{P.E. set to 0 at } r = \infty) \)

\[ E_n = \text{K.E.} + \text{P.E.} = \frac{1}{2} \left( \frac{q^2}{4 \pi \epsilon_0 r_n^2} \right) \]

\[ E_n = -\frac{m_0 q^4}{2(4 \pi \epsilon_0 n \hbar)^2} = -\frac{13.6}{n^2} \text{ eV} \]

\[ E_{m,n} = \text{const} \times \left( \frac{1}{m^2} - \frac{1}{n^2} \right) \]
Strange Experimental Observations
The Advent of Quantum Mechanics

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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

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

Presentation Outline
- Classical Systems
  » Particles
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  » 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.
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)

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

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

$E = hf$

- Light can be described by discrete particles of discrete energy
- Planck’s constant $\hbar$ (Planck constant)
- Light energy is not divisible
- Have to have minimum energy to kick out an electron from the bound state

$E_{\text{binding}} = hf_m$

$E_{\text{kinetic}} = E_{\text{light}} - E_{\text{binding}} = h(f_{\text{light}} - f_m) \geq 0$

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

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

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

\[ hf = pc \quad m_0=0 \text{ (photon rest mass)} \]

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

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- 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.
Which electrons contribute to device current?

Number of atoms/volume from crystal structure

Number of electrons available for conduction

Number of electrons/atoms

\[ n \neq \rho \times N \]

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

Do I really need Quantum Mechanics?

Original Problem Periodic Structure Electrons in periodic potential: Problem we want to solve

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 number = Number of states x filling factor

Chapters 2-3    Chapter 4

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

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• Why do we need quantum mechanics?
• Formulation of Schrödinger's Eq.
\[ E = \sqrt{m_0^2 c^4 + p^2 c^2} \approx m_0 c^2 \left[ 1 + \frac{p^2 c^2}{2 m_0^2 c^4} + \ldots \right] \]

\[ E - m_0 c^2 = V + \left( \frac{p^2}{2 m_0} \right) \]

\[ h f = \hbar \omega = V + \left( \frac{\hbar^2 k^2}{2 m_0} \right) \]

Assume,

\[ \Psi(x, t) = A \exp(-i(\omega t - kx)) \]

\[ \frac{d\Psi}{dt} = -i\omega \Psi \quad \text{and} \quad \frac{d^2 \Psi}{dx^2} = -k^2 \Psi \]

\[ i\hbar \frac{d\Psi}{dt} = \left( -\frac{\hbar^2}{2 m_0} \frac{d^2 \Psi}{dx^2} \right) + V \Psi \]
1. Given chemical composition and atomic arrangements, we can compute electron density by using quantum mechanics.

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.
Periodic Structure
Time-independent Schrödinger Equation

Assume

\[ -\frac{\hbar^2}{2m_0} \frac{d^2\psi}{dx^2} + U(x)\psi = i\hbar \frac{d\psi}{dt} \]

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

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

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

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

If \( E > U \), then ….

\[ k \equiv \sqrt{\frac{2m_0(E-U)}{\hbar}} \]

\[ \frac{d^2\psi}{dx^2} + k^2\psi = 0 \]

\[ \psi(x) = A\sin(kx) + B\cos(kx) \equiv Ae^{ikx} + Ae^{-ikx} \]

If \( U > E \), then ….

\[ \alpha \equiv \sqrt{\frac{2m_0(U-E)}{\hbar}} \]

\[ \frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \]

\[ \psi(x) = De^{-\alpha x} + Ee^{\alpha x} \]
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 2\textsuperscript{nd} order equation – pretty basic
- Interpret $|\psi|^2 = \psi \ast \psi$ as the probability of finding an electron at x
- Compute anything else you need, e.g.,

\[
p = \int_0^\infty \psi^\ast \left[ \frac{\hbar}{i} \frac{d}{dx} \right] \psi \, dx, \quad E = \int_0^\infty \psi^\ast \left[ -\frac{\hbar}{i} \frac{d}{dt} \right] \psi \, dx
\]

Presentation Outline

- Time Independent Schrödinger 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 Schrödinger’s equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)
- piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt
Case 1: Solution for Particles with $E \gg U$

1) Solution

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

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

2) Boundary condition

$$\psi(x) = A e^{ikx} \quad \text{positive going wave}$$

$$= A e^{-ikx} \quad \text{negative going wave}$$
\[ \psi(x) = A \sin(kx) + B \cos(kx) \]
\[ \equiv A_+ e^{ikx} + A_- e^{-ikx} \]
\[ \psi(x) = A_+ e^{ikx} \quad \text{positive going wave} \]
\[ = A_- e^{-ikx} \quad \text{negative going wave} \]

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

Momentum:
\[ p = \int_{-\infty}^{\infty} \psi^* \left[ \frac{\hbar}{i} \frac{d}{dx} \right] \psi \ dx = \hbar k \quad \text{or} \quad -\hbar k \]

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Free Particle...

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Full Problem Difficult: Toy Problems First

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Case 1:
Free electron
\[ E >> U \]

Case 2:
Electron in infinite well
\[ E << U \]

Case 3:
Electron in finite well
\[ E < U \]
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

Purdue Klimeck - ECE606 Fall 2012 - notes adopted from Alam

1-D Particle in a Box - A Solution Guess

- (Step 1) Formulate time independent Schrödinger equation

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

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

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

- (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

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

\begin{align*}
\text{\( n = 1 \)} & \quad x = 0 & \quad x = L_s \\
\text{\( n = 2 \)} & \quad x = 0 & \quad x = L_s \\
\text{\( n = 3 \)} & \quad x = 0 & \quad x = L_s \\
\text{\( n = 4 \)} & \quad x = 0 & \quad x = L_s
\end{align*}

Matches the condition we guessed at step 2!

But what do the NEGATIVE numbers mean?

• (Step 5) Plot corresponding electron densities

\[ \left| \psi_n(x) \right|^2 = A^2 \sin^2 \left( \frac{n \pi x}{L_s} \right), \ n = 1, 2, 3, \ldots \rightarrow \text{The distribution of SINGLE particle} \]

\begin{align*}
\text{\( n = 1 \)} & \quad x = 0 & \quad \text{\( \text{\textquotedblleft}s\text{-type}\) } x = L_s \\
\text{\( n = 2 \)} & \quad x = 0 & \quad \text{\( \text{\textquotedblleft}p\text{-type}\) } x = L_s \\
\text{\( n = 3 \)} & \quad x = 0 & \quad \text{\( \text{\textquotedblleft}d\text{-type}\) } x = L_s \\
\text{\( n = 4 \)} & \quad x = 0 & \quad \text{\( \text{\textquotedblleft}f\text{-type}\) } x = L_s
\end{align*}

ONE particle \( \rightarrow \) 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

\[ \int_0^{L_s} A^2 \sin^2 \left( \frac{n \pi x}{L_s} \right) dx = A^2 \int_0^{L_s} \frac{1 - \cos \left( \frac{2n \pi x}{L_s} \right)}{2} dx = A^2 \frac{L_s}{2} \]

\[ \therefore \ A = \frac{2}{\sqrt{L_s}} \]

Method 2) Integrate \( \left| \psi_n(x) \right|^2 \) over \( 0 \sim L_s \)

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

\[ \therefore \ \psi_n(x) = \sqrt{\frac{2}{L_s}} \sin \left( \frac{n \pi x}{L_s} \right), \ n = 1, 2, 3, \ldots \]

\[ 0 < x < L_s \]
1-D Particle in a Box - The Solution

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

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

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x) \]

\[ = E_n \]

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

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

Discrete Energy Levels!

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

- Quantum world \( \rightarrow \) 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.
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