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Title: Presentation Seminar

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Presentation Seminar

Presented by

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Theoretical Division (T-4)
Los Alamos National Laboratory

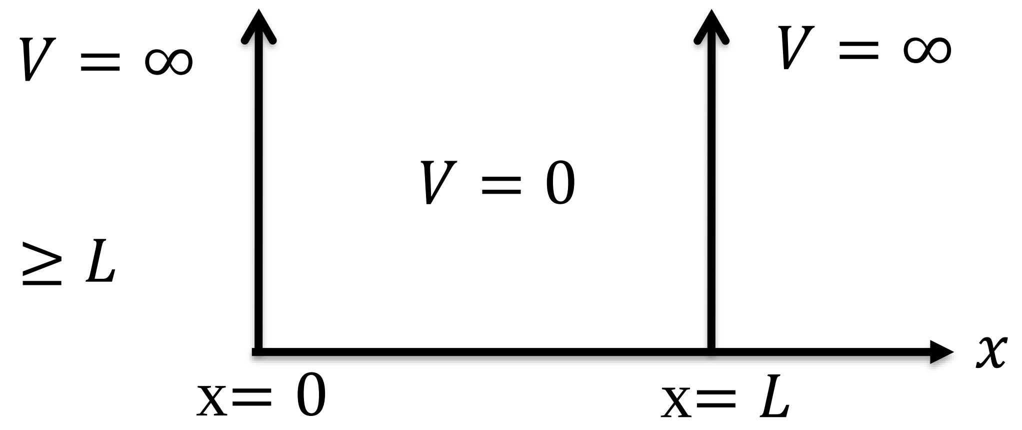
Date: 21/08/2023

Particle in a one-dimensional box

Particle in a one-dimensional box

Question:

$$V(x) = 0 \; for \; 0 < x < L$$
$$= \infty \; for \; x \leq 0 \; or \; x \geq L$$



- Consider an object of mass *m* is moving along the *x direction and* confined to a region between *x* = 0 and *x* = *L*. The potential energy is zero inside the "box" and infinite outside (see figure).

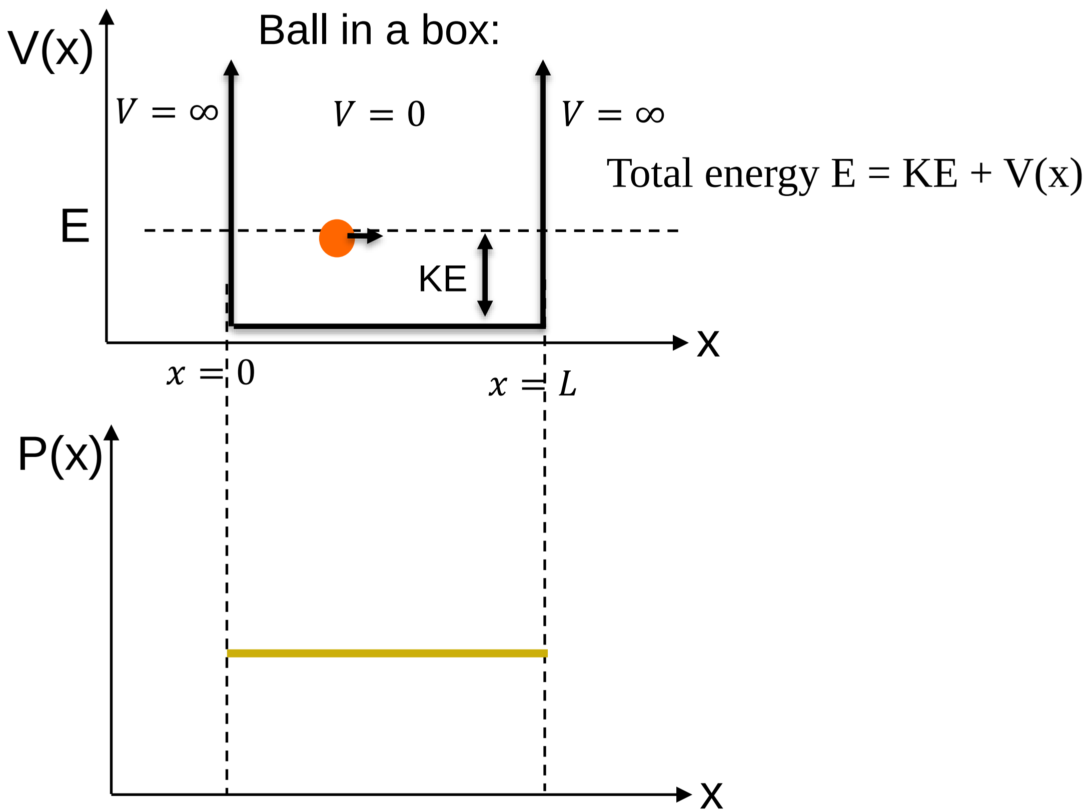
What is the probability of finding the object inside the box?

Particle in a one-dimensional box

Solution:

Let us start with the case when the mass of the object is large (~ kg)

Classical Picture



Probability is equally distributed

Particle in a one-dimensional box

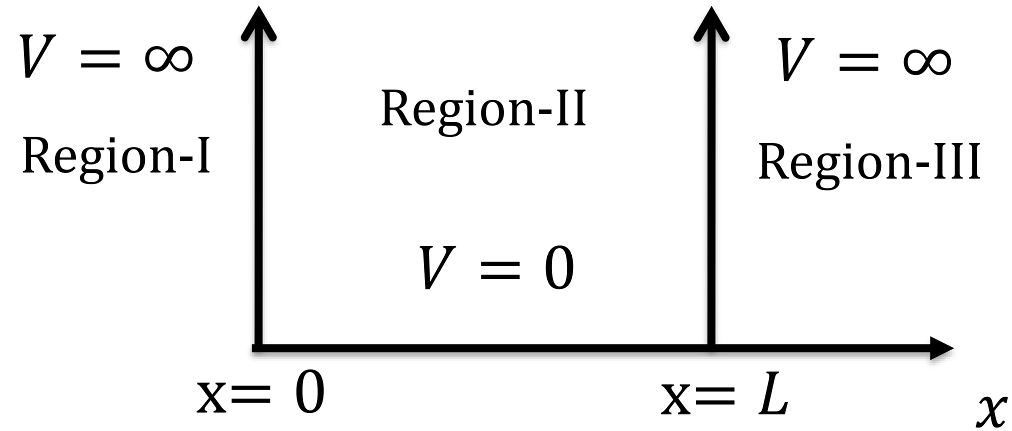
If we consider the object as an electron (~10^{-31} kg), does the previous result hold?

Particle behaves as a quantum particle, and we need to solve the problem quantum mechanically

Particle in a one-dimensional box

Solution:

$$V(x) = 0 \; for \; 0 < x < L$$
$$\quad = \infty \; for \; x \le 0 \; or \; x \ge L$$



Time Independent Schrödinger Equation

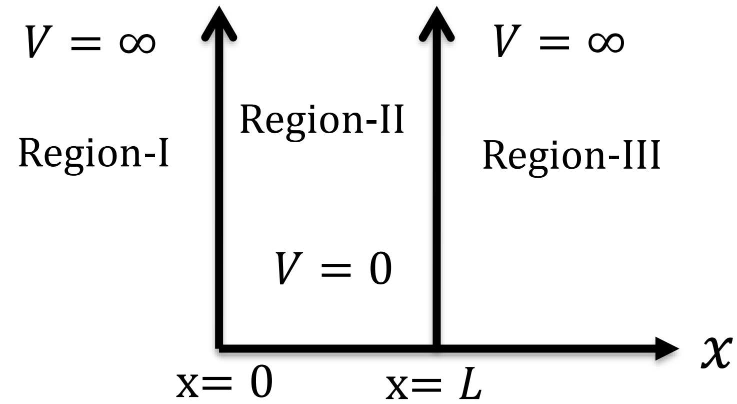
$$\underbrace{\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}}_{\text{KE}} + \underbrace{V(x)\psi}_{\text{PE}} = \underbrace{E\psi}_{\text{TE}}$$

Time-independent because the total energy is given

Regions I and III are identical, so we really only need to deal with two distinct regions, (i) outside, and (ii) inside the box

Particle in a one-dimensional box

Solution:



When V = 0 or ∞, what is ψ(x)?

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

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{Where } k^2 = \frac{2m(E-V)}{\hbar^2}$$

Second order homogeneous linear deferential equation

The solution is given by

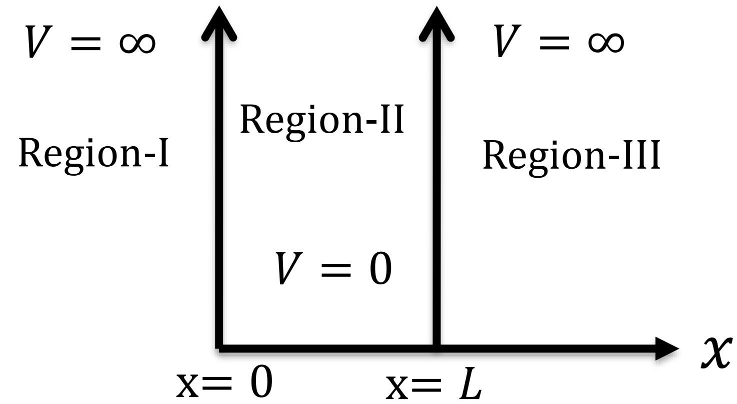
$$\psi_{II}(x) = A\sin kx + B\cos kx \quad \text{and} \quad \psi_I(x) = \psi_{III}(x) = 0$$

Otherwise, the energy would have to be infinite, to cancel U.

A and B are coefficients to be determined by the boundary conditions

Particle in a one-dimensional box

Solution:



Recall: The wave function ψ(x) must be continuous at all boundaries.

(i) *At x = 0:* $\psi_I(0) = \psi_{II}(0) = 0$

$$A \sin 0 + B \cos 0 = 0$$

Therefore, we must have $B = 0$ [Since $\sin 0 = 0$ and $\cos 0 = 1$]

(ii) *At x = L:* $\psi_{II}(L) = \psi_{III}(L) = 0;$ $A \sin L = 0$

- We must have either $A = 0$ or $\sin kL = 0$. The first solution ($A = 0$) is called the "**trivial solution**" and is not acceptable because this would make ψ_{II} equal to zero everywhere, which is not true.

- Then the acceptable solution is ($\sin kL = 0$) which can be true only when $kL = n\pi$ where $n = 1, 2, 3, \ldots$.
  Note that $n = 0$ is also a **trivial solution**.

Particle in a one-dimensional box

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Wave function for the particle inside the box in the **state *n***:

$$\psi_n = A \sin\left(\frac{n\pi x}{L}\right)$$

$n =$ quantum number of the state

A can be determined from the normalization condition

$$\int_0^L \psi_n \psi_n^* \, dx = 1 \quad \Rightarrow \quad A = \sqrt{2/L}$$

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

Energy Eigenvalue:

$$k = \frac{n\pi}{L} \quad \Rightarrow \quad E_n = \frac{n^2 h^2}{8mL^2}$$

Zero Point Energy $\Longrightarrow$ $E_1 = \dfrac{h^2}{8mL^2}$

Energy is *quantized*

Particle in a one-dimensional box

Energy

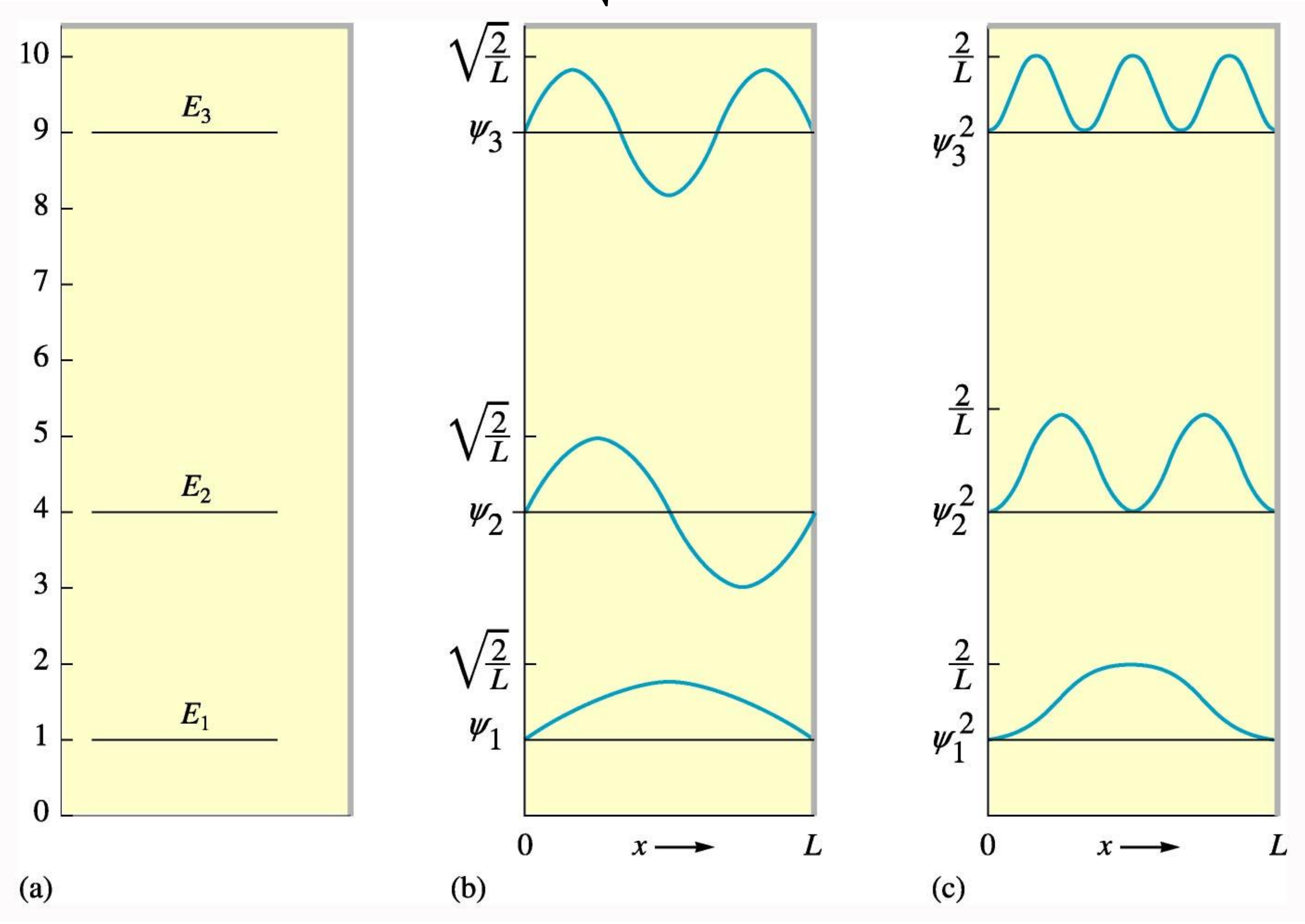
$$E_n = \frac{n^2 h^2}{8mL^2}$$

Wave Function

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

Probability

$$\psi_n(x)\psi_n^*(x)$$



Particle in a one-dimensional Box

Take Home Message

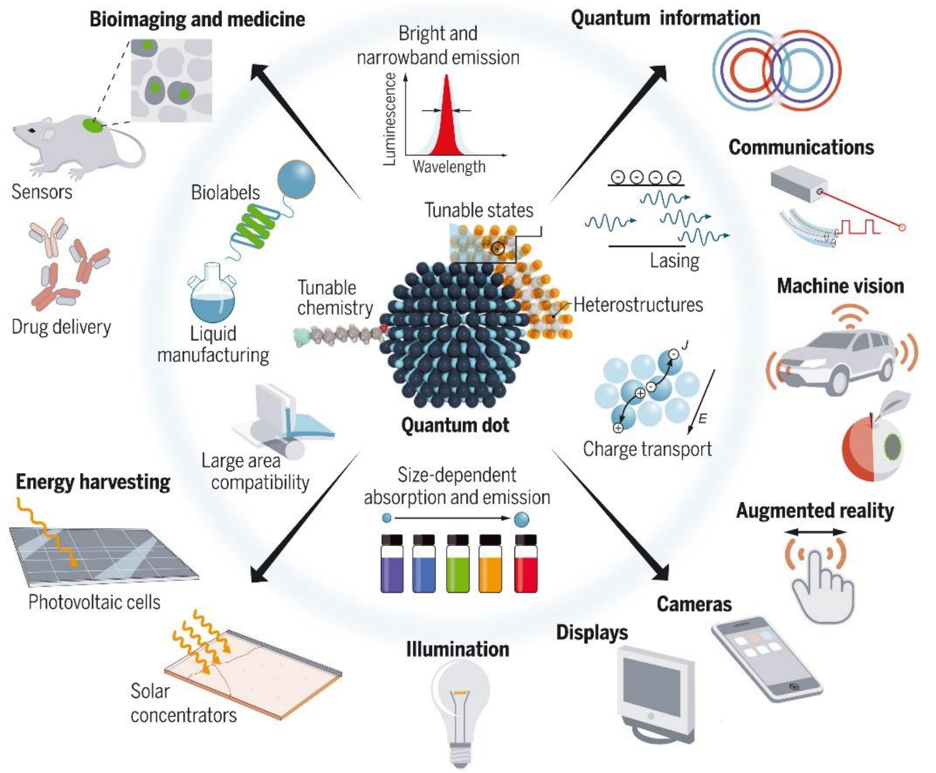
- The energy of a particle is quantized. This means it can only take on discreet energy values
- The lowest possible energy for a particle is **NOT** zero. This means the particle *always* has some kinetic energy.
- In classical physics, the probability of finding the particle is independent of the energy and the same at all points in the box.
- As E increases, number of nodes increases too (Number of node = n − 1)
- The probability changes with increasing energy of the particle and depends on the position in the box you are attempting to define the energy for

Particle in a one-dimensional Box

Real World Example

Quantum Dots Problem

- ❑ Quantum dots are nanoscale semiconductor, typically spheres of a few nanometers in diameter (10-50 nm)
- ❑ An electron in a quantum dot experiences quantum confinement in three dimensions (3D)
- ❑ **Can be thought of as a Particle in a 3D box problem**



García de Arquer et al., *Science* **373**, 640 (2021)

Teaching Proposal

Based on my research expertise, I would like to design and teach the following new courses

Introduction to Topological Condensed Matter Physics

Part-I: Concept of topology in condensed matter systems, polarization, Zak phase, Berry phase, phenomenology of topological phases in 1D (e.g., SSH model, edge state realization), topological phases in 2D, Chern insulator, quantum anomalous Hall effect, bulk-boundary correspondence, quantum spin Hall insulators.

Part-II: 3D topological insulators, Weyl semimetals and beyond, quantum anomalies, *transport phenomena* of topological semimetals using Boltzmann transport formalism and Kubo response theory, topological superconductivity, and its application to quantum computing.

Density Functional Theory and Beyond

Introduce basic concepts of density functional theory (DFT), success of DFT with examples, basics of correlated systems, disagreement between DFT results and experiments in correlated systems, introduction of many-body physics, and concept of dynamical mean field theory to solve many body problems.

Route to Detect Chiral Anomaly in Weyl Semimetal

Concept of Topology

- ❑ Topology: An abstract concept in mathematics
- ❑ Used to distinguish different objects

Gauss-Bonnet Theorem ⇨ $\int_S K_{Gauss}\, ds = 2(1-g)$

K_{Gauss}= Gauss Curvature
g = Genus

$\boldsymbol{g} = 0$

≠

$\boldsymbol{g} = 1$

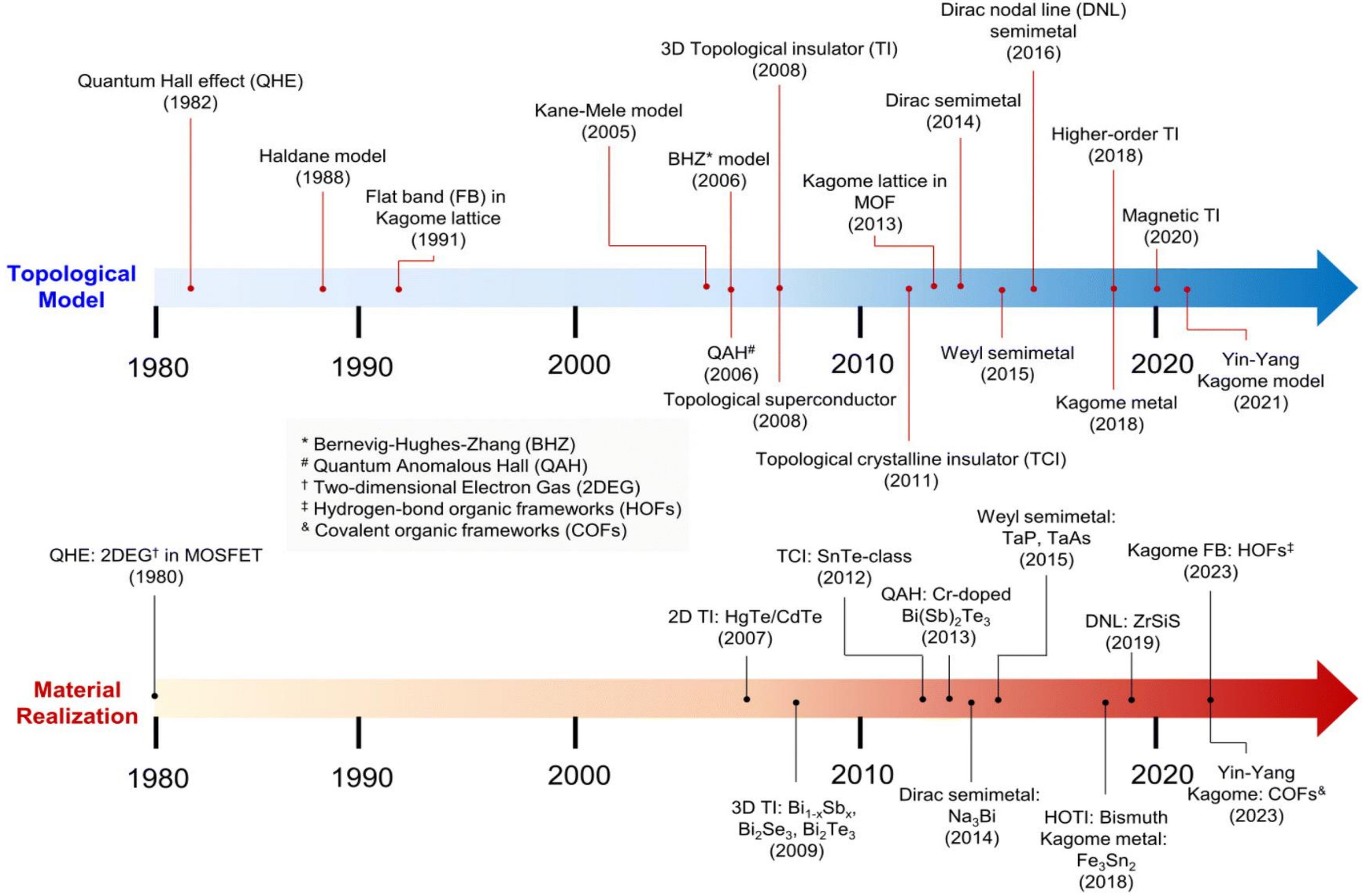
≠

$\boldsymbol{g} = 2$

Concept of Topology **?** **Condensed Matter Systems**

Overview

Topological Condensed Matter Physics



K-H. Jin *et al, Nanoscale* **15**, 12787 (2023); N. Kumar *et al, Chem. Rev.* **121**, 2780 (2021)

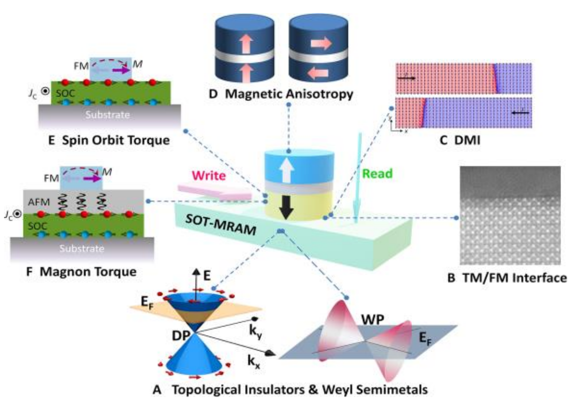
Why Topological Systems?

Fundamental Interests

- ❑ Most *robust* phases of nature (protected from local perturbations e.g., defects, impurities, material imperfections)
- ❑ Observables depend only on combinations of *fundamental constants*, like e, h, or c (Example: Hall conductivity of 2D insulators [e^2/h])
- ❑ Provide table-top experiment to detect the *quantum anomalies* linked with HEP
- ❑ Platform to realize experimentally the *fundamental Majorana quasiparticle*

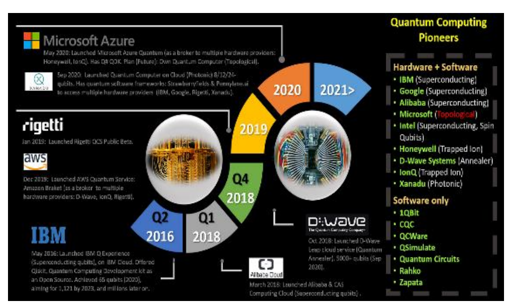
Technological Applications

Spintronics Applications



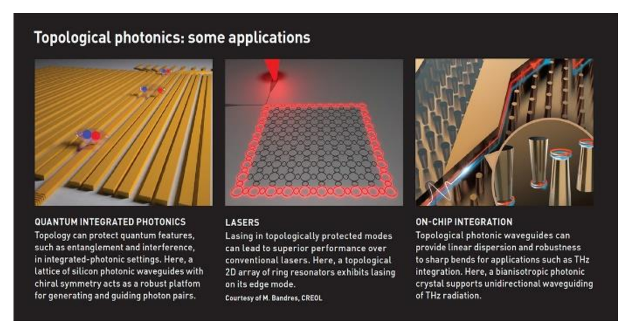
Y. Wang *et al Acc. Mater. Res.* **2**, 1061 (2022)

Quantum Computers



Picture: Google

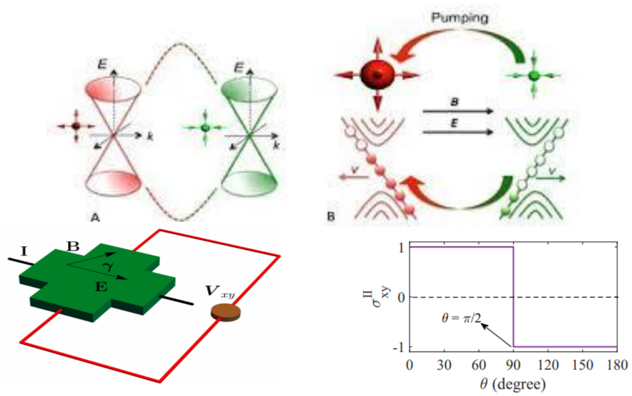
Photonics Applications



N. Kumar *et al Chem. Rev.* **121**, 2780 (2021)

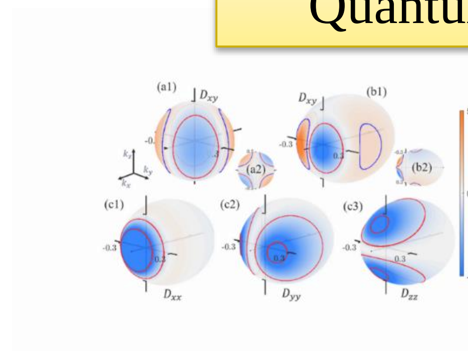
Research Directions

Topological Semimetals and Quantum Anomalies

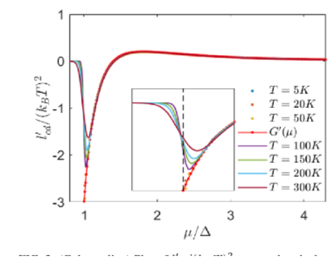


S. Nandy et. al., *Phys. Rev. Lett.* ***119***, 176804 (2017)
S. Nandy et. al., *Phys. Rev. B* ***100***, 115139 (2019)
S. Nandy et. al., *Phys. Rev. B* ***99***, 075116 (2019)
S. Nandy et. al., *Phys. Rev. B* ***106***, L041108 (2022)

Nonlinear Transport and Quantum Geometry



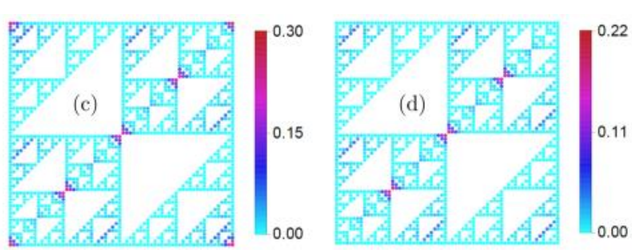
Nonlinear Hall Effect



New WF Law and Mott Relation

S. Nandy et. al., *Phys. Rev. Lett.* ***125***, 266601 (2020)
S. Nandy *et al, Phys. Rev. B* ***100***, 195117 (2019) [*ES*]
CZ, **S. Nandy** et. al., *Phys. Rev. Res. 2*, 032066 (R) (2020)
S. Nandy et. al., *Phys. Rev. B* ***104***, 205124 (2021)
CZ*, **S. Nandy***et al, *Phys. Rev. B* ***99***, 075116 (2022) [ES]

Topological Superconductivity



Search for Majorana Quasiparticle

SM**, S. Nandy** et. al., *Phys. Rev. B* ***105***, L201301 (2022)

Weyl Semimetals and Quantum Anomalies

S. Nandy et. al., *Phys. Rev. Lett.* ***119***, 176804 (2017)
S. Nandy et. al., *Phys. Rev. B* ***100***, 115139 (2019)
S. Nandy et. al., *Phys. Rev. B* ***99***, 075116 (2019)
S. Ghosh, A. Sahoo and **S. Nandy**, *arXiv: 2209.11217 (Accepted in SciPost Physics)*

Weyl Fermions and High Energy Physics

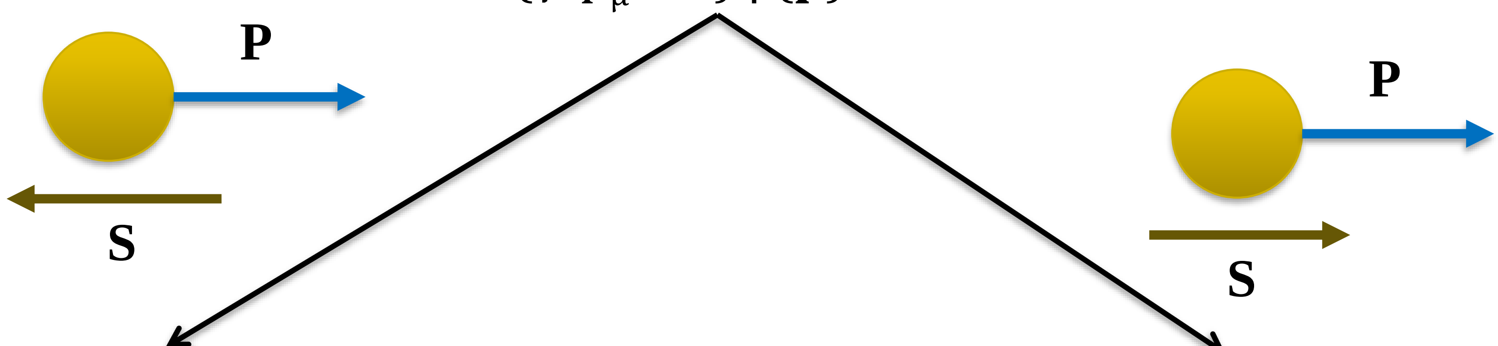
Hermann Weyl

- Weyl Fermion: Introduced in High Energy Physics in 1929.
- Massless spin-1/2 particles

Weyl, H. Elektron und Gravitation. I. *Z. Physik* **56,** 330–352 (1929)

Massless solution to the Dirac equation

$$(\gamma^{\mu} p_{\mu} - mc)\psi(\mathbf{p}) = 0$$



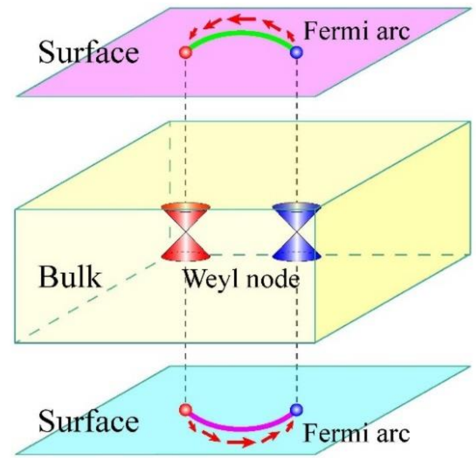
Left chirality Weyl Fermions

Right chirality Weyl Fermions

Peskin & Schroeder, An Introduction to Quantum Field Theory

Can Weyl Fermion appear in condensed matter systems?

- Appear as a low-energy quasiparticles near the touching point of a pair of linearly dispersing nondegenerate bands



- Low-energy Hamiltonian near a Weyl node

$$H^{\chi}(\boldsymbol{k}) = \chi \sum_{i=1}^{3} v_i(k_i)\sigma_i$$

N. P. Armitage et. al., *Rev. Mod. Phys*. **90**, 015001 (2018)

- Monopole Charge (Topological Invariant) ➡ $\chi = \frac{1}{2\pi}\int_{\Sigma} d\boldsymbol{S} \cdot \boldsymbol{\Omega} = \pm 1$

$\boldsymbol{\Omega}$ =Berry Curvature

First Discovery in 2015

Material: TaAs

Other Materials

TaP, NbP, NbAs, Mn_3Sn, $Co_3Sn_2S_2$, WTe_2

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S-.Y. Xu… M.Z. Hasan *et al* Science **349**, 9297 (2015); B-.Q. Lv… **H. Ding** *et al* PRX **5**, 031013 (2015)

Quantum Anomalies in WSM

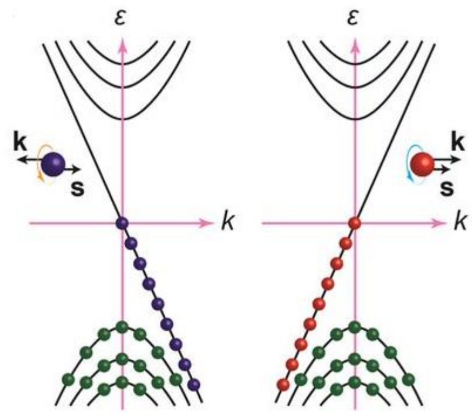
Quantum Anomalies

Quantum Anomaly refers to the violation of a “classical” symmetry, i.e., symmetry of the Lagrangian, once the second quantization is performed

Weyl Semimetal in a Magnetic Field

Left- and right-handed chiral fermions expected to have equal populations

$\chi = -1$



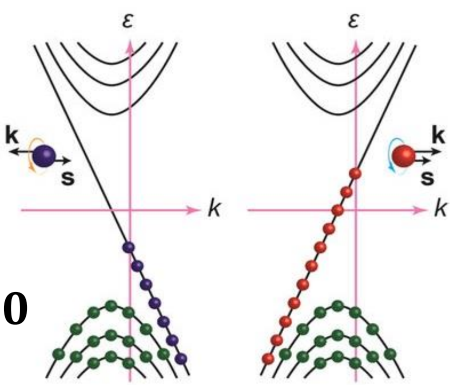
$\chi = +1$

$\boldsymbol{E} = 0$
$\mathbf{B} \neq 0$

Chiral Anomaly or Adler-Bell-Jackiw Anomaly

$\chi = -1$

$\mathbf{E} \neq 0$
$\mathbf{B} \neq 0$
$\mathbf{E} \cdot \mathbf{B} \neq \mathbf{0}$



$\chi = +1$

$$\partial_\mu J_\mu{}^\chi = \frac{e^2}{\hbar^2}\boldsymbol{E} \cdot \boldsymbol{B}$$

Technological Application

- ❖ Dissipationless information processing
- ❖ Chiral Photonics

Adv. Funct. Mater.2021, **31**, 2104192

*J. S. Bell and R. A. Jackiw, Nuovo Cimento A **60**, 47 (1969); V. Aji, Phys. Rev. B **85**, 241101 (2012); S. Adler, Phys. Rev. **177**, 2426 (1969)*

Key Science Question?

How to unambiguously identify the signature of the chiral anomaly in condensed matter experiments?

Existing Works

Negative Longitudinal Magnetoresistance

Son and Spivak, Phys. Rev. B **88**, 104412 (2013)
J. Xiong et. Al., *Science* **350,** 413–416 (2015)
X. Huang et. Al., . *Phys. Rev. X* **5**, 031023 (2015)
N. P. Armitage et. Al., *Rev. Mod. Phys*. **90**, 015001 (2018)

Experimental Concerns

- Current jetting effect
- Weak localization
- Negative off-diagonal effective mass

N.P. Ong and S. Liang, *Nat. Rev. Phys*. **3**, 394 (2021)
Y. Li et al., *Front. Phys*. **12**, 127205 (2017)
F. Arnold et. Al., *Nat. Commun*. **7**, 11615 (2016)
R. D. dos Reis et. al., New J. Phys. 18, 085006 (2016)

Difficult to separate topological contribution from non-topological origin

Chiral Anomaly in WSM

Planar Hall Effect

S. Nandy et. al., *Phys. Rev. Lett.* ***119***, 176804 (2017)

Appearance of an in-plane transverse voltage when the co-planar electric and magnetic fields are not perfectly aligned

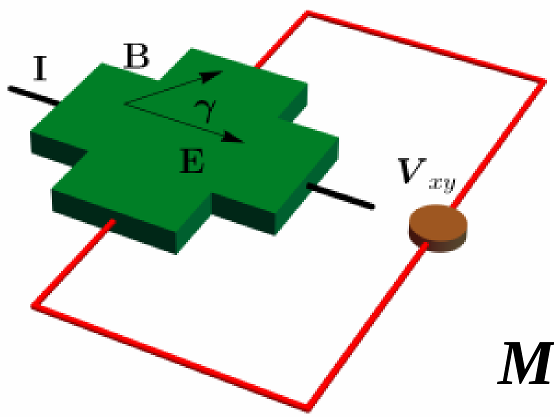


Illustration of planar Hall effect geometry

Method: Quasiclassical Boltzmann Transport Theory

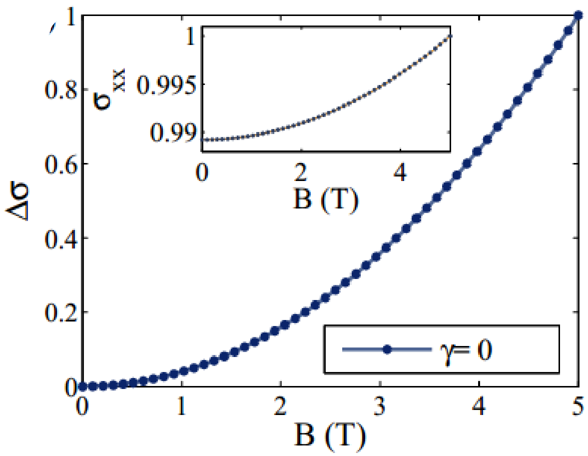
$$\sigma_{yx}^{ph} = e^2 \int [d\boldsymbol{k}] D\tau \left(-\frac{\partial f_{eq}}{\partial \varepsilon}\right)\left[v_y + \frac{eB\sin\theta}{\hbar}(\boldsymbol{v_k}\cdot\boldsymbol{\Omega_k})\right]\left[v_x + \frac{eB\cos\theta}{\hbar}(\boldsymbol{v_k}\cdot\boldsymbol{\Omega_k})\right]$$

- ❑ Does not satisfy the anti-symmetry property of regular Hall conductivity

$$\sigma_{yx}^{ph} \neq -\sigma_{xy}^{ph}$$

Chiral Anomaly in WSM

S. Nandy et. al., *Phys. Rev. Lett.* ***119***, 176804 (2017)

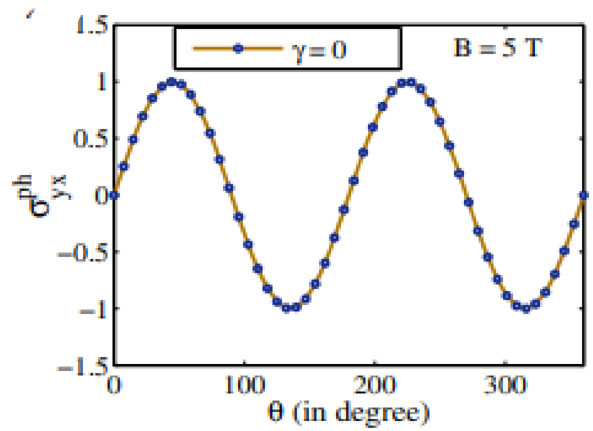


$$\sigma_{yx}^{ph} = \Delta\sigma \sin\theta \cos\theta$$

$$\Delta\sigma \propto B^2$$

↓

Magnitude of PHC



γ= Tilt Parameter

Origin: *Chiral Anomaly*

Recent Experimental Confirmation

❖ GdPtBi, Cd_3As_2, WTe_2, $PdTe_2$, $MoTe_2$, $ZrTe_5$, $Pr_2Ir_2O_7$ and so on…

N. Kumar et. al., Phys. Rev. B **98**, 041103(R) (2018)
P. Li et. al., Phys. Rev. B **98**, 121108(R) (2018)
N. Wadehra et. al., *Nat. Comm*. **11**, 874 (2020)

G. Yin et al., PRL **122**, 106602 (2019)
J. Zhong et. Al., Chin. Phys. B 32, 047203 (2023)

Future Directions

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Interplay Between Topology and Correlation

- Interplay between topology and electronic correlation and their consequences on transport and its application to real materials

Detecting Quantum Anomalies

- Proposing anomaly-induced new transport quantities linear-in-B that can shed light on distinguishing topological and non-topological contributions.

- Exploring PHE by including both the ferromagnetic and anomaly-induced contributions to gain deeper insight into ongoing experiments in recently discovered magnetic WSM

Quantum Geometry Induced Nonlinear Transport

- Revealing the role of disorder to higher-order responses in both 2D and 3D systems by considering different types of disorder (scalar disorder and beyond) and other scattering mechanisms (e.g., electron-phonon coupling) .


Thank You..

Why We Study this Problem?

Energy ∝ n 2 , not equally spaced
As E increases, number of nodes increases too (Number of node = n − 1.)
The probability |ψ(x)| 2 is more localized in the center at n = 1 and then spread out as n
The zero point energy is h 2 8mn2

Energy ∝ 1 a 2 , so when size of the box increases, the energy drops rapidly
Return to classical state at n → ∞

Also note that as the energy of the particle becomes greater, the quantum mechanical model breaks down as the energy levels get closer together and overlap, forming a continuum. This continuum means the particle is free and can have any energy value. At such high energies, the classical mechanical model is applied as the particle behaves more like a continuous wave.