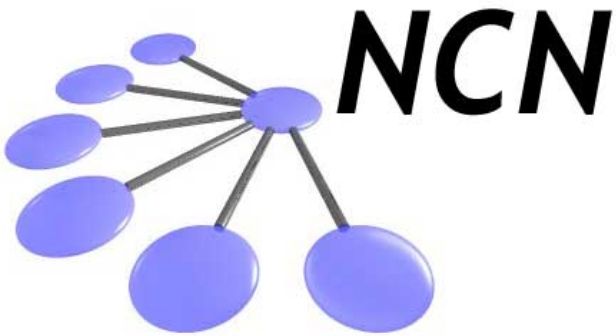

Introduction to Quantum Dot Lab

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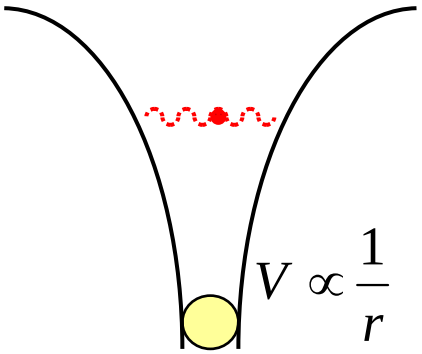
Analytical Solutions to the Schrödinger Equation

- Mathematical interpretation of Quantum Mechanics(QM)

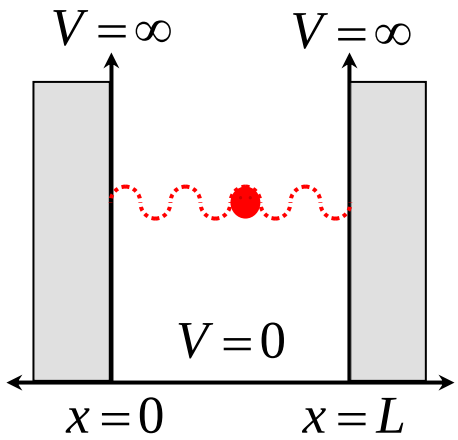
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

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



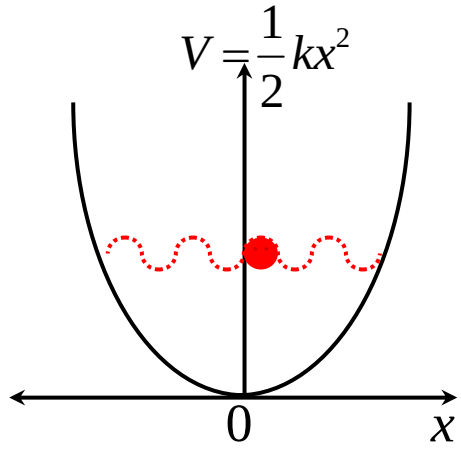
Coulomb Potential
by nucleus in an atom

$$\Psi_n(r) = AR_n(r)Y_n(\theta,\varphi)$$



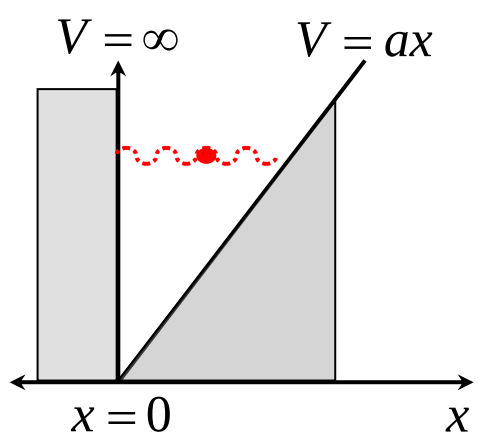
Particle in a box

$$\Psi_n(x) = A\sin(k_n x)$$



Harmonic Oscillator

$$\Psi_n(x) = A\frac{1}{\sqrt{2^n n!}}H_n(Bx)e^{-\frac{Cx^2}{2}}$$



Triangular Potential Well

$$\Psi_n(x) = N\mathrm{Ai}(\xi_n)$$

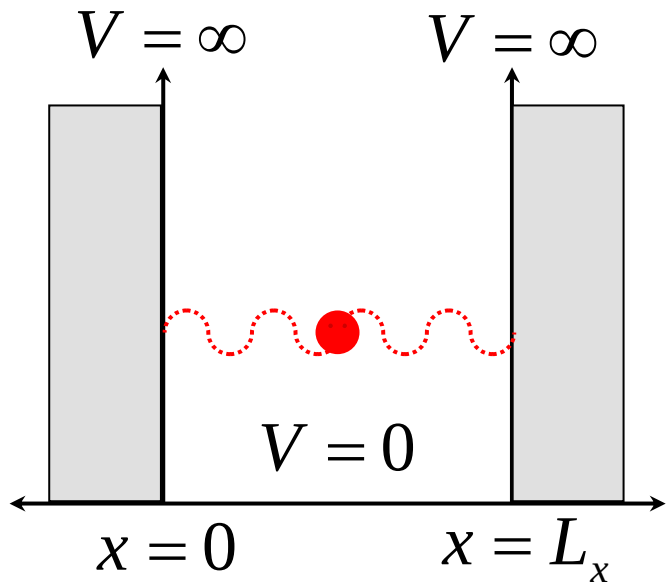
1-D Particle in a Box – A Solution Guess

- (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,

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



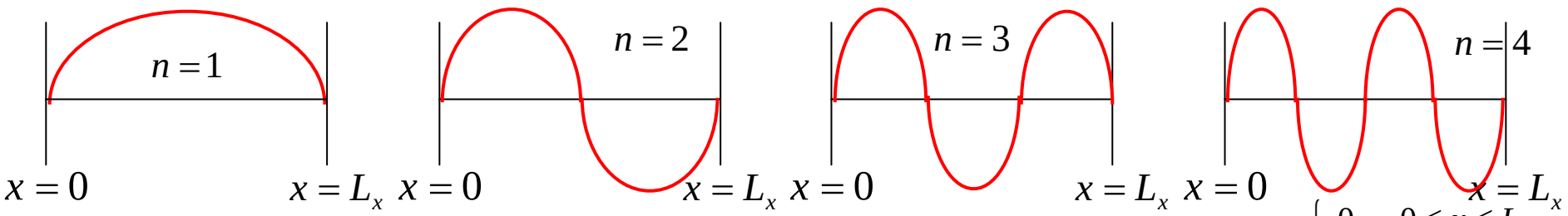
- (Step 3) Think of a solution in the well as:

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

1-D Particle in a Box – Visualization

- (Step 4) Plot first few solutions

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



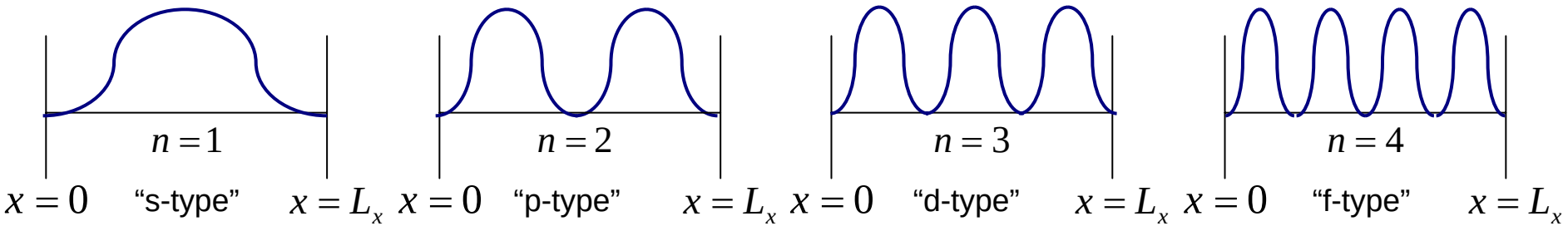
$$\psi(x) = \begin{cases} 0 & 0 \le x \le L_x \\ \neq 0 & \text{in the well} \end{cases}$$

Matches the condition we guessed at step 2!

But what do the NEGATIVE numbers mean?

- (Step 5) Plot corresponding electron densities

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



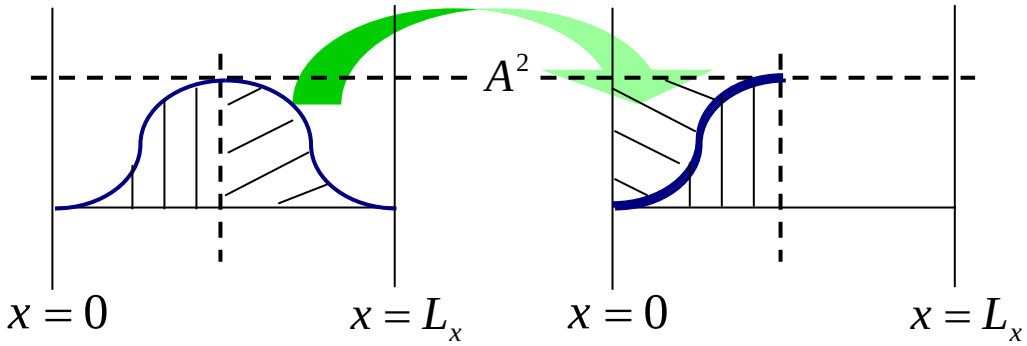
ONE particle => density is normalized to ONE

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

(Step 6) Normalization (determine the constant A)

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

Method 1) Use symmetry property of sinusoidal function



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

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

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

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

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

1-D Particle in a Box - The Solution

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

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

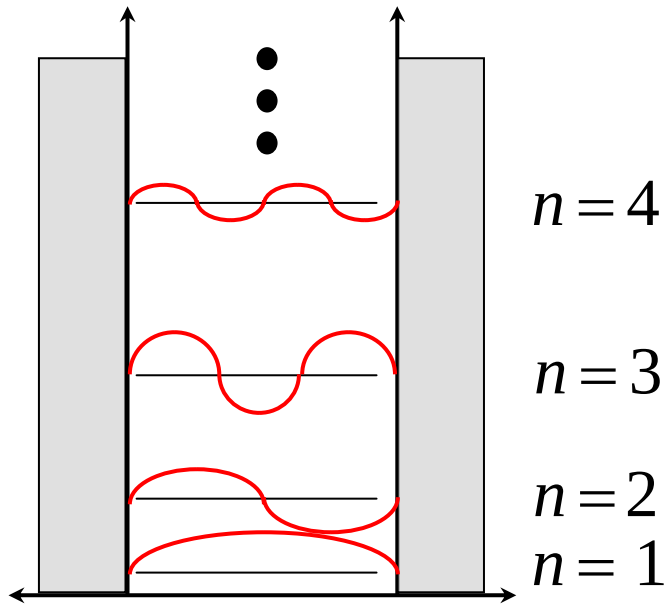
$$\frac{\hbar^2}{2m}\frac{n^2\pi^2}{L_x^{\,2}} = E_n$$

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

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

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

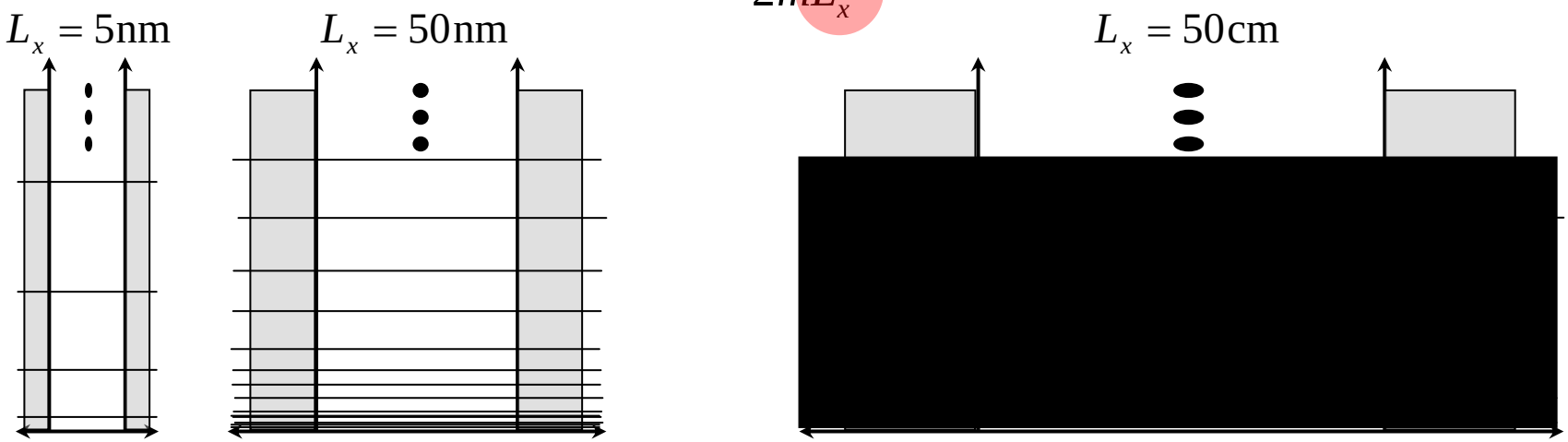
Discrete Energy Levels!



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?

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

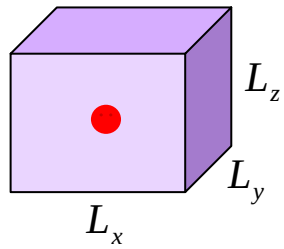


- Energy level spacing goes smaller and smaller as physical dimension increases.
- In macroscopic world, where the energy spacing is too small to resolve, we see continuum of energy values.
- Therefore, the quantum phenomena is only observed in nanoscale environment.

3-D Particle in a Box

- What will happen if a particle is confined in a cube?
  - » Schrödinger equation in full 3-D representation

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)=E\psi(x,y,z)$$



  - » Energy confinement in 3-D

$$V(x)=\begin{cases}0 & 0<x<L_x\ ,0<y<L_y,\ 0<z<L_z\\ \infty & \text{elsewhere}\end{cases}$$

- Similar to 1-D problem, we can conceive a set of solutions in a similar form:

$$\psi_{n_x n_y n_z}(x,y,z)=\sqrt{\frac{2}{L_x}\frac{2}{L_y}\frac{2}{L_z}}\sin\left(\frac{n_x\pi}{L_x}x\right)\sin\left(\frac{n_y\pi}{L_y}y\right)\sin\left(\frac{n_z\pi}{L_z}z\right)$$

$$E_{n_x n_y n_z}=\frac{\hbar^2\pi^2}{2m}\left(\left(\frac{n_x}{L_x}\right)^2+\left(\frac{n_y}{L_y}\right)^2+\left(\frac{n_z}{L_z}\right)^2\right)$$

$$n_x,n_y,n_z=1,2,3,\ldots,\quad 0<x<L_x,0<y<L_y,0<z<L_z$$

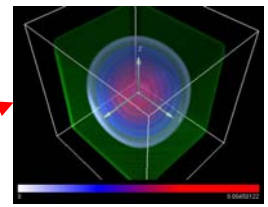
3-D Particle in a Cube

- Let $L_x = L_y = L_z = L$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right) \equiv K\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right)$$

$$\psi_{n_x n_y n_z} = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right)$$

n_x	n_y	n_z
1	1	1



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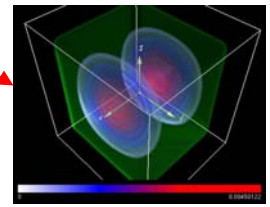
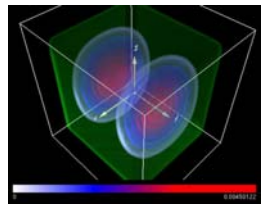
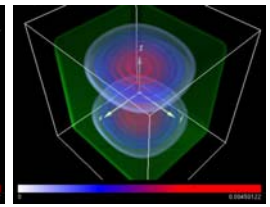






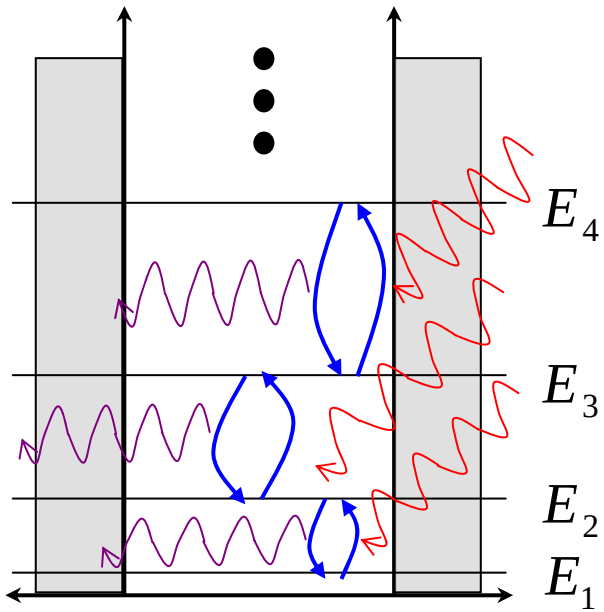
px py pz

- Degenerate energy values
  - same energy level
  - multiple wavefunctions

Transition Energy

Q: can a confined electron confined hop over energy states?

A: In principle, YES. It is *possible* "only if" we add appropriate amount of energy (i.e. shining light with certain frequency, thermal energy, etc.) to the system.

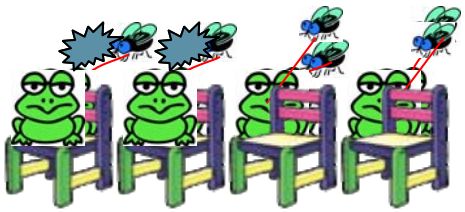


- Energy values of interest?
  - » Difference between discrete energy levels (i.e. E_4-E_3, E_3-E_2, E_2-E_1,…,E_4-E_1)
  - » Loses energy to settle at lower energy state by emitting light
  - » Absorbs energy to jump up to higher state
- Transition Energy $E_{nm} = E_m - E_n \ (= hf)$
  - » Energy needed to excite/relax an electron from initial state n to final state m
  - » LED,Laser (light emission)
  - » Photo detectors (energy excitation)
  - » Other energy values: Nothing happens!

Available States

Q: In a real Quantum Dot(QD), is it possible for electrons to hop around the energy levels freely if you apply Transition Energy?

A: NO! Because there are limited number of “states” in each energy level. Here’s an example.



100% Excitation!

(50% absorption)

“Available” state

Electron(frog) “occupied” state.

Any source of energy that helps an electron(frog) to jump up to the higher energy level

- Applying transition energy to the QD is not enough!
  - » Need available states for electrons to sit on.
- How do we know the occupancy at given energy level?

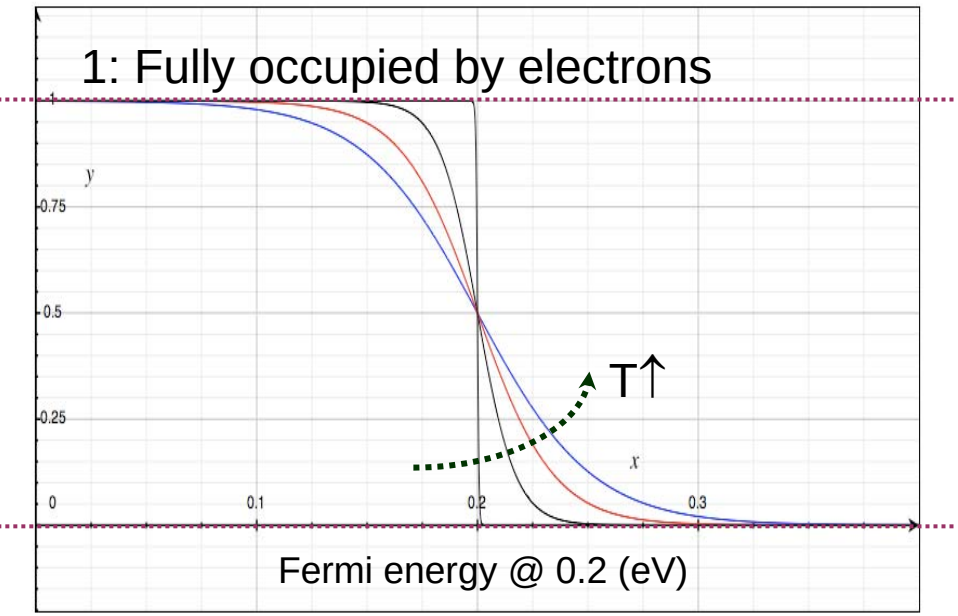
Fermi-Dirac Distribution Function

Fermi-Dirac Distribution Function

- Indicates the occupancy of states by electrons in equilibrium at given temperature and energy.

$$f(E) = \frac{1}{1 + \exp\left[\left(E - E_F\right)/k_B T\right]}$$

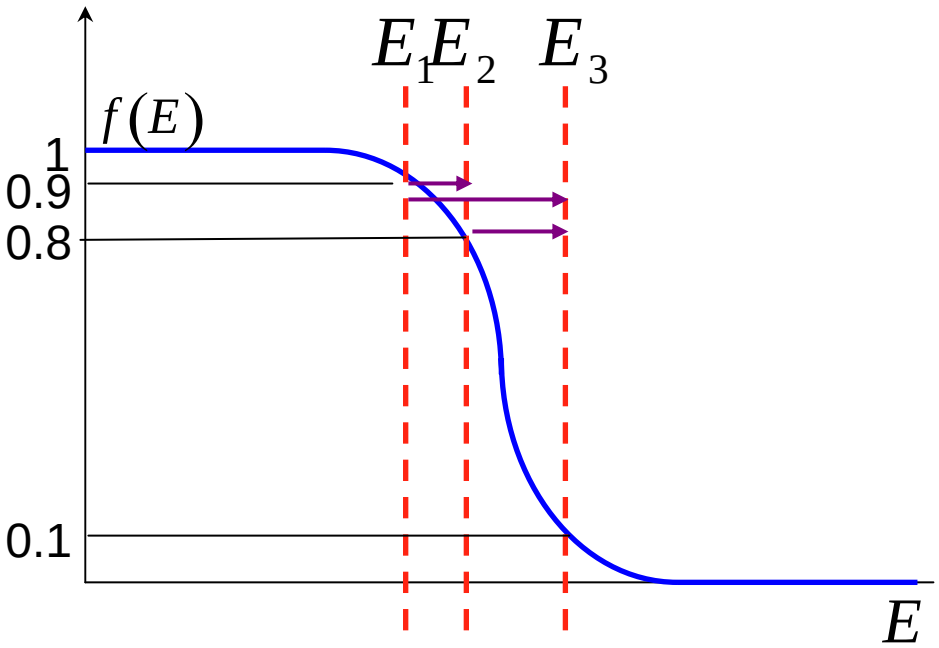
E_F : Fermi energy (eV)
k_B : Boltzmann constant (eV/K)
T : Temperature (K)



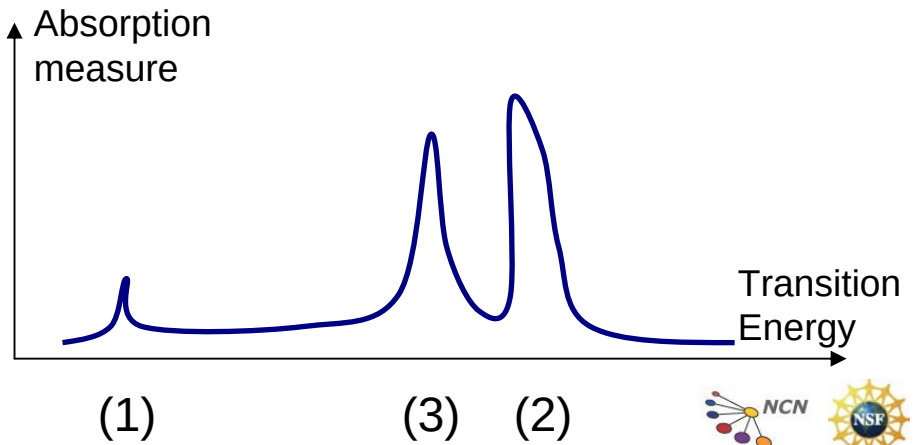
- Electrons tend to occupy from the lowest energy levels (T=0K)
- As thermal energy increases, more electrons near Fermi level are excited to occupy higher energy states (T>0K)

Energy Absorption Example

- Think of a nanostructure that has following properties:
  - » Energy levels are discretized
  - » Device is operating in finite temperature (>0K)
  - » Number of states are kept constant regardless of energy level
  - » Let's shine light and see what happens



State Transition	Transition Energy	Absorption
1 => 2	E2-E1 (1)	small
1 => 3	E3-E1 (2)	large
2 =>3	E3-E2 (3)	large

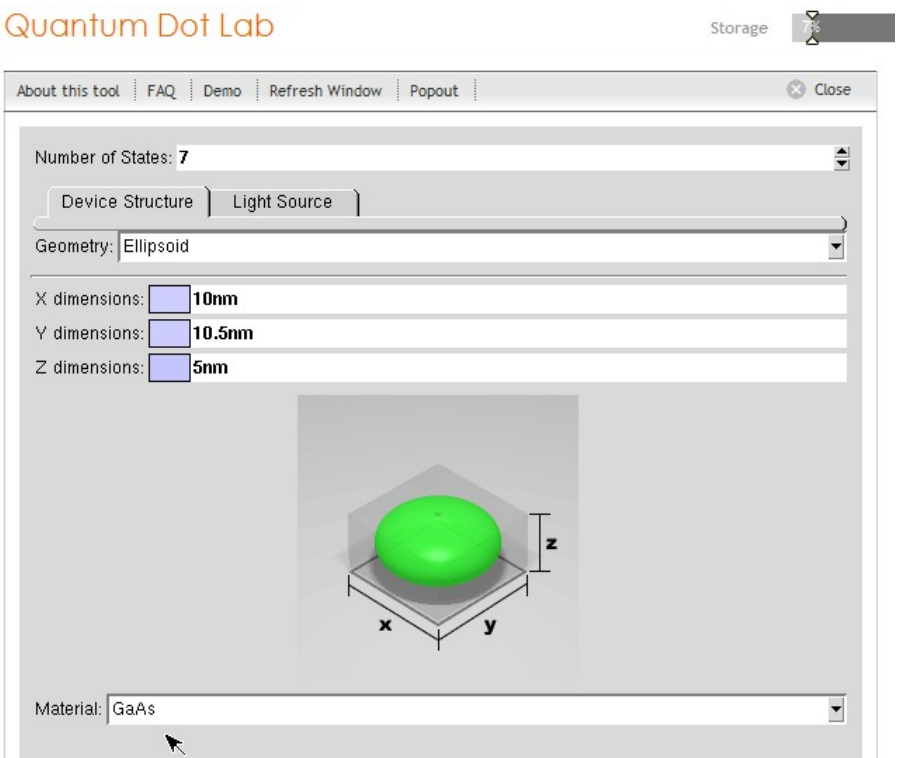


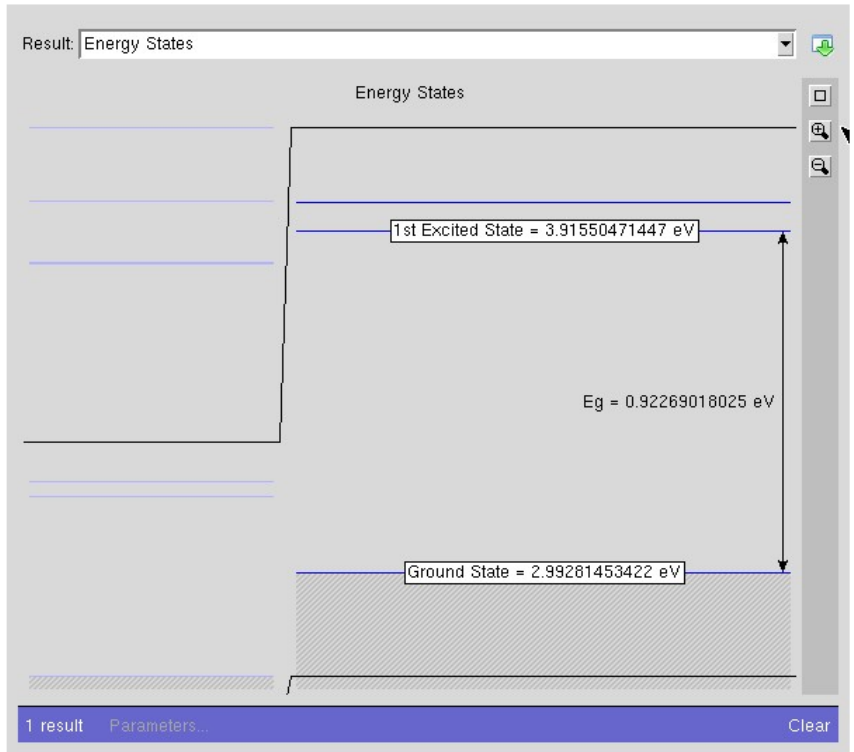
Quantum Dot Lab

- Now, let's try examples to enhance your understandings
- We can verify all the items we have learned through "Quantum Dot Lab"
- http://www.nanohub.org/tools/qdot/

Quantum Dot Lab
Simple Overview

- Analytical solutions are not always easy to obtain.
  - » What if we were interested in an “Ellipsoid shape” quantum dot?
  - » Can be easily computed with Quantum Dot Lab.





Exercise 1 :

Compute first 9 electron energy states in GaAs cubic Quantum Dot with Lx = 5nm Ly = 5.5nm and Lz = 6nm. Follow given procedure.

(Step 1) Run Rappture.

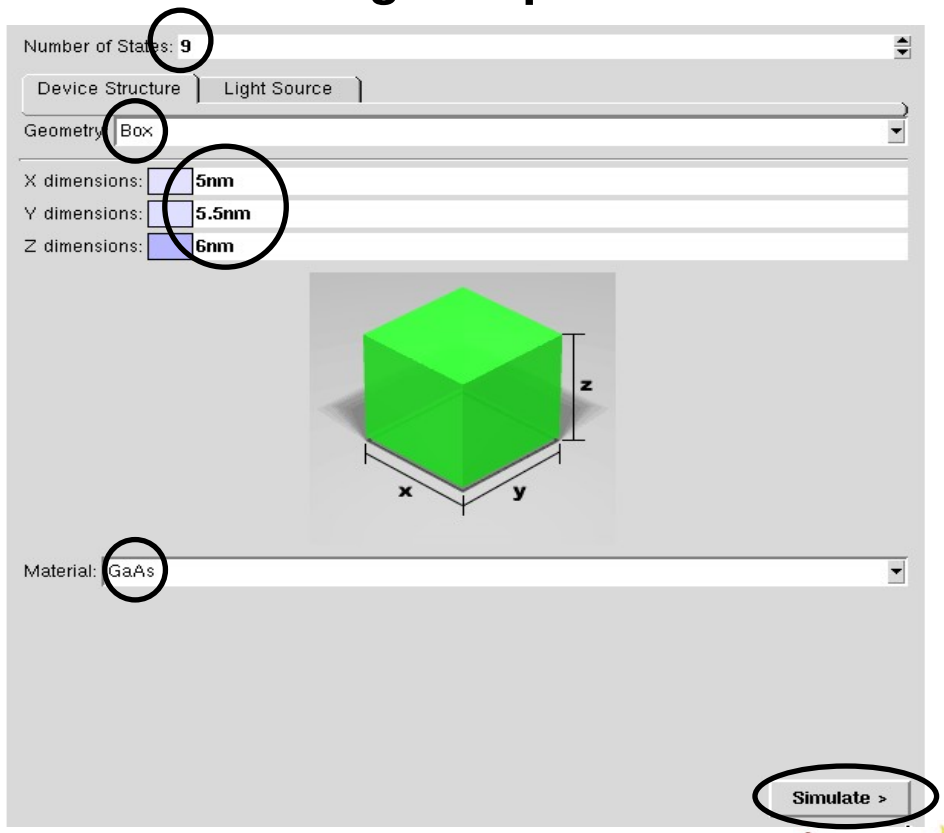
(Step 2) In 'Device Structure' tab, Choose the number of energy levels.

(Step 3) Select geometry of QD.

(Step 4) Set size of QD.

(Step 5) Select material of QD.

(Step 6) Simulate!

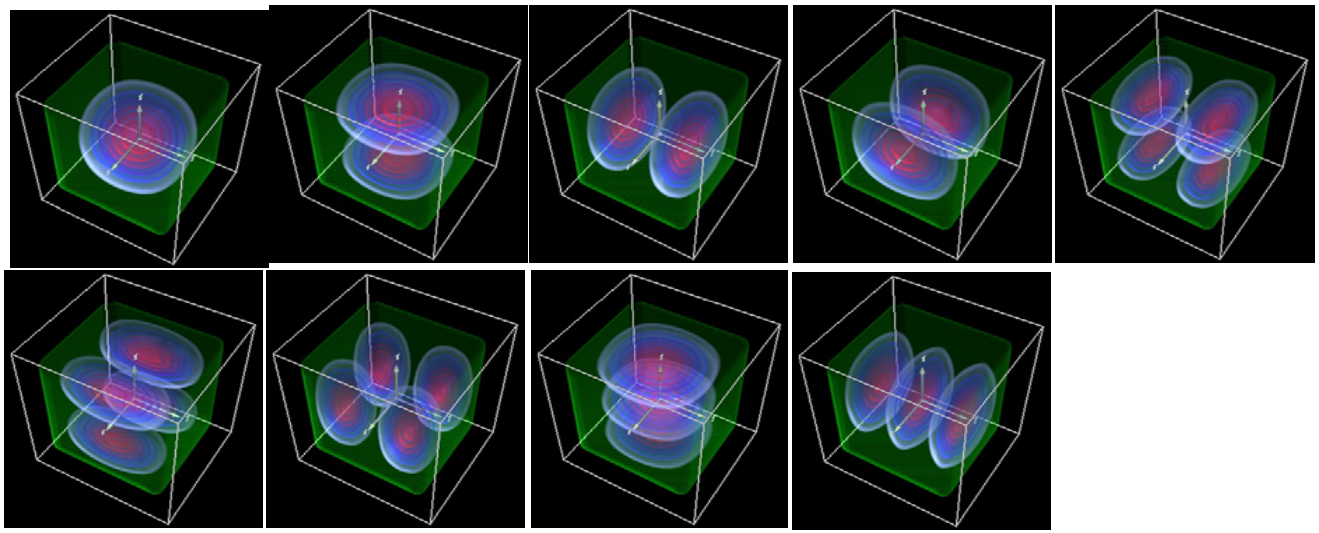


Exercise 1
3d box - Eigenstates

- **Computed Energy Level**

Ground	3.3099 (eV)	5th Excited	7.0171 (eV)
1st Excited	4.8655 (eV)	6th Excited	7.2794 (eV)
2nd Excited	5.1278 (eV)	7th Excited	7.3575 (eV)
3rd Excited	5.4615 (eV)	8th Excited	8.0197 (eV)
4th Excited	6.6834 (eV)		

- **Electron wave function at each energy level**



State 1, 2, 3, 4, 5

State 6, 7, 8, 9

Exercise 2 and 3

Exercise 2 :

Compute the first 20 eigenstate of an InAs cubic quantum dot with Lx = 7nm, Ly = 7.5nm and Lz = 2nm.

Tabulate corresponding energy values.

Exercise 3 :

Compute the first 20 eigenstates of GaAs pyramid quantum dot with Lx = 10nm, Ly = 10.5nm and Lz = 5nm.

Tabulate corresponding energy values.

Optical Property of Quantum Dot

- Optical Transition can be also computed with Quantum Dot Lab.

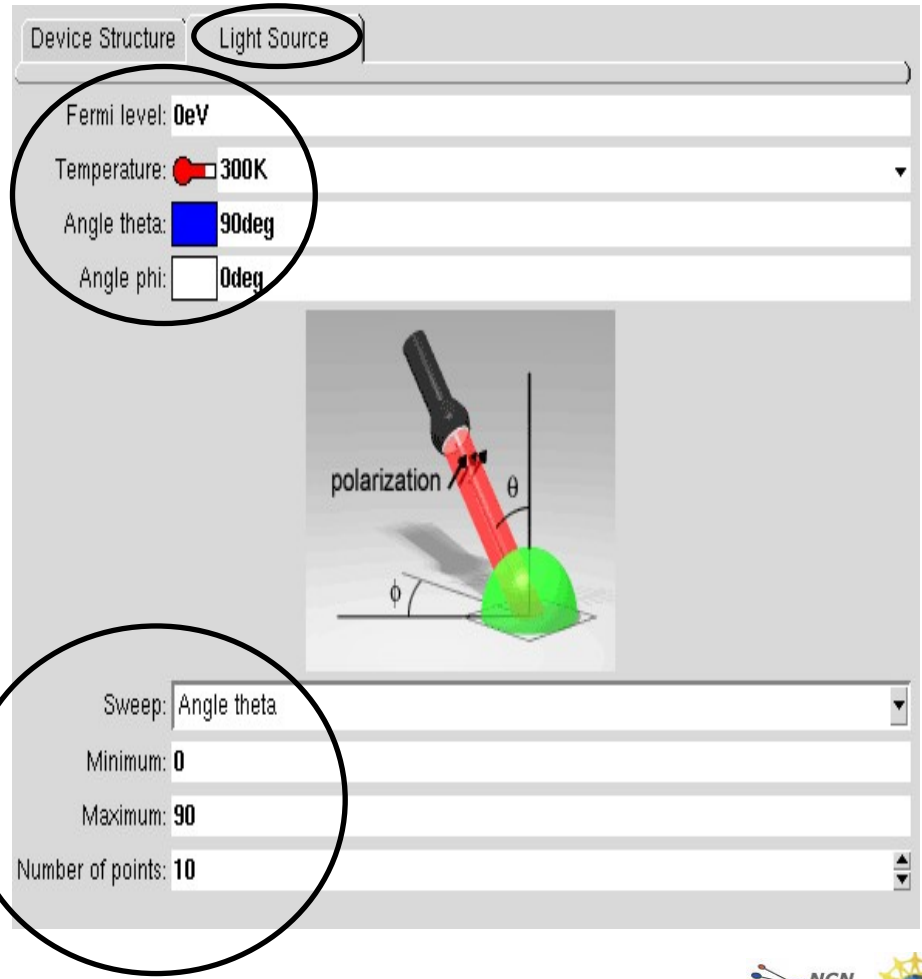
(Step 1) Select 'Light Source' Tab

(Step 2) Set Initial condition of simulation

- Location of Fermi Level
- Temperature
- Angle of Incident Light

(Step 3) Variation of optical properties is computed by sweeping one of following parameters

- Angle Theta
- Angle Phi
- Fermi Level



Optical Property of Quantum Dot - Example

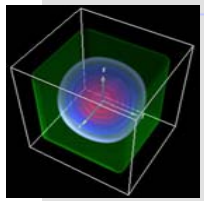
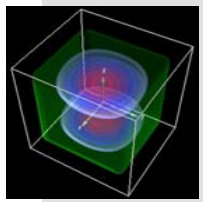
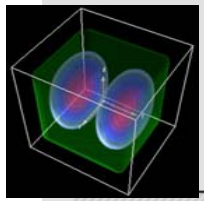
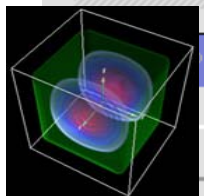
Example Problem
expansion to exercise 1

Cubic GaAs Quantum Dot
Lx = 5nm Ly = 5.5nm and Lz = 6nm
Only FOUR (4) eigenstates.

Use (theta = phi = Fermi E = 0)

Ground	3.3099 (eV)
1st Excited	4.8655 (eV)
2nd Excited	5.1278 (eV)
3rd Excited	5.4615 (eV)

First 4 energy levels

Optical Property of Quantum Dot - Example

Example Problem
expansion to exercise 1

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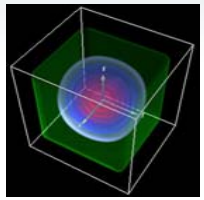
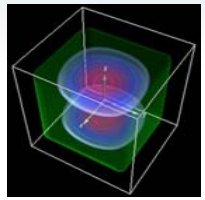
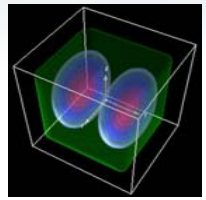
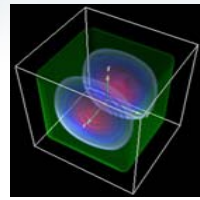
Only FOUR (4) eigenstates.

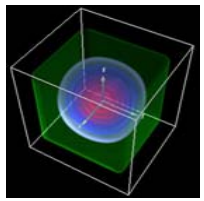
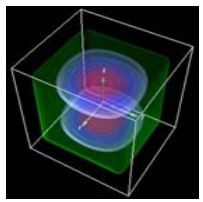
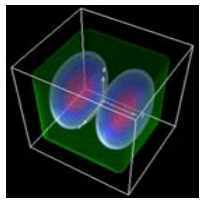
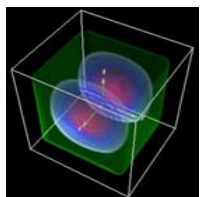
Use (theta = phi = Fermi E = 0)

Ground	3.3099 (eV)
1st Excited	4.8655 (eV)
2nd Excited	5.1278 (eV)
3rd Excited	5.4615 (eV)

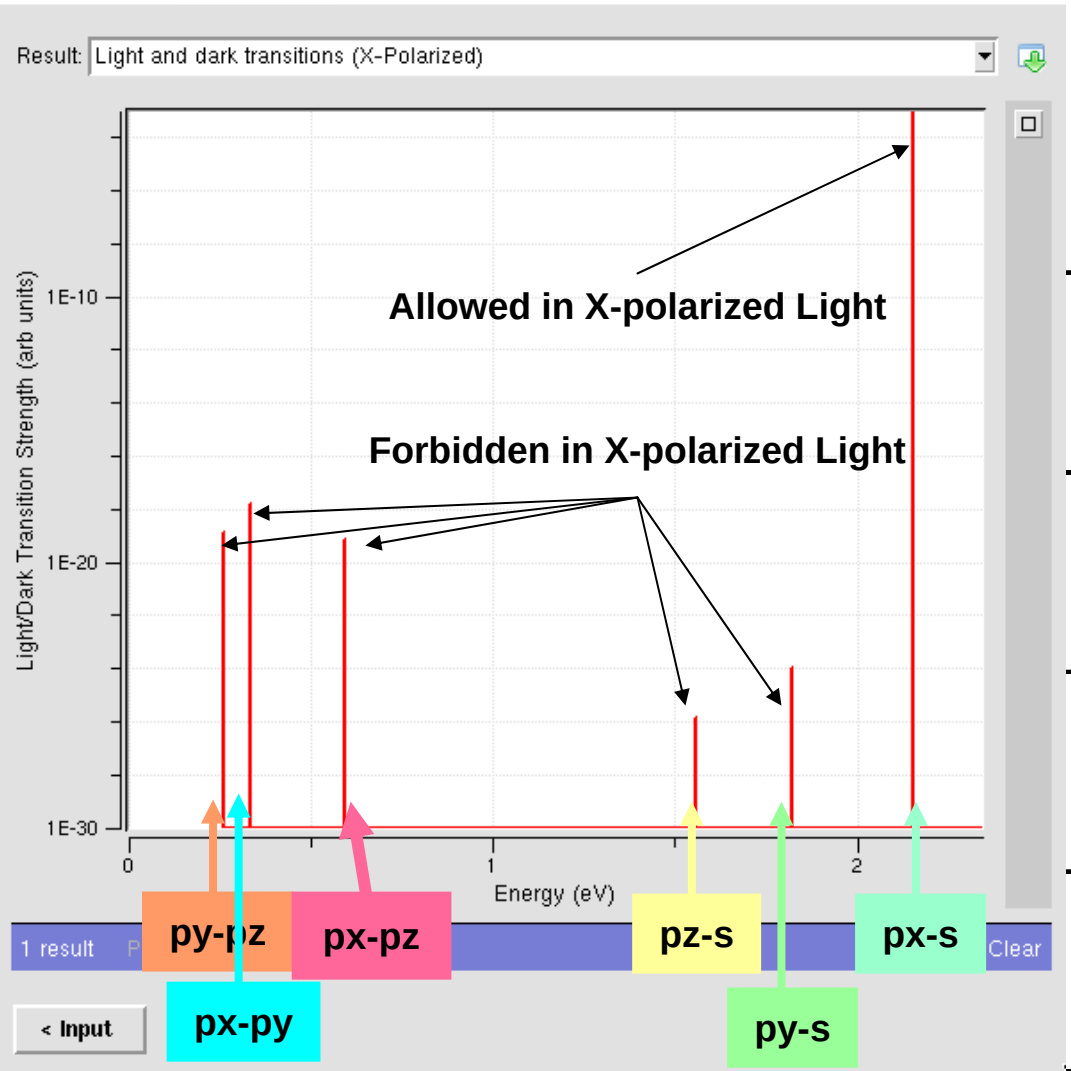
First 4 energy levels

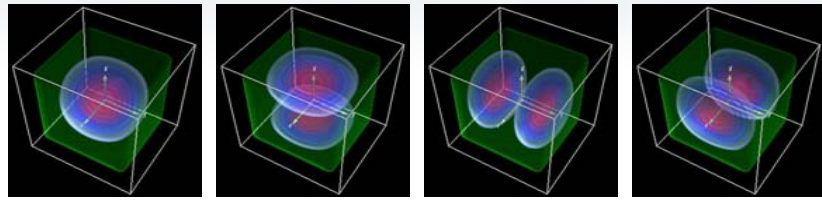
6 transition energies

	s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
 s E1 3.3099		E2-E1 1.5556 pz-s	E3-E1 1.8179 py-s	E4-E1 2.1516 px-s
 pz E2 4.8655			E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
 py E3 5.1278				E4-E3 0.3337 px-py
 px E4 5.4615				

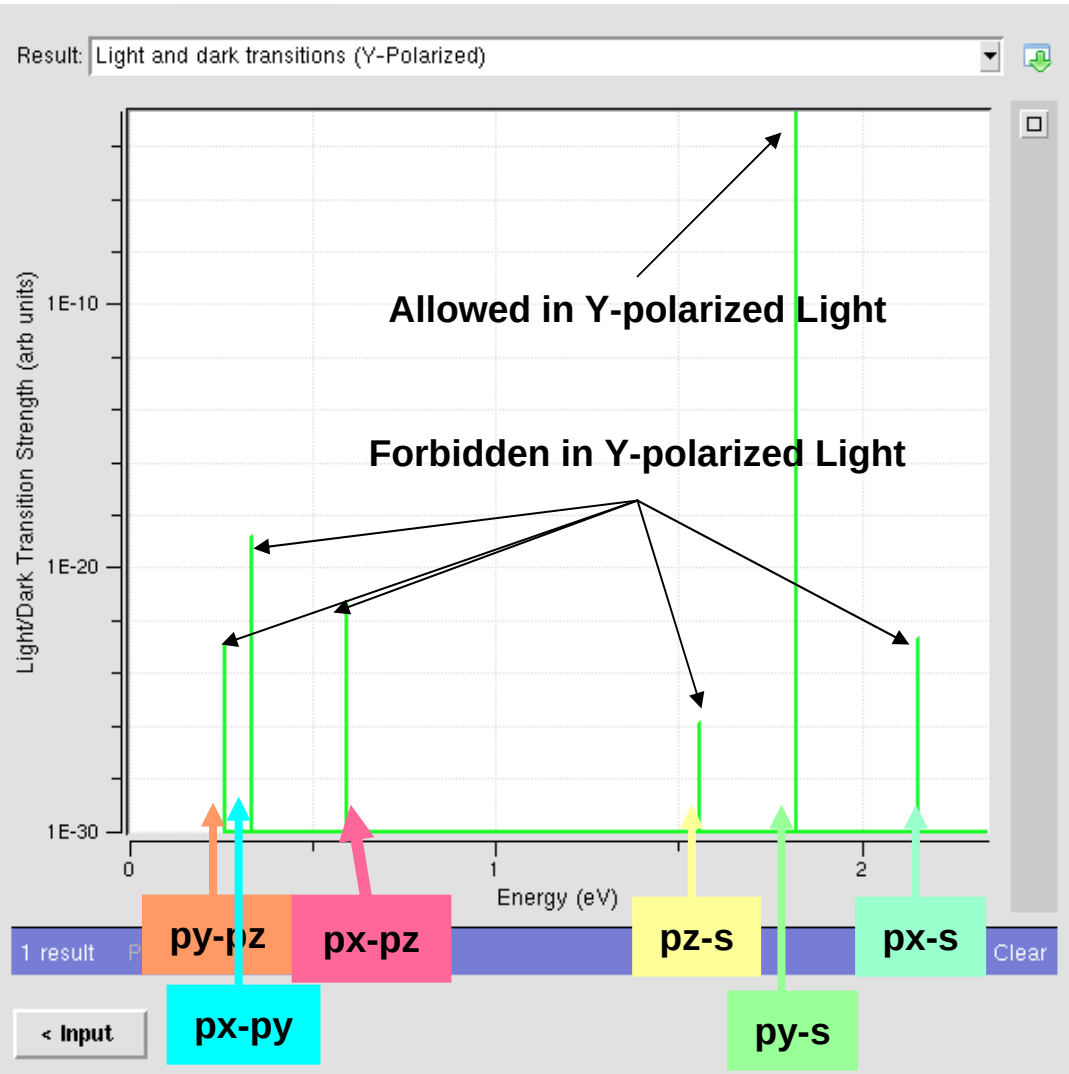
Optical Property of Quantum Dot – X-Polarized Light

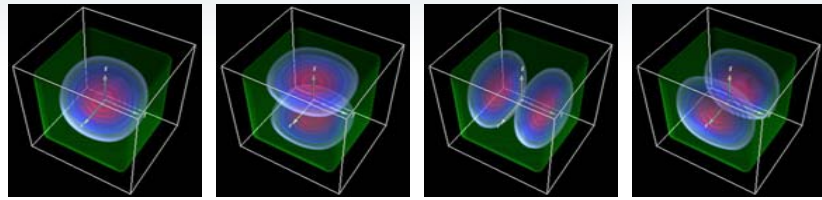




s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s	E3-E1 1.8179 py-s	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

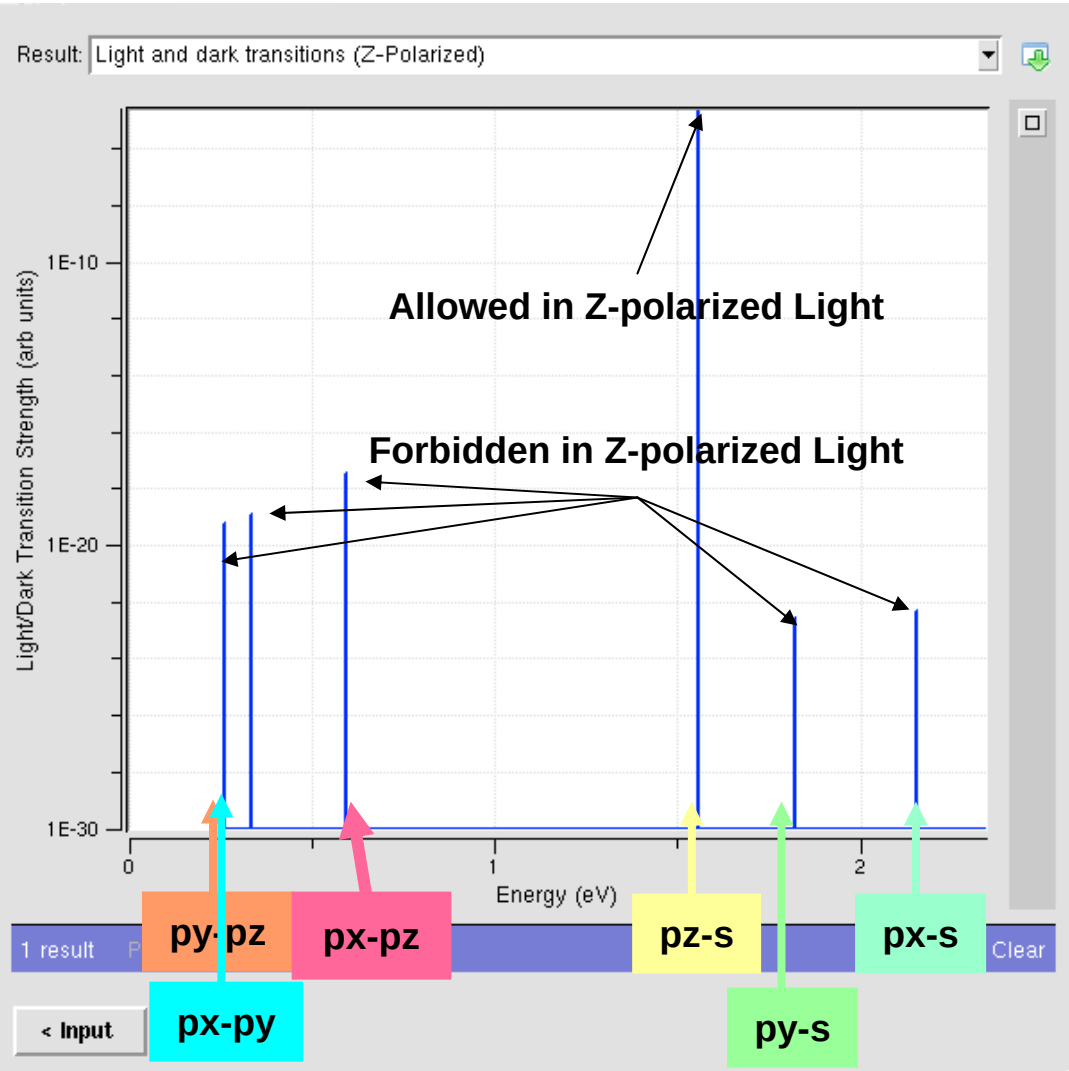
Optical Property of Quantum Dot – Y-Polarized Light

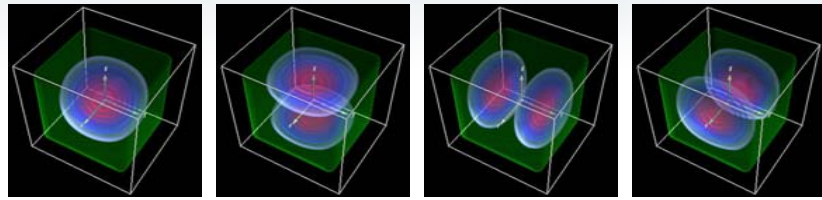




s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

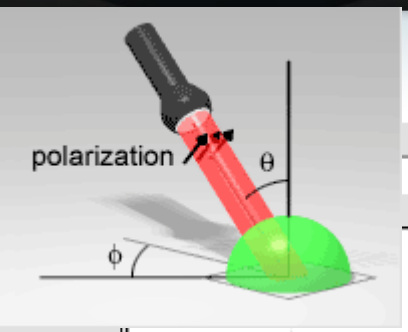
Optical Property of Quantum Dot – Z-Polarized Light



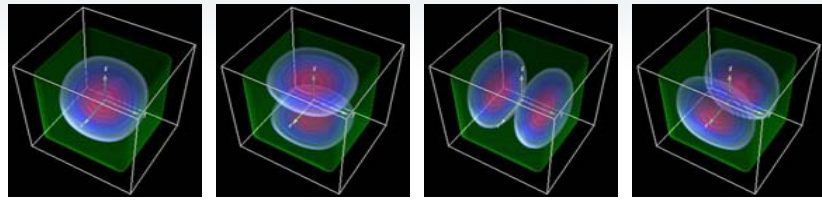


s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Optical Property of Quantum Dot - X-Pol - orthogonal

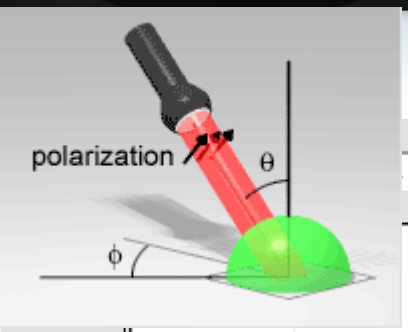


$\Phi = 0 \quad \theta = 0$

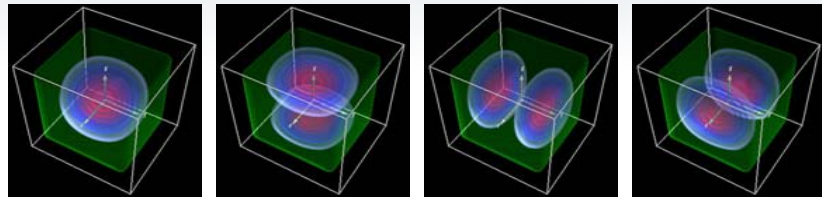


s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Optical Property of Quantum Dot – Angle Variation

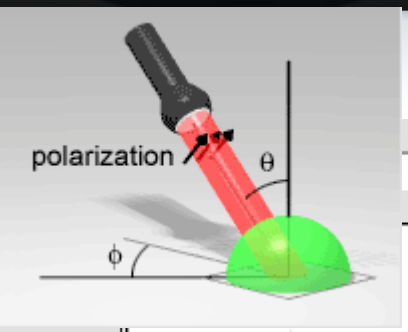


$\Phi = 0 \quad \theta = 0..90$

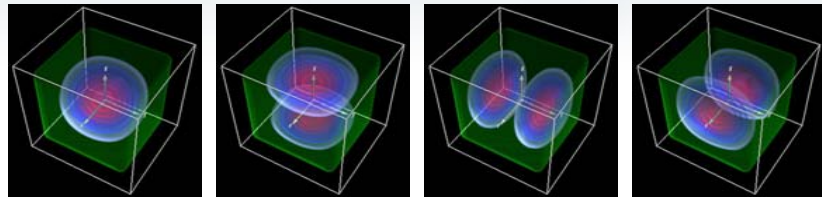


s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Optical Property of Quantum Dot – 45 Degree shift

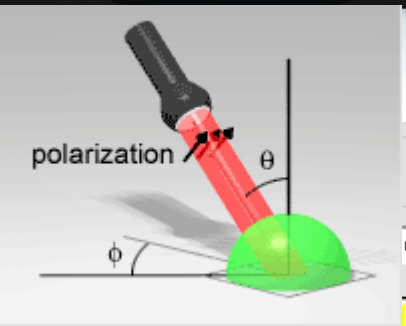


Φ=45 θ=0..90

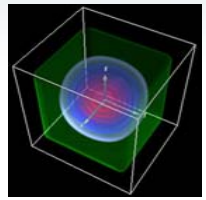
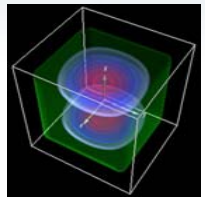
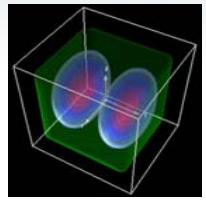
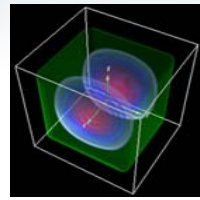


s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Optical Property of Quantum Dot – Many more states

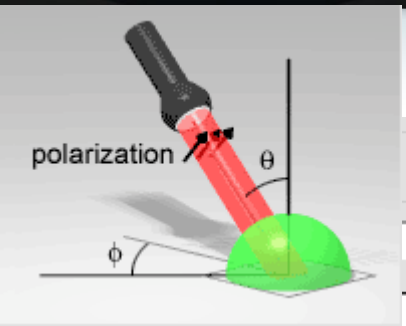


$\Phi = 45$ $\theta = 0$ **20 states**

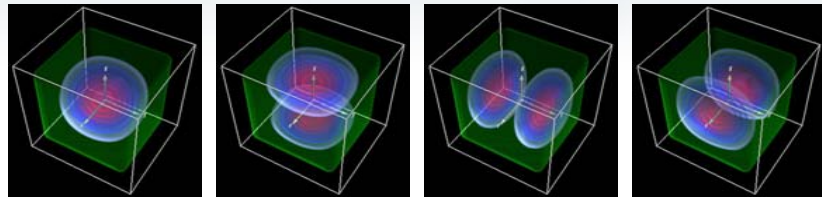





	s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
s E1 3.3099		E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
pz E2 4.8655			E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
py E3 5.1278				E4-E3 0.3337 px-py
px E4 5.4615				

Optical Property of Quantum Dot – Many more states

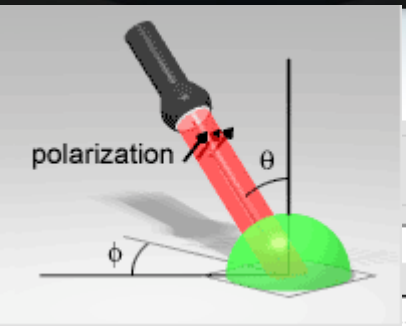


Φ=45 θ=0 20 states

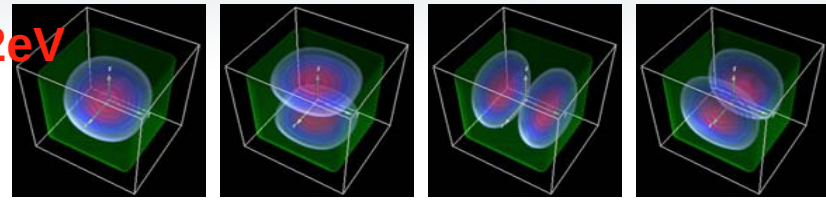


s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Optical Property of Quantum Dot – Increasing the Fermi Level



$\Phi = 45$ $\theta = 0$ 20 states Ef=2.2eV



s E1 3.3099	pz E2 4.8655	py E3 5.1278	px E4 5.4615
	E2-E1 1.5556 pz-s **Z**	E3-E1 1.8179 py-s **Y**	E4-E1 2.1516 px-s **X**
		E3-E2 0.2623 py-pz	E4-E2 0.596 px-pz
			E4-E3 0.3337 px-py

Homework Assignment - Project

1) For a pyramidal quantum dot with vertical absorption (theta=0 degree), design a quantum dot that has the highest absorption energy as close as possible to 1eV.
2) How does the absorption change as a function of incident angle?
3) What happens if the Fermi level is increased to 1eV?
4) What if more states (>20) are included in the design calculation?
5) extra credit:
    1) Simulate a cubic quantum dot where 5nm=Lx=Ly <> Lz=6nm. What happens with the px and py states? What happens to the Lz state?
    (hint: some states are degenerate, make sure you search for at least 10 states.)
    2) Simulate a cubic quantum dot where 5nm=Lx=Lz <> Ly=6nm. What happens with the px and py states?
    (hint: some states are degenerate, make sure you search for at least 10 states.)
    3) Simulate a cubic quantum dot with 5nm=Lx=Ly=Lz. What happens to the px, py and pz states?
    (hint: some states are degenerate, make sure you search for at least 10 states.)
    4) Why are certain absorption lines forbidden and others allowed?

Questions & Answers