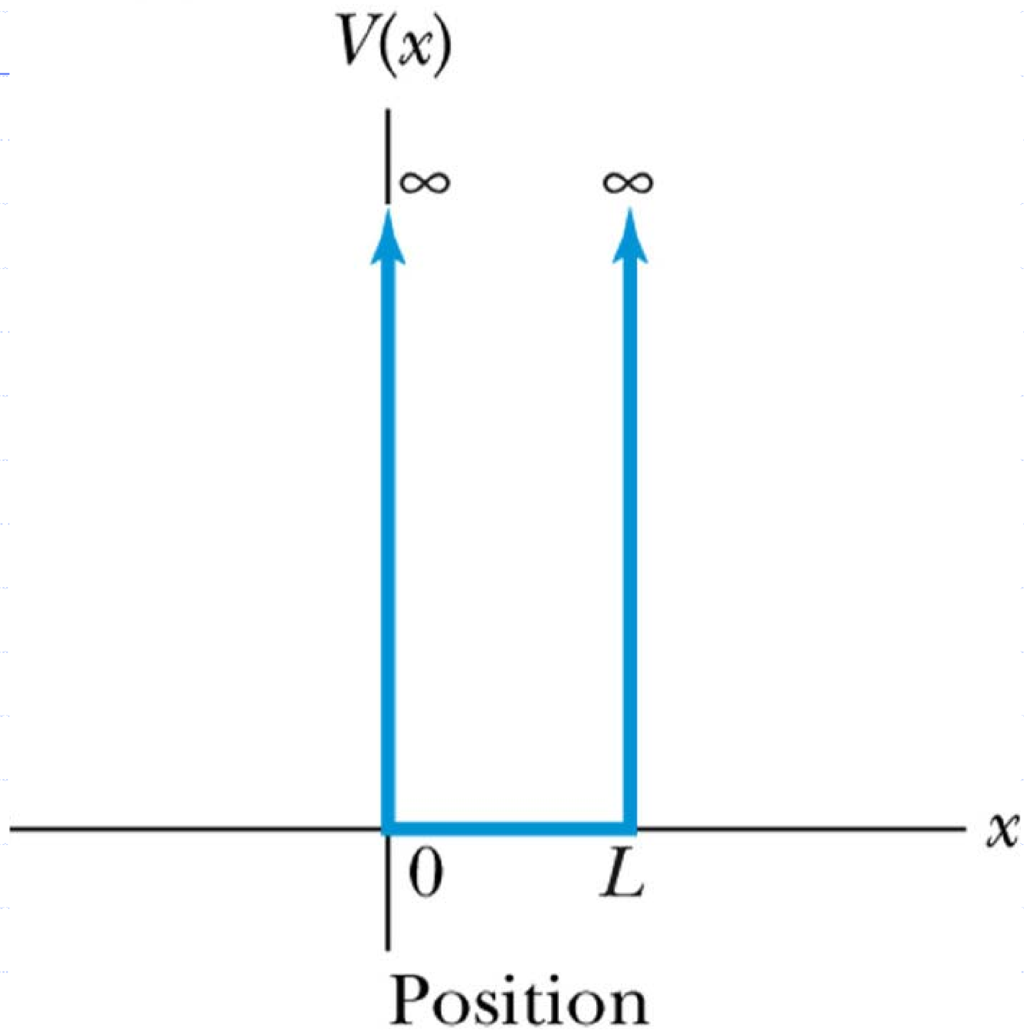
Infinite Square Well



Infinite Square Well

- We can use the time independent Schrodinger equation
- Outside the well

$$\psi(x) = 0$$

- Inside the well

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \text{ where } k = \frac{\sqrt{2mE}}{\hbar}$$

$$\text{Try solutions } \psi(x) = A\sin kx + B\cos kx$$

Infinite Square Well

- Typically the constants are determined by the boundary conditions (and normalization)
- In this case the boundary conditions needed to ensure continuity of ψ are

$$\psi(0) = \psi(L) = 0$$

- Thus

$$\text{Since } \psi(0) = A\sin 0 + B\cos 0 = 0,\ B = 0$$

$$\text{Since } \psi(L) = A\sin kL = 0, \text{ then } kL = 0, \pm\pi, \pm 2\pi, \ldots$$

$$k \text{ cannot be } 0, \text{ so solutions have } k_n = \frac{n\pi}{L}, \text{ n} = 1,2,3,\ldots$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\pi^2 \hbar^2}{2mL^2}; \text{energy is quantized!!}$$

Infinite Square Well

- What about the normalization of ψ_n?

$$\int_0^L dx |\psi_n|^2 = \int_0^L dx |A|^2 \sin^2 kx$$

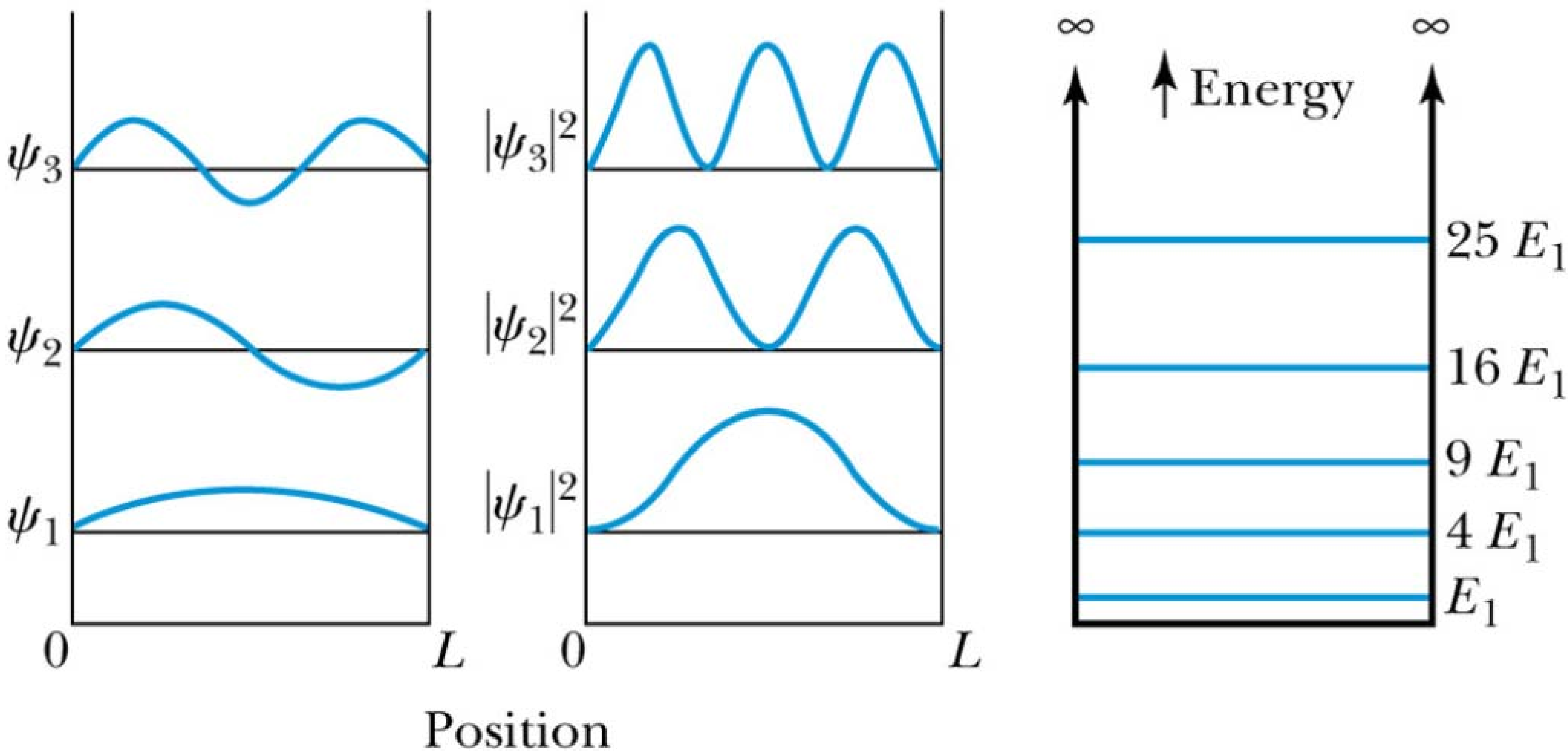
$$= |A|^2 \left(\frac{x}{2} - \frac{\sin 2kx}{4k} \right)_{x=0}^{x=L}$$

$$= |A|^2 \frac{L}{2} = 1$$

thus $A = \sqrt{\frac{2}{L}}$

so the solutions are $\psi_{\text{n}} = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L} \right)$

Infinite Square Well



Infinite Square Well

Comments

- Ψ and dΨ/dx must be continuous at all boundaries except where the potential is infinite
- As n increases, λ decreases, E increases

$$k_n = \frac{n\pi}{L} = \frac{2\pi}{\lambda}$$

$$\lambda = \frac{2L}{n}$$

- Number of nodes in the n'th eigenfunction = n-1
- The eigenfunctions are alternating even and odd functions about the symmetry axis

Infinite Square Well

- Comments
  - Energy states are

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1$$

  - The lowest energy bound state has non-zero energy (zero point energy)
  - The excitation/de-excitation energy is E_{final}-$E_{initial}$

Infinite Square Well

➢ Comments

- The eigenfunctions ψ are mutually orthogonal (recall postulate #4)

$$\int_0^a dx\, \psi_i^* \psi_j = \frac{2}{L}\int_0^L dx \sin\frac{i\pi x}{L}\sin\frac{j\pi x}{L} = \delta_{ij}$$

- Please look at the calculation of expectation values in Thornton-Rex (Example 6.8)
  - What would you expect for <x>?, <p>?, $\langle p^2 \rangle$?

Infinite Square Well

- **Comments**
  - What are the possible momentum states?

Look at the eigenvalue equation

$$-i\hbar\frac{\partial f_n(x)}{\partial x} = p_n f_n(x) = \pm\hbar k_n f_n(x)$$

Solutions are $f_n(x) = Ae^{\pm ik_n x}$

Makes sense since our energy eigenfunctions can be written as

$$\sin k_n x = \frac{1}{2i}\left(e^{ik_n x} - e^{-ik_n x}\right)$$

Infinite Square Well

Comments

- The stationary states of the infinite well are

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar} \text{ where } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

- A general solution to the time dependent Schrodinger equation (see postulate #4) is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar}$$

- Given an initial condition the coefficients c_n can be determined

$$c_n = \sqrt{\frac{2}{L}} \int_0^L dx \sin\left(\frac{n\pi x}{L}\right) \Psi(x,0)$$

Infinite Square Well

- Problem
  - Let $$\psi(x) = \frac{1}{\sqrt{5L}}\sin\frac{\pi x}{L} + \frac{3}{\sqrt{5L}}\sin\frac{3\pi x}{L}$$
  - What are the possible results of an energy measurement?
  - What are the probabilities?
  - What is the form of the wave function immediately after an energy measurement?

Infinite Square Well

Problem

- What is the ratio of probabilities for the particle to be at $x=L/3$ to $x=L/4$?

Infinite Square Well

- Problem
  - Let

$$\Psi(x,0) = A\{\psi_1(x) + \psi_2(x)\}$$

  - Normalize ψ
  - Calculate $|\psi(x,t)|^2$
  - Calculate <x>
  - Calculate <H>

Infinite Square Well

- Note to myself
  - www.phys.uri.edu/~yoon/deep**well**main.html

Infinite Square Well

- In three dimensions, Schrodinger's equation becomes

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x},\ \hat{p}_y = -i\hbar\frac{\partial}{\partial y},\ \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

$$\vec{p} = -i\hbar\vec{\nabla} \text{ and } \hat{p}^2 = -\hbar^2\nabla^2$$

$$\text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

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

$$\text{and } \Psi(x,t) \rightarrow \Psi(\vec{r},t)$$

Infinite Square Well

- Free particle in a box
  - An infinite well in 3 dimensions

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \quad (1)$$

Try $\psi = A\sin k_1 x \sin k_2 y \sin k_3 z$

Boundary conditions give

$$k_1 = \frac{n_1\pi}{L_1} \qquad k_2 = \frac{n_2\pi}{L_2} \qquad k_3 = \frac{n_3\pi}{L_3}$$

Since $\frac{\partial^2\psi}{\partial x^2} = -k_1^2\psi$ (1) becomes

$$\frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right)\psi = E\psi$$

Infinite Square Well

- Free particle in box
  - Continuing

$$E = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right)$$

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right)$$

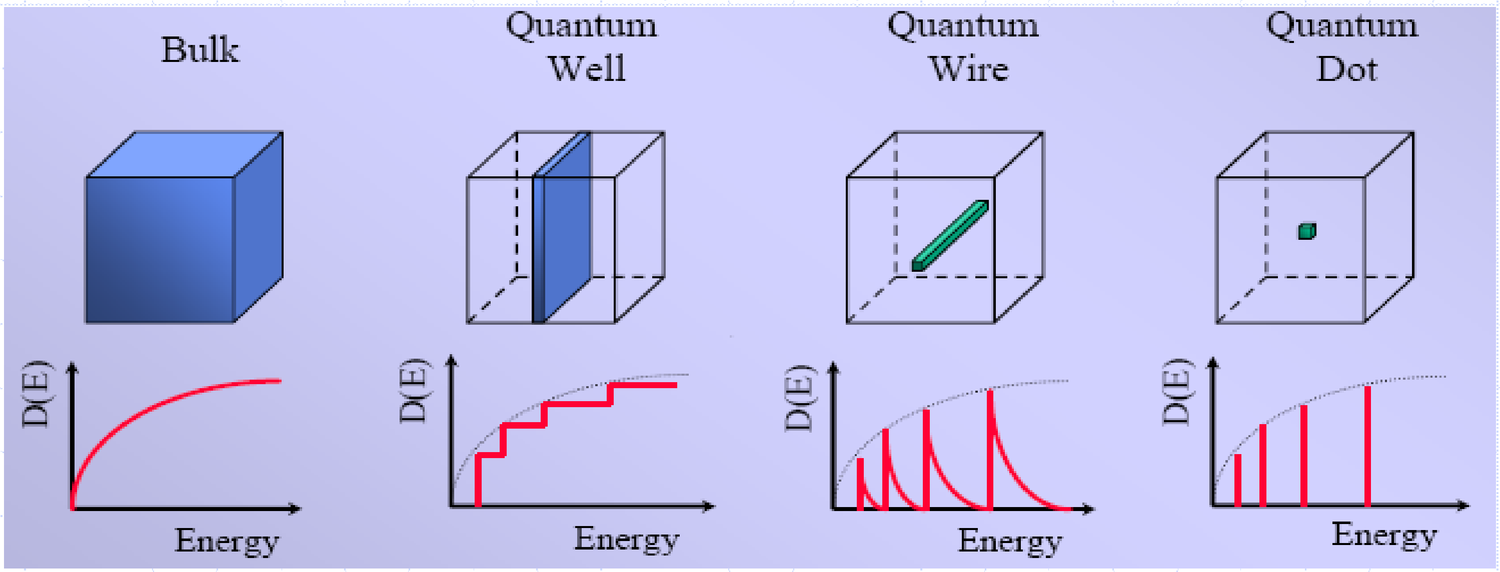
$$\text{for } L_1 = L_2 = L_3 = L$$

$$E = \frac{\pi^2\hbar^2}{2mL^2}\left(n_1^2 + n_2^2 + n_3^2\right)$$

- States with different quantum numbers but the same energy are called degenerate

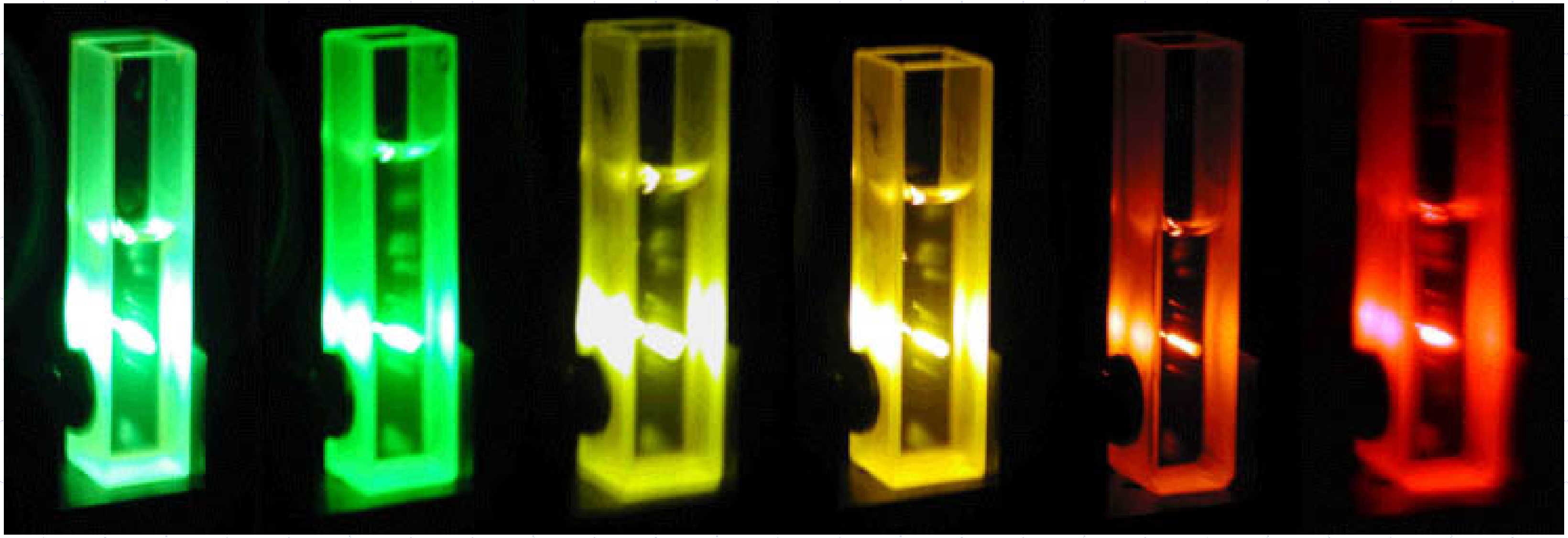
Quantum Dots

- Quantum dots are semiconductor nanostructures that confine 1-1000 conduction electrons in all three dimensions (just like the particle in a box)



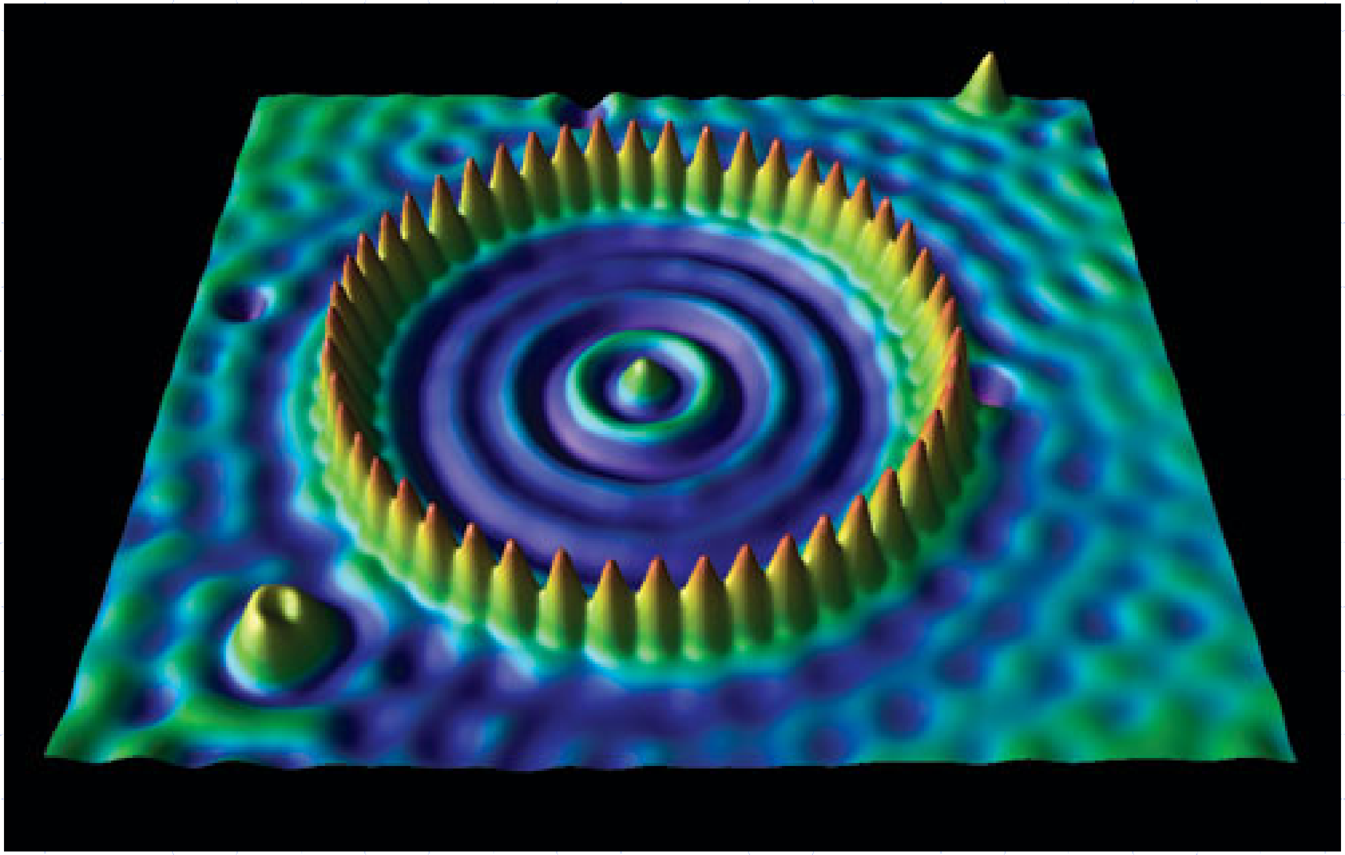
Quantum Dots

- CdSe quantum dots in solution under exposure to UV light
- Which sample has the largest quantum dots?



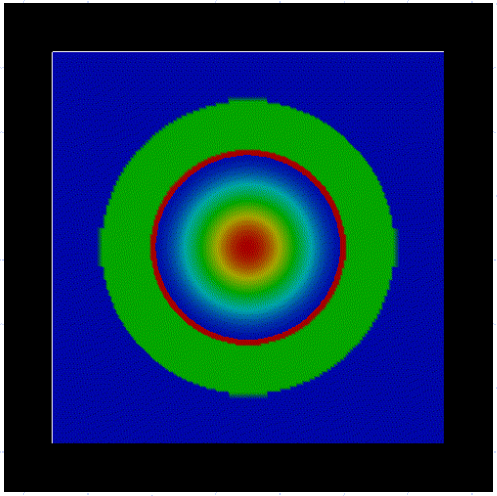
Quantum Corrals

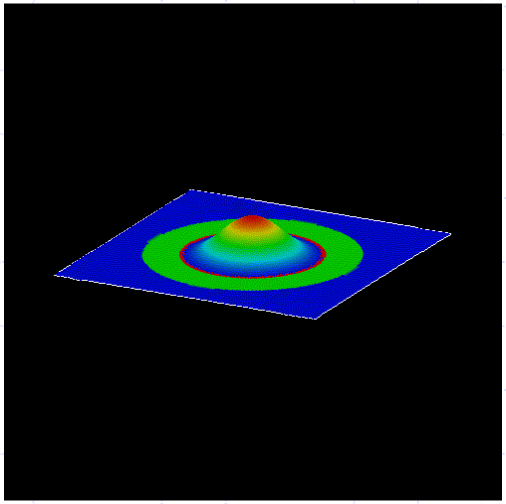
- Electron in a corral of iron atoms on copper

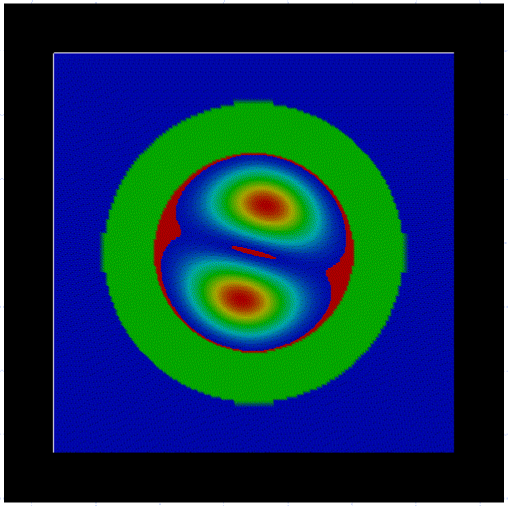


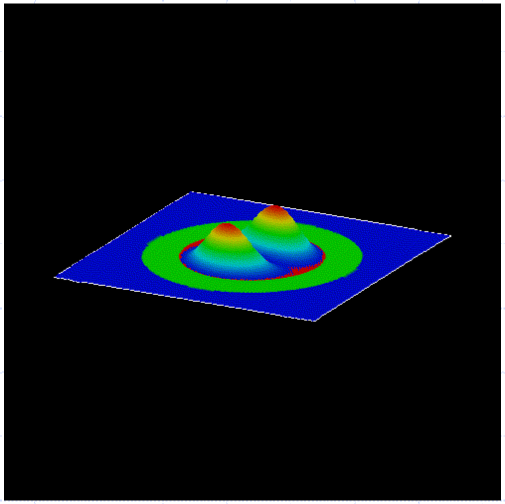
Quantum Corrals

- Electron in a corral of iron atoms









Quantum Corrals