The Schrödinger Equation (Part 3)
Applications, Review and 2D

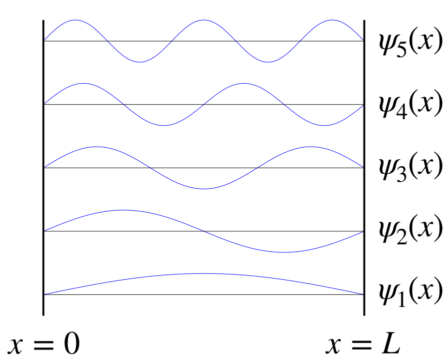
$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t}$$

Kinetic Energy + Potential Energy = Total Energy

Infinite Potential Well: Particle in a Box

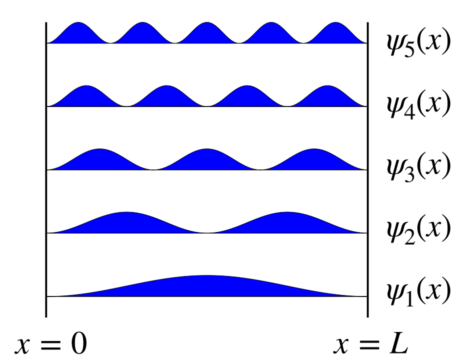
Wave Function

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



Probability Density

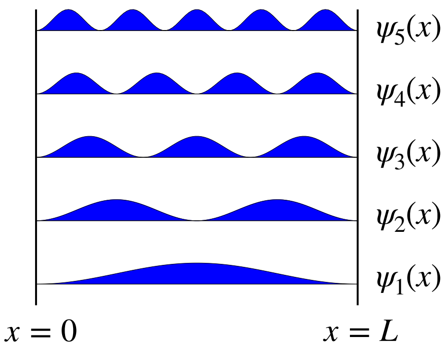
$$|\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$$

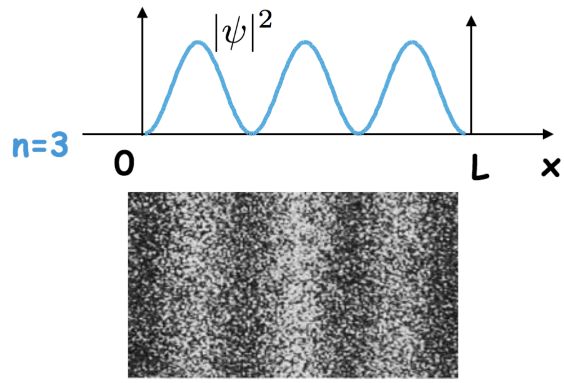


Probability Density describes the chances of detecting the particle at a particular point in space.

Probability Density

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

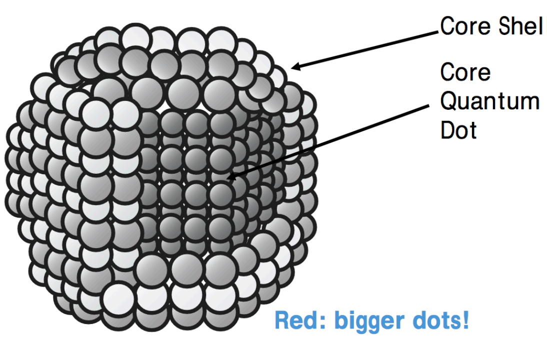




Application: Quantum Dots

<u>*Semiconductor Nanoparticles*</u>

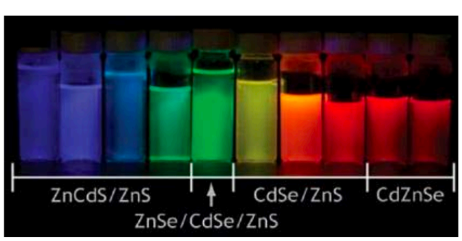
(aka: Quantum Dots)



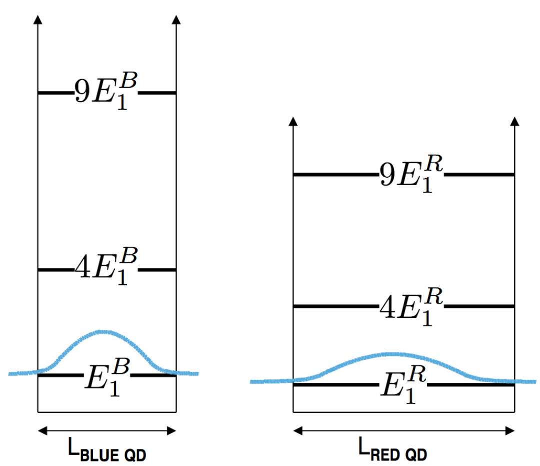
Determining QD energy using the Schrödinger Equation

$$E_1 = n^2 E_1 \qquad E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}$$

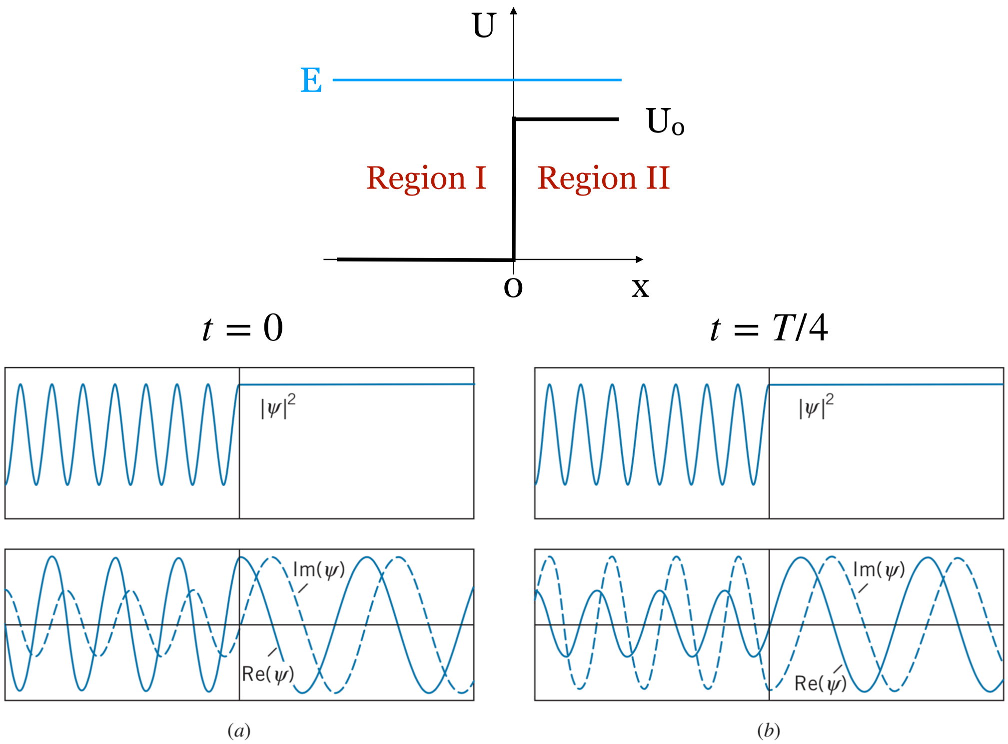
Red: bigger dots!
Blue: smaller dots!



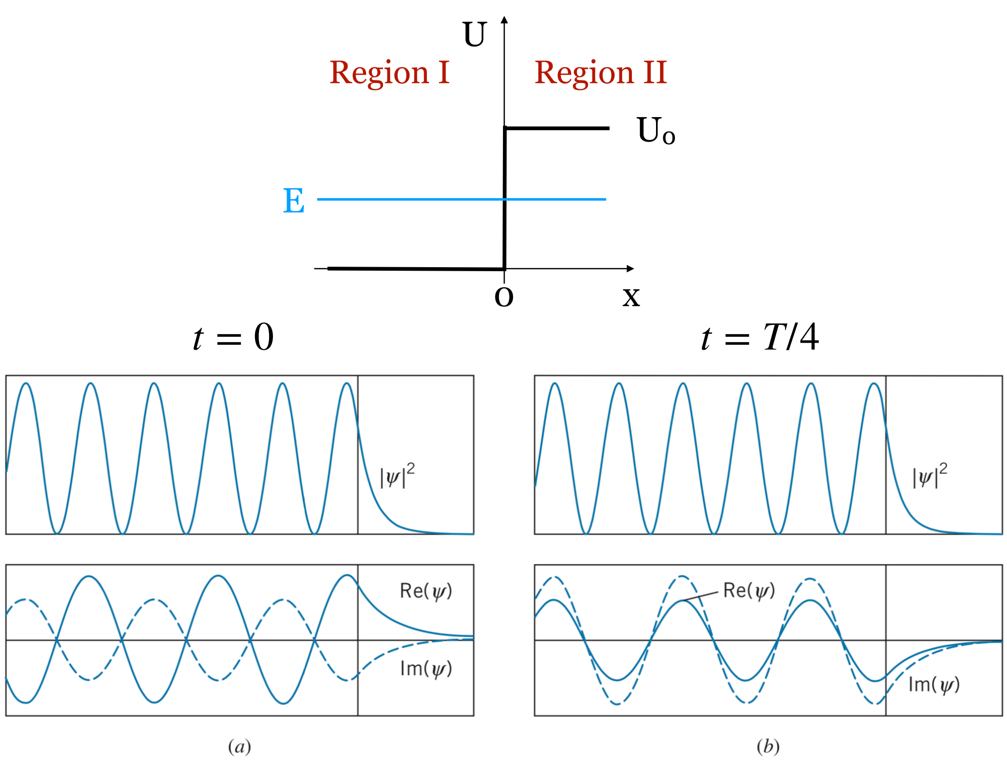
3KRWR E\ - +DSHUW &RXUWHV\ RI 0 %DZHQGL *URXS &KHPLVWU\ 0,7



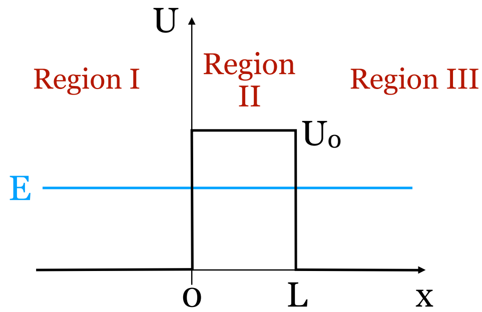
General Constant Potential: $E > U_o$



General Constant Potential: $E < U_o$



Quantum Tunneling



Region I $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$

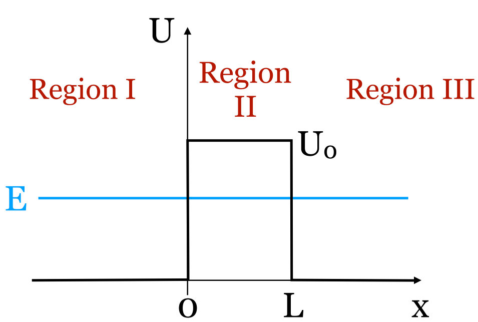
Region II $\psi_{II}(x) = Ce^{ik'x} + De^{-ik'x}$

Region III $\psi_{III}(x) = Ee^{ikx} + Fe^{-ikx}$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

Probability of Quantum Tunneling



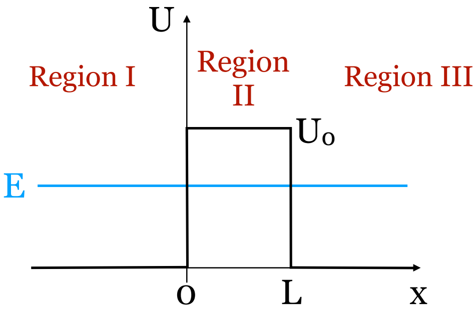
$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

$$T \approx \left(\frac{k^2 + k'^2}{2k'k}\right)^2 e^{-2k'L}$$

$$T \approx \frac{16E(U_0 - E)}{U_0^2} e^{-2k'L}$$

Example: Electron with 6 eV of K.E. approaches a potential barrier with height 12 eV and width 0.18 nm. Find the tunneling probability.



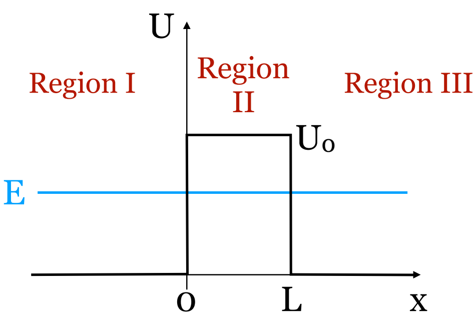
$$k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

$$T \approx \frac{16E(U_0 - E)}{U_0^2} e^{-2k'L}$$

$$k' = \frac{\sqrt{2(9.11 \times 10^{-31}\ \text{kg})(12 - 6\ \text{eV})}}{1.055 \times 10^{-34}} = 1.25 \times 10^{10}\text{m}^{-1} \quad \Rightarrow \quad 2k'L = 4.5$$

$$T = \frac{16 \cdot 6 \cdot 6}{12^2} e^{-4.5} = 0.044 \qquad \boxed{4.4\%}$$

Example: Electron with 6 eV of K.E. approaches a potential barrier with height 12 eV and width 0.18 nm. Find the tunneling probability.

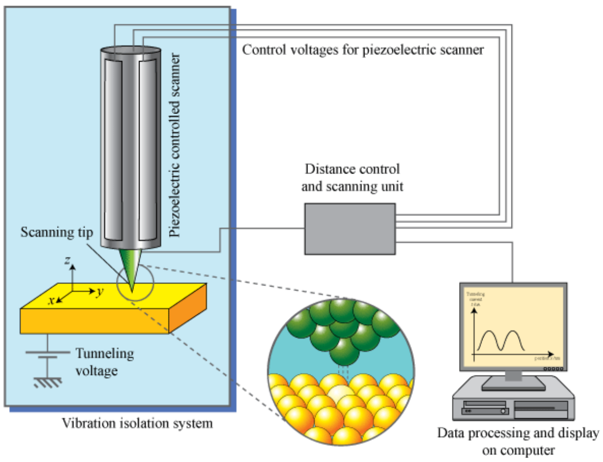


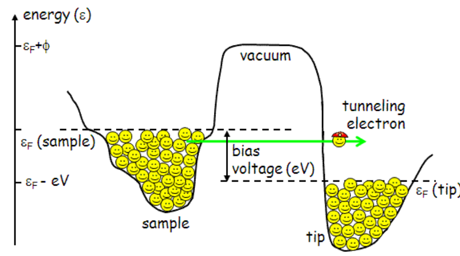
$$k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

$$T \approx \frac{16E(U_0 - E)}{U_0^2} e^{-2k'L}$$

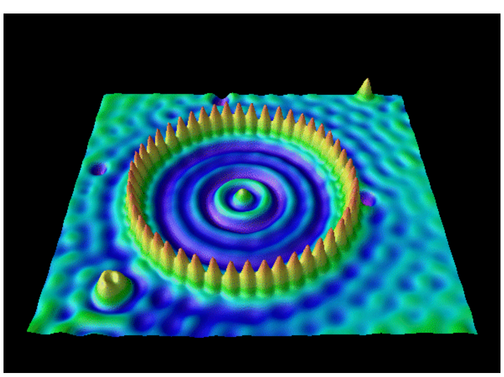
How does this probability change if the barrier width is doubled?

Scanning, Tunneling Microscope





Scanning, Tunneling Microscope



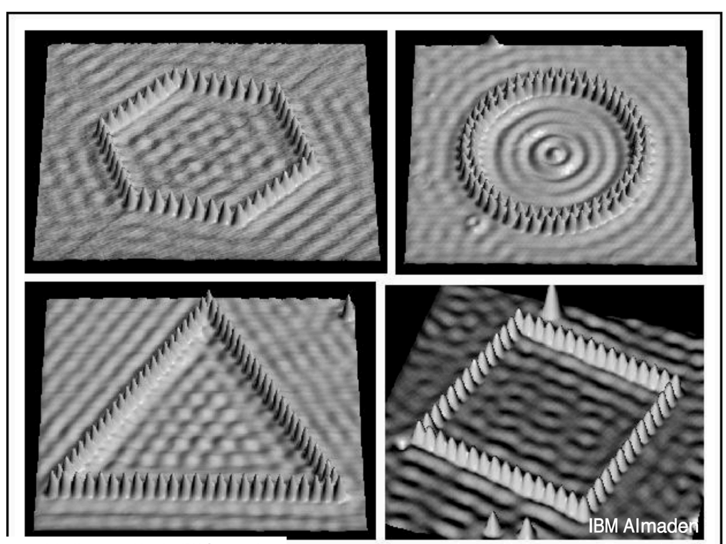
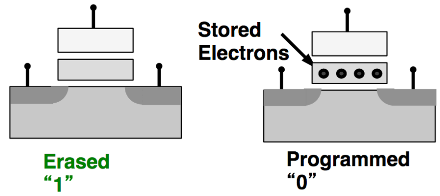
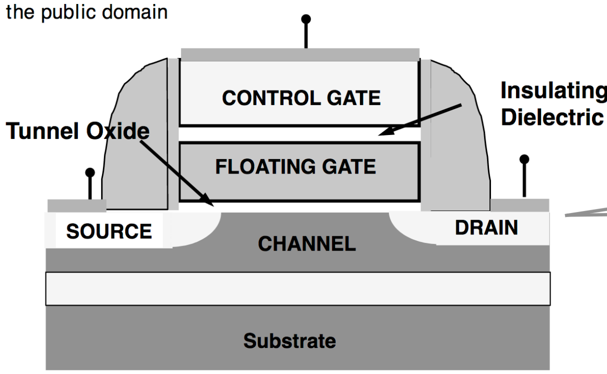


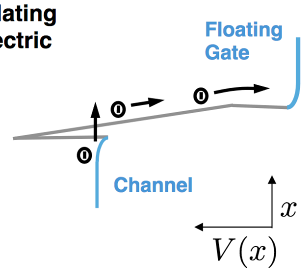
Image originally created by the IBM Corporation.

Flash Memory

Image is in the public domain







Electrons tunnel preferentially when a voltage is applied

The Schrödinger Equation in Higher Dimensions

1D: $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

2D: $$-\frac{\hbar^2}{2m}\left[\frac{d^2\psi(x,y)}{dx^2} + \frac{d^2\psi(x,y)}{dy^2}\right] + U(x,y)\psi(x,y) = E\psi(x,y)$$

3D: $$-\frac{\hbar^2}{2m}\left[\frac{d^2\psi(x,y,z)}{dx^2} + \frac{d^2\psi(x,y,z)}{dy^2} + \frac{d^2\psi(x,y,z)}{dz^2}\right] + U(x,y)\psi(x,y,z) = E\psi(x,y,z)$$

The Schrödinger Equation in Higher Dimensions

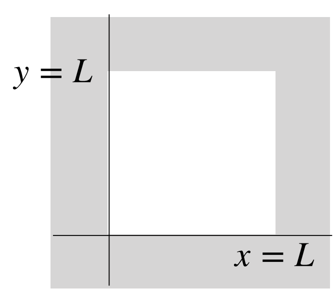
$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(x,y,z)\psi = E\psi$$

Laplacian Operator $\quad \nabla^2\psi = \frac{d^2\psi(x,y,z)}{dx^2} + \frac{d^2\psi(x,y,z)}{dy^2} + \frac{d^2\psi(x,y,z)}{dz^2}$

Two-Dimensional Infinite Potential Well

$U(x,y) = 0 \quad$ for $\quad 0 \le x \le L\,,\ \ 0 \le y \le L$

$U(x,y) = \infty \quad$ otherwise



Look for solutions of the form $\quad \psi(x,y) = f(x)g(y)$

where $\quad f(x) = A\sin(k_x x) + \cancel{B\cos(k_x x)}$

$$g(x) = C\sin(k_y y) + \cancel{D\cos(k_y y)}$$

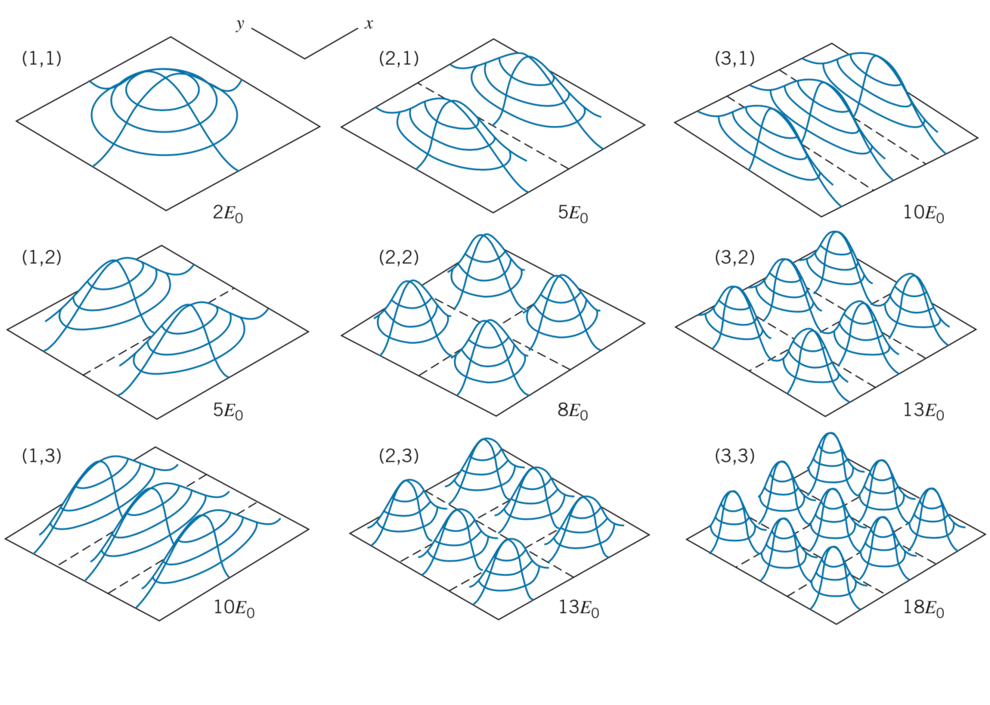
Two-Dimensional Infinite Potential Well

Solutions: $\psi(x,y) = \frac{2}{L}\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)$

$$E_n = \frac{h^2}{8\pi m L^2}(n_x^2 + n_y^2)$$

Two-Dimensional Infinite Potential Well

$$\psi(x,y) = \frac{2}{L}\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)$$



Two-Dimensional Infinite Potential Well

$$E_n = \frac{h^2}{8\pi m L^2}(n_x^2 + n_y^2)$$

	1	2	3	4
1				
2				
3				
4				

Energy Levels