Modern Physics

Unit 5: Schrödinger's Equation and the Hydrogen Atom

Lecture 5.1: Schrödinger's Equation in 2 Dimensions

Ron Reifenberger
Professor of Physics
Purdue University

If we know the wavefunction, we know everything it is possible to know

For every dynamical system, there exists a wavefunction Ψ that is a continuous, square-integrable*, single-valued function of the <u>coordinates of all the particles</u> and of time. If you know Ψ, all possible predictions about the physical properties of the system can be obtained.

"The coordinates of all the particles"?

For a single particle in one dimension: $\boxed{\Psi(x)}$

For a single particle moving in one dimension: $\boxed{\Psi(x,t)}$

For a single particle in a superposition of two quantum states, a and b (state vector): $\boxed{\Psi(x,t) = A\Psi_a(x,t) + B\Psi_b(x,t)}$

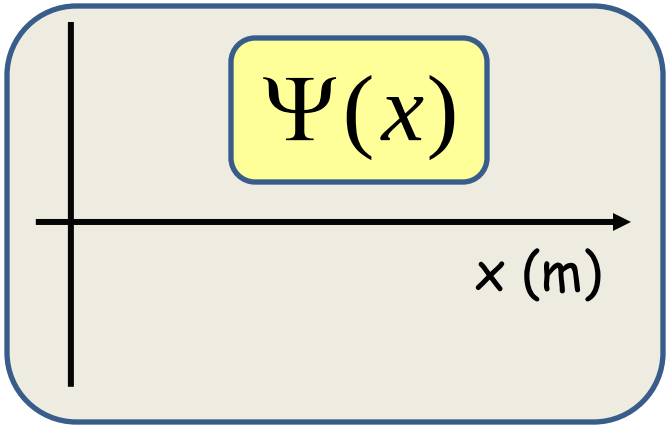
For a single particle moving in three dimensions: $\boxed{\Psi(\vec{\mathbf{r}},t)}$

For **two** particles moving in three dimensions: $\boxed{\Psi(\vec{\mathbf{r}}_1,\vec{\mathbf{r}}_2,t)}$

*Square-integrable means that the normalization integral is finite

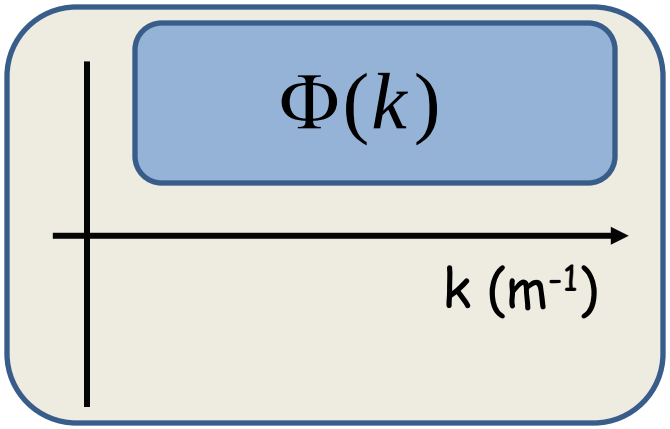
Real space vs. k-space

real space



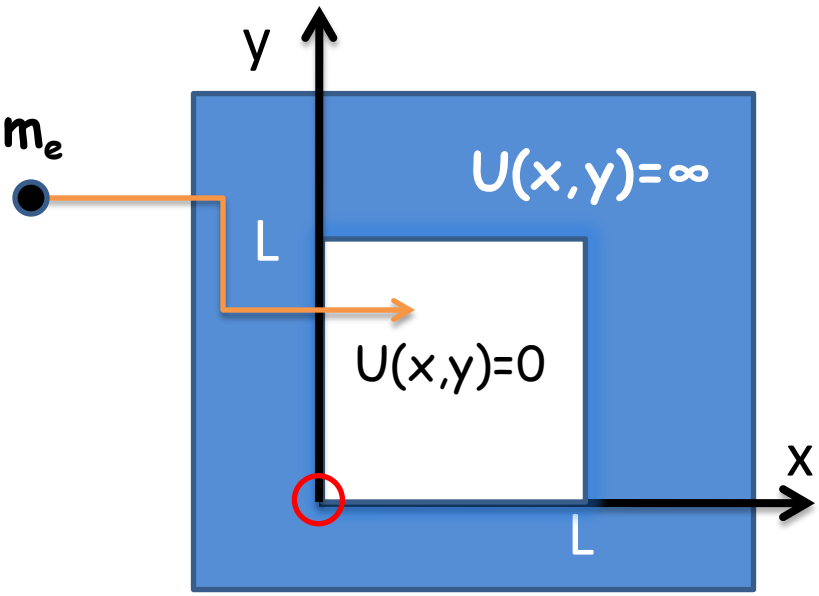
$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x) e^{-ikx} dx$$

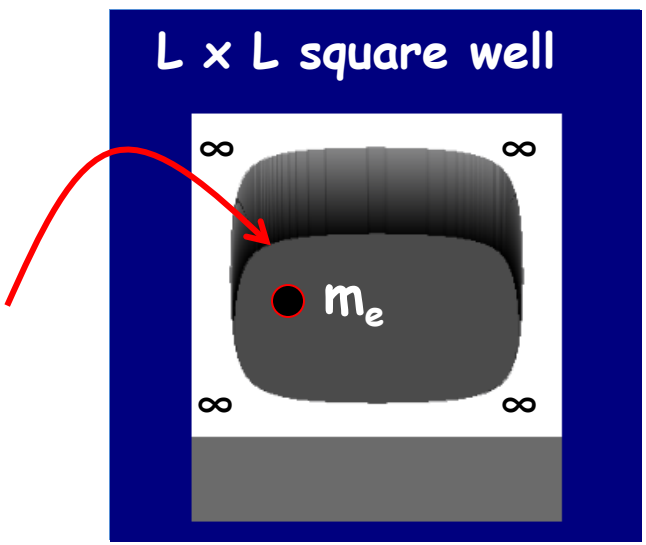
$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi(k) e^{ikx} dk$$



k-space
or
wavevector space
or
reciprocal space
or
inverse space

A particle of mass m_e in a rigid 2-d square box





$$-\frac{\hbar^2}{2m_e}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+U(x,y)\right]\Psi = E\Psi$$

for $0 < x < L$ *and* $0 < y < L,\ \ U(x,y) = 0$

we then have

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2} = -\frac{2m_e}{\hbar^2}E\Psi$$

Suppose $\Psi(x,y) = X(x)Y(y)$ *then,*

$$\frac{\partial^2\Psi}{\partial x^2} = Y(y)\frac{d^2X(x)}{dx^2}$$

$$\frac{\partial^2\Psi}{\partial y^2} = X(x)\frac{d^2Y(y)}{dy^2}$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}=-\frac{2m_e}{\hbar^2}E\Psi \quad \textit{now becomes}$$

$$Y(y)\frac{d^2X(x)}{dx^2}+X(x)\frac{d^2Y(y)}{dy^2}=\left[-\frac{2m_e}{\hbar^2}E\right]X(x)Y(y)$$

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2}+\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}=\left[-\frac{2m_e}{\hbar^2}E\right]$$

This must be true for **<u>any</u>** (x,y) such that 0<x<L and 0<y<L

This equation is of the form:

(function of x only) + (function of y only) = some constant

Separation constants

$$\therefore \quad \frac{1}{X(x)}\frac{d^2X(x)}{dx^2}=\text{constant}_1=-k_x^2$$

$$\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}=\text{constant}_2=-k_y^2$$

$$\frac{d^2X(x)}{dx^2}=-k_x^2X(x)$$

$$\frac{d^2Y(y)}{dy^2}=-k_y^2Y(y)$$

I. Boundary Conditions

$$X(x=0)=X(x=L)=0$$

$$Y(y=0)=Y(y=L)=0$$

Try the solutions:

$$X(x)=A\sin\left(k_x x\right) \qquad Y(y)=B\sin\left(k_y y\right)$$

To match boundary conditions:

$$k_x=\frac{n\pi}{L};\ n=1,2,3... \qquad k_y=\frac{m\pi}{L};\ m=1,2,3...$$

II. Solution for Ψ

$$\begin{aligned}\Psi(x,y)&=X(x)Y(y)\\&=AB\sin(k_x x)\sin(k_y y)\\&=AB\sin\frac{n\pi x}{L}\sin\frac{m\pi y}{L}\end{aligned}$$

III. Allowed Energies

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2}+\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}=\left[-\frac{2m_e}{\hbar^2}E\right]$$

$$-\frac{n^2\pi^2}{L^2}-\frac{m^2\pi^2}{L^2}=-\frac{2m_e}{\hbar^2}E$$

$$\boxed{E=\frac{\hbar^2}{2m_e}\cdot\frac{\pi^2}{L^2}\left[n^2+m^2\right]=E_o\left[n^2+m^2\right]}$$

Systematically pick various n,m values to determine allowed energy levels. Note: Can't choose either n or m =0. Why?

n	m	E	Degeneracy
1	1	$2E_o$	nondegenerate
1	2	$5E_o$	2-fold degenerate
2	1		
2	2	$8E_o$	nondegenerate
1	3	$10E_o$	2-fold degenerate
3	1		

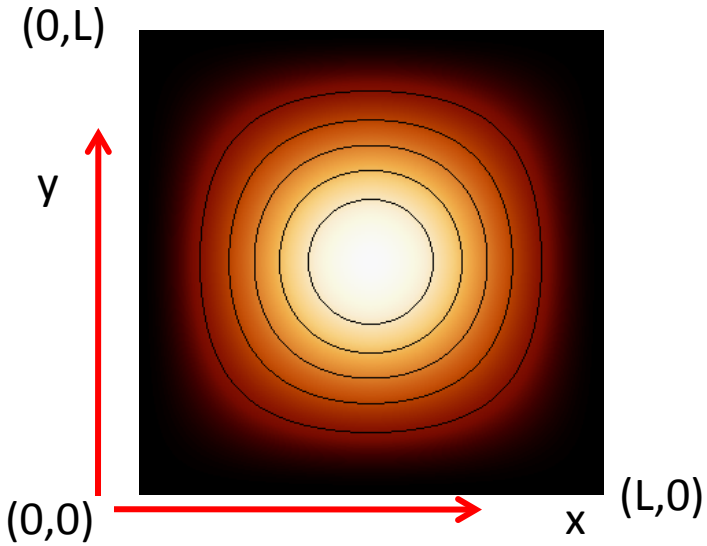
Two different quantum states that happen to have the same energy!

A quantum state is called degenerate when there is more than one wave function for a given energy.

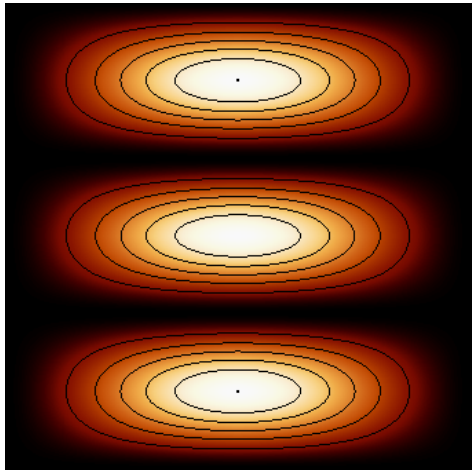
Plots of Ψ*Ψ for various energy eigenvalues

$$\Psi(x,y) = C \sin\frac{n\pi x}{L} \sin\frac{m\pi y}{L}$$

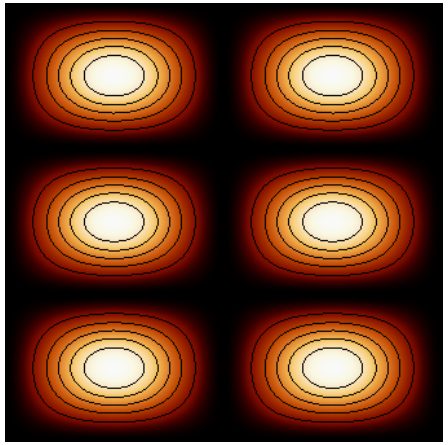
n=1; m=1; E=2E$_o$



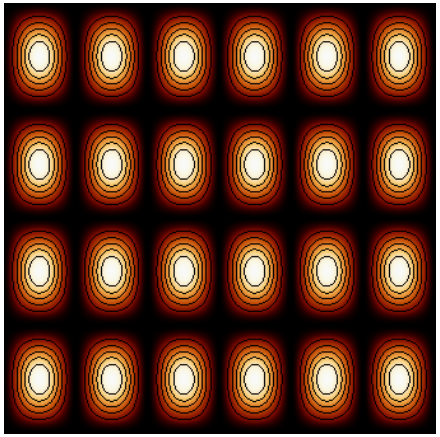
n=1; m=3 ; E=10E$_o$



n=2; m=3; E=13E$_o$



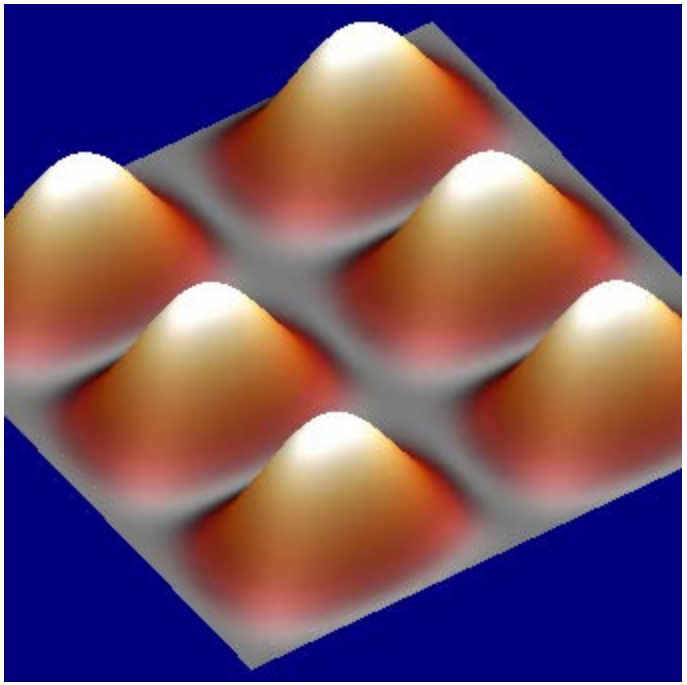
n=6; m=4; E=52E$_o$



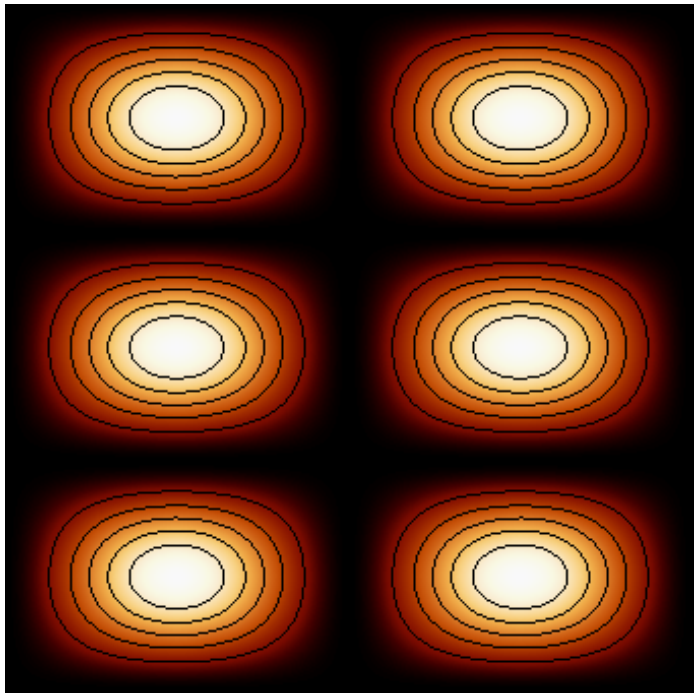
Plot of Ψ*Ψ

n=2; m=3

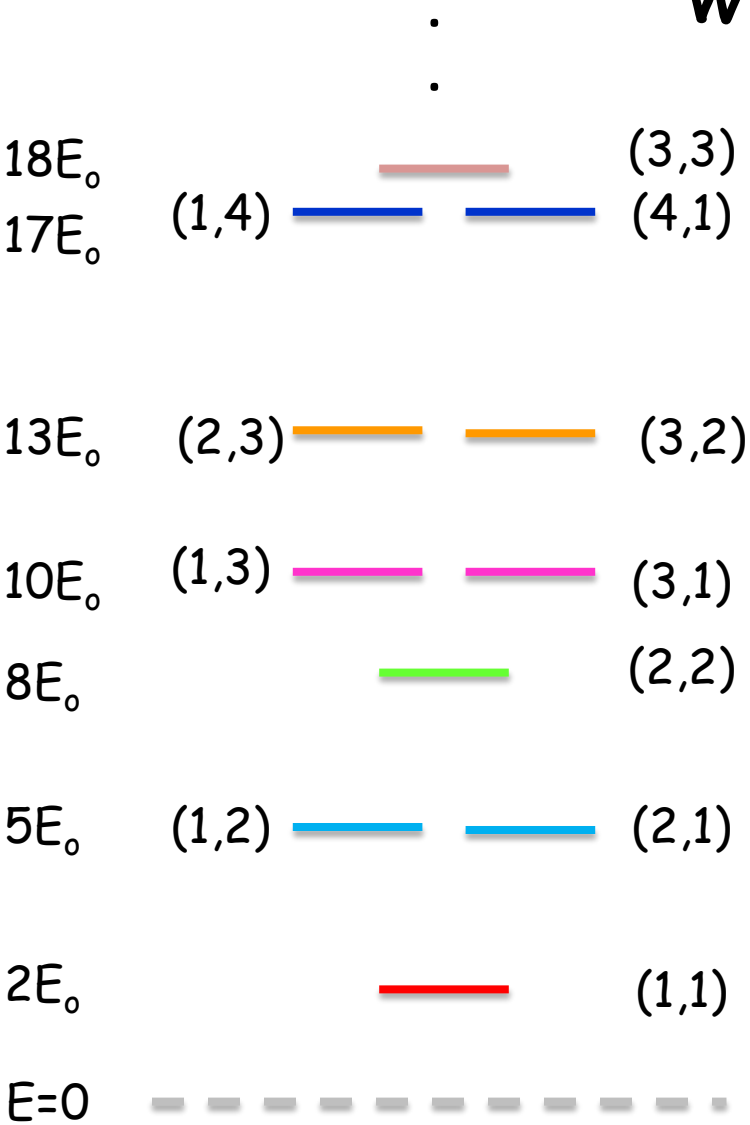
3-dimensional



Top view – false color w. contours

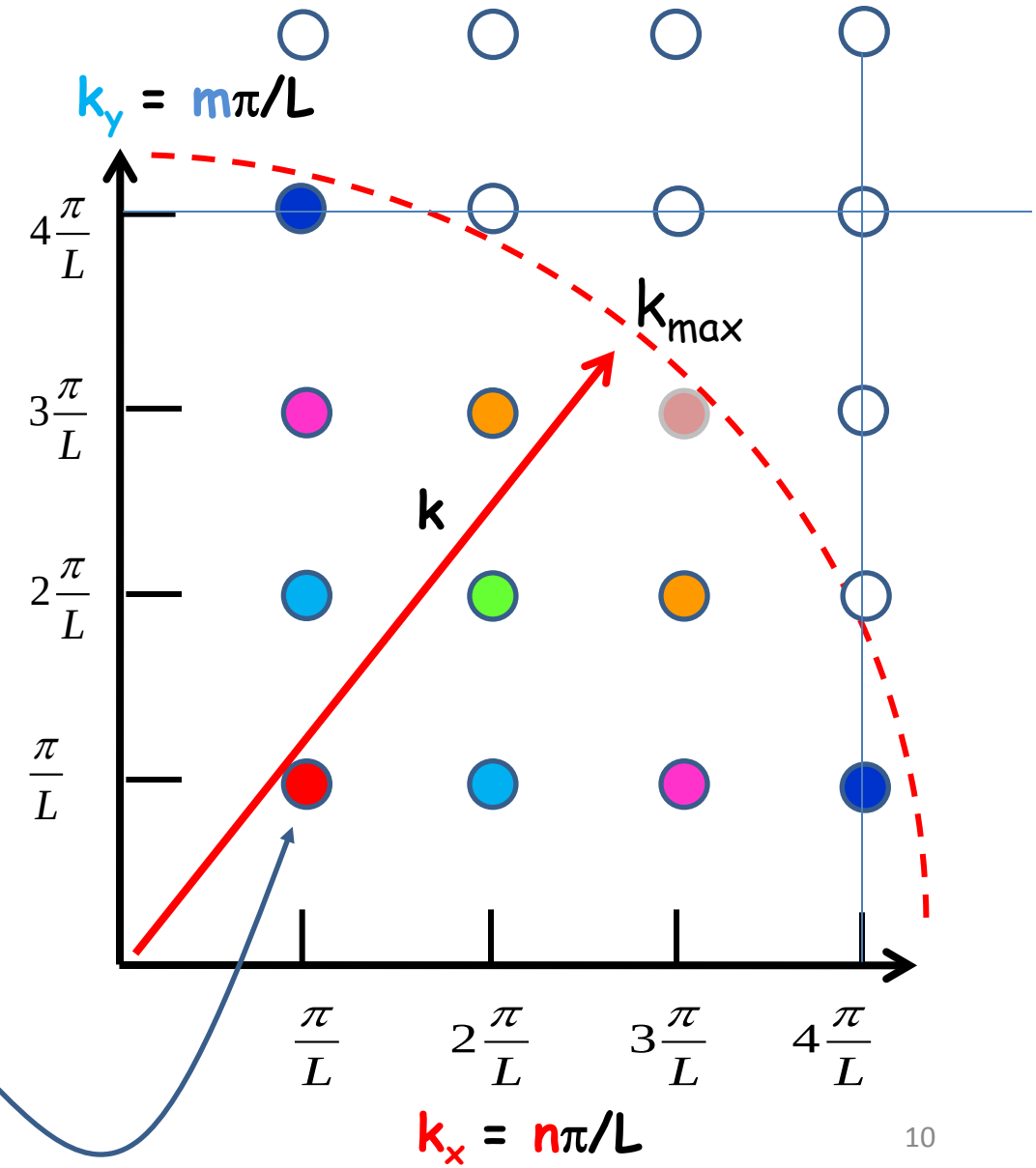


What it means

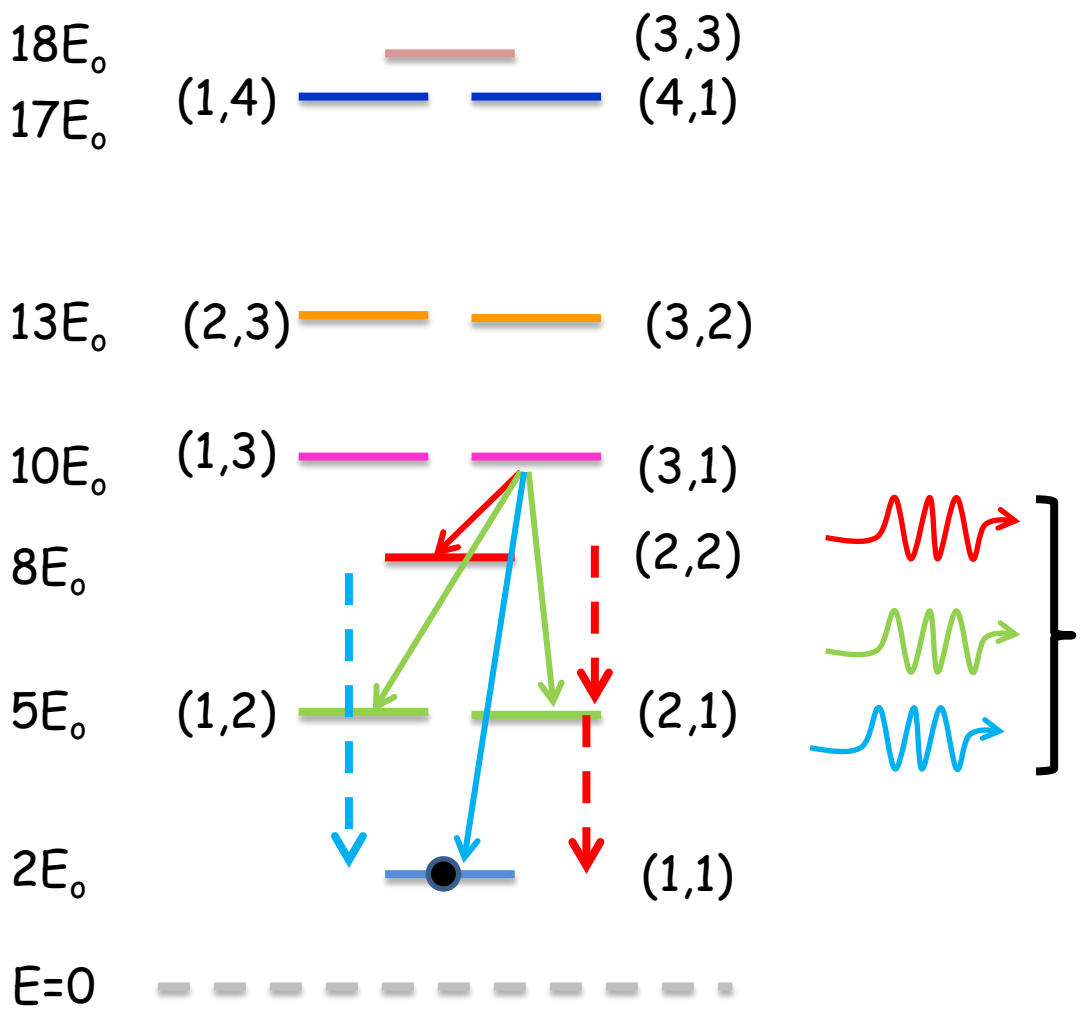


Each dot represents a quantum state

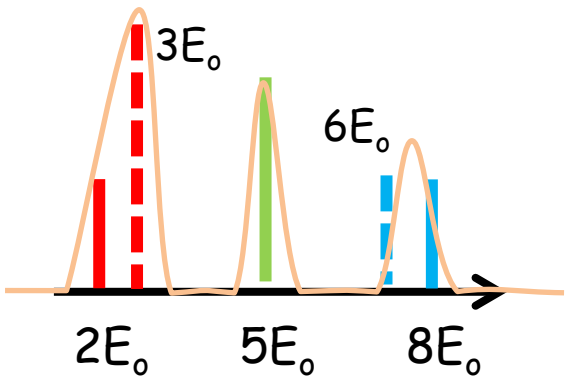
filled vs. empty states in "k-space"



Checking the theory



Check against experiment

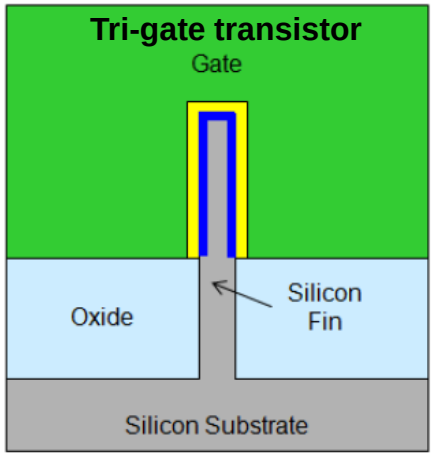


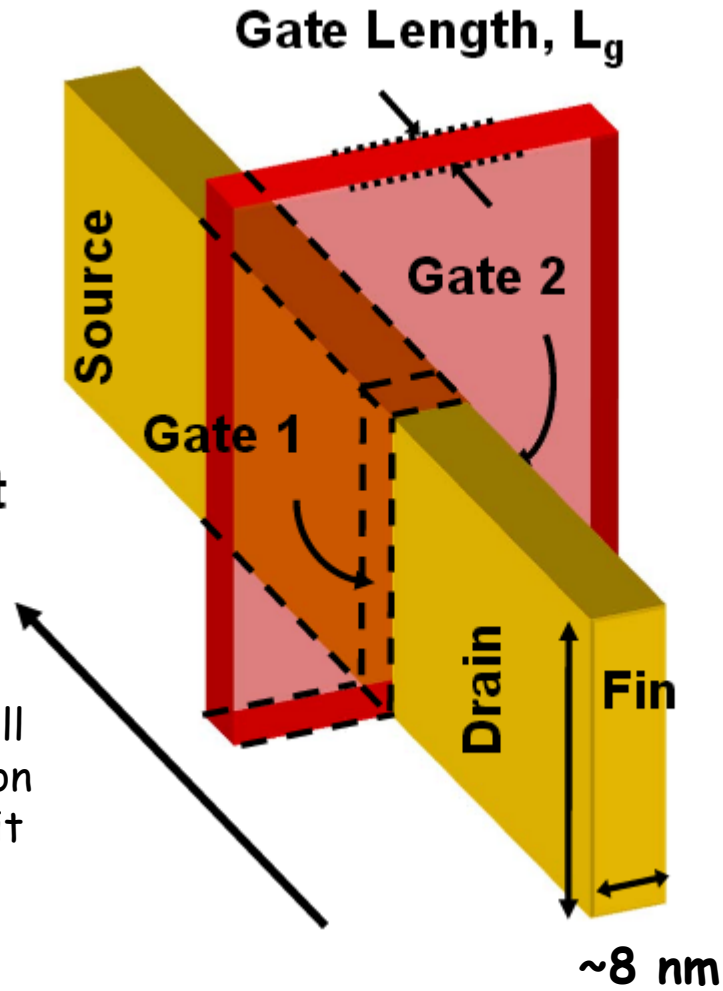
Assumes transitions radiate light

two clicks

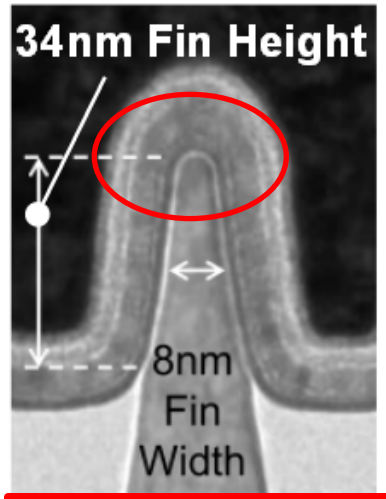
2d Application: FinFET Concept and Implementation

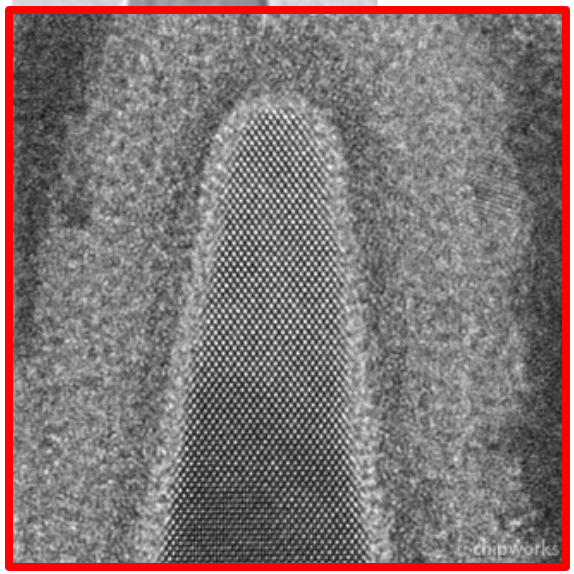
On May 4, 2011, Intel announced what it called the most radical shift in semiconductor technology in 50 years.





(Intel)





New 3-dimensional transistor design will enable the production of integrated-circuit chips that operate faster with less power...

http://electroiq.com/chipworks_real_chips_blog/2012/04/

C. Auth, VLSI-T (2012)

Up Next – counting quantum states