Modern Physics

Unit 5: Schrödinger’s Equation and the Hydrogen Atom
Lecture 5.1: Schrödinger’s Equation in 2 Dimensions

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

For every dynamical system, there exists a wavefunction $\Psi$ that is a continuous, square-integrable*, single-valued function of the coordinates of all the particles and of time. If you know $\Psi$, 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:

For $\Psi(x)$

For a single particle moving in one dimension:

For $\Psi(x,t)$

For a single particle in a superposition of two quantum states, a and b (state vector):

$\Psi(x,t) = A\Psi_a(x,t) + B\Psi_b(x,t)$

For a single particle moving in three dimensions:

For $\Psi(\vec{r},t)$

For two particles moving in three dimensions:

For $\Psi(\vec{r}_1,\vec{r}_2,t)$

*Square-integrable means that the normalization integral is finite
Real space vs. k-space

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

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

\[ \Phi(k) \quad \text{or} \quad \text{wavevector space or reciprocal space or inverse space} \]

real space

k (m^{-1})

x (m)
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,

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

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

This must be true for any \((x,y)\) 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

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

\[
\frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = \text{constant}_2 = -k_y^2
\]
I. Boundary Conditions

\[ X(x = 0) = X(x = L) = 0 \]
\[ Y(y = 0) = Y(y = L) = 0 \]

Try the solutions:

\[ X(x) = A \sin(k_x x) \quad Y(y) = B \sin(k_y y) \]

To match boundary conditions:

\[ k_x = \frac{n\pi}{L}; \quad n = 1, 2, 3... \quad k_y = \frac{m\pi}{L}; \quad m = 1, 2, 3... \]

II. Solution for $\Psi$

\[ \Psi(x, y) = X(x)Y(y) \]
\[ = AB \sin(k_x x) \sin(k_y y) \]
\[ = AB \sin \left( \frac{n\pi x}{L} \right) \sin \left( \frac{m\pi y}{L} \right) \]
III. Allowed Energies

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

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

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

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

<table>
<thead>
<tr>
<th>n</th>
<th>m</th>
<th>$E$</th>
<th>Degeneracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>$2E_o$</td>
<td>nondegenerate</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>$5E_o$</td>
<td>2-fold degenerate</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
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<td>2-fold degenerate</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>$8E_o$</td>
<td>nondegenerate</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>$10E_o$</td>
<td>2-fold degenerate</td>
</tr>
</tbody>
</table>

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 $\Psi^*\Psi$ for various energy eigenvalues

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

- $n=1; m=1; E=2E_0$
- $n=2; m=3; E=13E_0$
- $n=1; m=3; E=10E_0$
- $n=6; m=4; E=52E_0$
Plot of $\Psi^*\Psi$

$n=2; \ m=3$

3-dimensional

Top view – false color w. contours
What it means

filled vs. empty states in “k-space”

Each dot represents a quantum state

$E=0$

$E=2E_o$

$E=3E_o$

$E=4E_o$

$E=5E_o$

$E=6E_o$

$k_y = m\pi/L$

$k_x = n\pi/L$

$k_{max}$

$\pi/L$

$2\pi/L$

$3\pi/L$

$4\pi/L$

$k$

$k_{max}$

$k_y = m\pi/L$

$k_x = n\pi/L$
Checking the theory

- 18E₀
- 17E₀
- 13E₀
- 10E₀
- 8E₀
- 5E₀
- 2E₀
- E=0

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.

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