PHY 114 A General Physics II
11 AM-12:15 PM TR Olin 101

Plan for Lecture 23 (Chapter 40-42):
Some topics in Quantum Theory
1. Particle behaviors of electromagnetic waves
2. Wave behaviors of particles
3. Quantized energies

Part of SPS zone 5 conference
April 20-21, 2012

Time, Einstein, and the Coolest Stuff in the Universe
A free public lecture by Nobel Laureate
Dr. William Phillips
National Institute of Standards and Technology
8:00 PM Friday, April 20
Brenkle Recital Hall
Wake Forest University
www.wfu.edu/physics/SPS/SPSzone52012conf/welcome.html

Offer 1 point extra credit for attendance*

*After the lecture, email me that you attended. In the following email exchange you will be asked to answer one question about the lecture.
Webassign hint:

\[ d \sin \theta = m \lambda \]

For \( N = 4160 \) grooves/cm, \( d = \frac{1}{N} \)

Webassign hint:

Incident beam

The incident beam can reflect from different planes of slits.

Upper and Lower planes

Condition for bright spot:

\[ 2d \sin \theta = m \lambda = \lambda \]

If you have not already done so – please reply to my email concerning your intentions regarding Exam 4.

The material you have learned up to now in PHY 113 & 114 was known in 1900 and is basically still true. Some details (such as at high energy, short times, etc.) have been modified with Einstein’s theory of relativity, and with the development of quantum theory.
Which of the following technologies do not need quantum mechanics.
A. X-ray diffraction
B. Neutron diffraction
C. Electron microscope
D. MRI (Magnetic Resonance Imaging)
E. Lasers

Which of the following technologies do not need quantum mechanics.
A. Scanning tunneling microscopy
B. Atomic force microscopy
C. Data storage devices
D. Microwave ovens
E. LED lighting

Image of Si atoms on a nearly perfect surface at T=7 K.

Image made using atomic force microscopy.

From Physical Review Letters
March 20, 2000 – Volume 84, Issue 12, pp. 2642-2645

Quantum physics –
- Electromagnetic waves sometimes behave like particles
  - one “photon” has a quantum of energy $E=hf$ and momentum $p=h/\lambda=hf/c$

- Particles sometimes behave like waves
  - “wavelength” of particle related to momentum: $\lambda=h/p$
  - quantum particles can “tunnel” to places classically “forbidden”
  - Stationary quantum states have quantized energies
Classical physics

Wave equation for electric field in Maxwell's equations (plane wave boundary conditions):

\[ \frac{\partial^2 \mathbf{E}}{\partial t^2} = c^2 \frac{\partial^2 \mathbf{E}}{\partial x^2} \text{ for example: } \mathbf{E}(x, t) = E_{\text{max}} \sin(kx - \omega t) \]

Equation for particle trajectory \( r(t) \) in conservative potential \( U(r) \) and total energy \( E \):

\[ \frac{1}{2} m \left( \frac{dr}{dt} \right)^2 + U(r) = E \]

for example: \( r(t) = r_0 + v_0 t - \frac{1}{2} \omega \hat{k} t^2 \)

---

Particle ↔ wave properties in classical physics

<table>
<thead>
<tr>
<th>Particle properties</th>
<th>Wave properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position as a function of time is known -- ( r(t) )</td>
<td>Phenomenon is spread out over many positions at an instant of time.</td>
</tr>
<tr>
<td>Particle is spatially confined when ( E \leq U(r) ).</td>
<td>Notion of spatial confinement non-trivial.</td>
</tr>
<tr>
<td>Particles are independent.</td>
<td>Interference effects.</td>
</tr>
</tbody>
</table>

---

Mathematical representation of particle and wave behaviors.

Consider a superposition of periodic waves at \( t=0 \):

\[ E(x, t) = \sum_{i} E_{\text{max}} \sin(k_i x) \]

---

4/19/2012
\[ [E(x,0)]^2 = \left( \sum_{i} E_{\text{max}}(k_i) \sin(k_i x) \right)^2 \]

\[ \Delta x \Delta k = 2\pi \]

\[ \Delta x \text{ smaller } \rightarrow \text{ more particle like} \]
\[ \Delta k \text{ smaller } \rightarrow \text{ more wave like} \]

\[ \Delta x \Delta k = 2\pi \rightarrow \text{Heisenberg's uncertainty principle} \]

De Broglie's particle wavelength relation:
\[ p = \frac{\hbar}{\lambda} \]
\[ \frac{\hbar}{\lambda} = \frac{\hbar}{2\pi} = \hbar k \]

Heisenberg's hypotheses:
\[ \Delta x \Delta p \geq \frac{\hbar}{2} \]
\[ \Delta x \Delta E \geq \frac{\hbar}{2} \]

\[ \hbar = 6.6 \times 10^{-34} \text{ Js} = 4.14 \times 10^{-15} \text{ eVs} \]

Wave equations

Electromagnetic waves:
\[ \frac{\partial^2 E}{\partial x^2} = \frac{\epsilon c^2}{\epsilon_0} \frac{\partial^2 E}{\partial t^2} \]

Matter waves: (Schrödinger equation)
\[ -i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi(x,t) \]
Comparison of different wave equations

<table>
<thead>
<tr>
<th>Electromagnetic waves</th>
<th>Matter waves</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vector – E or B fields</td>
<td>Scalar – probability amplitude</td>
</tr>
<tr>
<td>Second order t dependence</td>
<td>First order t dependence</td>
</tr>
<tr>
<td>Examples:</td>
<td>Examples:</td>
</tr>
<tr>
<td>$E_x(t, x) = E_{max} \sin(kt - \omega t)$</td>
<td>$\Psi(x, t) = \Psi_0 \sin(kt)e^{-\frac{iE_0x}{\hbar}}$</td>
</tr>
<tr>
<td>$B_z(t, x) = \frac{E_{max}}{c} \sin(kt - \omega t)$</td>
<td>$\Psi(r, t) = \frac{1}{\sqrt{</td>
</tr>
<tr>
<td>$E_0 = \frac{e^2}{8\hbar^2\omega_0}$</td>
<td>$</td>
</tr>
</tbody>
</table>

What is the meaning of the matter wave function $\Psi(x, t)$?

- $\Psi(x, t)$ is not directly measurable
- $|\Psi(x, t)|^2$ is measurable – represents the density of particles at position $x$ at time $t$.
- For a single particle system – represents the probability of measuring particle at position $x$ at time $t$.
- For many systems of interest, the wave function can be written in the form $\Psi(x, t) = \psi(x)e^{-i\omega t}$
- $|\Psi(x, t)|^2 = |\psi(x)|^2$
- $\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$

Wave-like properties of particles

Louis de Broglie suggested that a wavelength could be associated with a particle's momentum

$$p = \frac{\hbar}{\lambda} \Rightarrow -i \hbar \frac{\partial}{\partial x} \Psi(x) = -i\hbar \frac{\partial}{\partial x} \Psi(x, t)$$

"Wave" equation for particles – Schrödinger equation

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

Stationary state wavefunctions: $\Psi(r, t) = \psi(r)e^{-i\omega t}$

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi(x, t) = E\Psi(x, t)$$
Example -- free particle -- $U(r) = 0$: $\Psi(r, t) = \psi(r) e^{i \omega t}$

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

$$\Psi(x, t) = \Psi_0 \sin(\beta x) e^{i \omega t}$$

$$E = \frac{\hbar^2 \beta^2}{2m}$$

$$k = \frac{2\pi}{\lambda} \Rightarrow \lambda = \frac{\hbar}{\sqrt{2mE}} \text{ or } E = \frac{\hbar^2}{2m\lambda^2}$$

Example: Suppose we want to create a beam of electrons ($m = 9.1 \times 10^{-31} \text{kg}$) for diffraction with $\lambda = 1 \times 10^{-10} \text{m}$. What is the energy $E$ of the beam?

$$E = \frac{\hbar^2}{2m\lambda^2} = \frac{\left(6.6 \times 10^{-34} \text{J} \cdot \text{s} \right)^2}{2 \cdot 9.1 \times 10^{-31} \text{kg} \cdot \left(10^{-10} \text{m} \right)^2} = 2.4 \times 10^{-17} \text{J} = 150 \text{eV}$$

Electron microscope

Typically $E = 120,000$–$200,000 \text{ eV}$ for high resolution EM

From Microscopy Today article May 2009

Electrons in an infinite box:

$$E \psi(x) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right] \psi(x) \text{ for } 0 \leq x \leq L$$

$$\psi(x) = \Psi_0 \sin \left( \frac{\pi n x}{L} \right) \quad n = 1, 2, 3 \ldots$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$
Electrons in a finite box:

finite probability of electron existing outside of classical region

Why would it be interesting to study electrons in a finite box?
A. It isn’t
B. It is the mathematically most simple example of quantum system
C. Quantum well systems can be manufactured to design new devices

Tunneling of electrons through a barrier

surface region   tip   vacuum
How a scanning tunneling microscope works:

Developed at IBM Zurich by Gerd Binnig and Heinrich Rohrer who received Nobel prize in 1986.

Visualization of $|\psi(x)|^2$

A surface if a nearly perfect Si crystal


The physics of atoms --

Features are described by solutions to the matter wave equation – Schrödinger equation:

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

"reduced" mass of electron and proton

Stationary-state wavefunctions: $\Psi(r,t) = \psi(r)e^{-iE/\hbar}$

Solutions: $E_n = \frac{Z^2\beta^2}{8\pi\varepsilon_0\varepsilon_n} - \frac{1}{n^2} = -\frac{13.6Z^2}{n^2}\text{eV}$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.0529\text{ nm}$$
Form of probability density for ground state \( n = 1 \)

\[
P_1 = 4\pi r^2 |\psi(r)|^2
\]

Angular degrees of freedom

- Since the force between the electron and nucleus depends only on distance and not on angle, angular momentum \( \mathbf{L} = \mathbf{r} \times \mathbf{p} \) is conserved. Quantum numbers associated with angular momentum:

\[
L_z^2 = h^2 \ell (\ell + 1)
\]

\[
L_z = \hbar m
\]

\( \ell = 0, 1, 2, ..., (n-1) \)

Notation:

\( \ell = 0 \Rightarrow s, \quad 1 \Rightarrow p, \quad 2 \Rightarrow d \)

Summary of results for H-atom:

\[
E_n = -13.6 \frac{Z^2}{n^2} \text{eV}
\]

Balmer series spectra

Degeneracy associated with each \( n \): \( 2\ell^2 \)
Atomic states of atoms throughout periodic table:

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>Li</td>
<td>Be</td>
<td>B</td>
<td>C</td>
<td>N</td>
<td>O</td>
<td>F</td>
<td>Ne</td>
<td>Na</td>
</tr>
<tr>
<td>Li</td>
<td>Be</td>
<td>B</td>
<td>C</td>
<td>N</td>
<td>O</td>
<td>F</td>
<td>Ne</td>
<td>Na</td>
<td>Mg</td>
</tr>
<tr>
<td>Na</td>
<td>Mg</td>
<td>Al</td>
<td>Si</td>
<td>P</td>
<td>S</td>
<td>Cl</td>
<td>Ar</td>
<td>K</td>
<td>Ca</td>
</tr>
<tr>
<td>K</td>
<td>Ca</td>
<td>Sc</td>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
</tr>
<tr>
<td>Sc</td>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
</tr>
<tr>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
</tr>
<tr>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
</tr>
<tr>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
</tr>
<tr>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
<td>Br</td>
</tr>
<tr>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
<td>Br</td>
<td>Kr</td>
</tr>
<tr>
<td>Ni</td>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
<td>Br</td>
<td>Kr</td>
<td>Xe</td>
</tr>
<tr>
<td>Cu</td>
<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
<td>Br</td>
<td>Kr</td>
<td>Xe</td>
<td>Rn</td>
</tr>
</tbody>
</table>

\[ E\psi(r) = -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} + U(r) \right) \psi(r) \]

Example: Cu (Z=29) \[1s^22s^22p^63s^23p^63d^{10}4s^1 \]

- S
- P
- D

Radial density for Cu

\[ 4\pi r^2 |\psi(r)|^2 \]