Lecture Outline

• Introduction to quantum mechanics (Chap.2)

• Quantum theory for semiconductors (Chap. 3)
  • Allowed and forbidden energy bands (Chap. 3.1)
Classical Mechanics and Quantum Mechanics

**Mechanics**: the study of the behavior of physical bodies when subjected to forces or displacements.

- **Classical Mechanics**: describing the motion of *macroscopic* objects. *Macroscopic*: measurable or observable by naked eyes.
- **Quantum Mechanics**: describing behavior of systems at atomic length scales and smaller.
Inconsistency with classical light theory

According to the classical wave theory, maximum kinetic energy of the photoelectron is only dependent on the incident intensity of the light, and independent on the light frequency; however, experimental results show that the kinetic energy of the photoelectron is dependent on the light frequency.

Concept of “energy quanta”
Energy Quanta

• Photoelectric experiment results suggest that the energy in light wave is contained in discrete energy packets, which are called energy quanta or photon

• The wave behaviors like particles. The particle is photon

Planck’s constant: \( h = 6.625 \times 10^{-34} \text{ J-s} \)

Photon energy = \( h\nu \)

Work function of the metal material = \( h\nu_o \)

Maximum kinetic energy of a photoelectron: \( T_{max} = h(\nu - \nu_o) \)
Electron’s Wave Behavior

Davisson-Germer experiment

Electron as a particle has wave-like behavior
Wave-Particle Duality

Particle-like wave behavior
(example, photoelectric effect)

Wave-like particle behavior
(example, Davisson-Germer experiment)

Wave-particle duality

Mathematical descriptions:

The momentum of a photon is:
\[ p = \frac{h}{\lambda} \]

The wavelength of a particle is:
\[ \lambda = \frac{h}{p} \]

\( \lambda \) is called the de Broglie wavelength
Quantum Theory for Semiconductors

How to determine the behavior of electrons in the semiconductor?

• Use the wave theory to describe the electron motion

• Mathematical description of wave theory in quantum mechanics — Schrödinger’s Equation

• Solution of Schrödinger’s Equation → energy band structure of electrons
Schrödinger’s Equation

One dimensional Schrödinger’s Equation:

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x)\Psi(x, t) = j\hbar \frac{\partial \Psi(x, t)}{\partial t}
\]

\(\Psi(x, t)\) : Wave function

\[|\Psi(x, t)|^2 \, dx\] , the probability to find a particle in \((x, x+dx)\) at time \(t\)

\[|\Psi(x, t)|^2\] , the probability density at location \(x\) and time \(t\)

\(V(x)\) : Potential function

\(m\) : Mass of the particle
Probability Density for One-Electron Atom

\[ \psi(r, \theta, \phi) = \psi_{nlm}(r, \theta, \phi) \quad E_n \propto \frac{1}{n^2} \]

For the lowest energy state, \( n=1, l=0, m=0 \)

\[ \psi_{100} = \frac{1}{\sqrt{\pi}} \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0} \]

\[ a_0 = \frac{4\pi \epsilon_0 \hbar^2}{m_0 e^2} = 0.529 \text{ Å} \quad \text{Bohr's radius} \]
# Table for Atom Orbits

<table>
<thead>
<tr>
<th></th>
<th>s (l=0)</th>
<th>p (l=1)</th>
<th>d (l=2)</th>
<th>f (l=3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n=1</td>
<td><img src="image1" alt="s-orbit" /></td>
<td><img src="image2" alt="p-orbit" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n=2</td>
<td><img src="image3" alt="s-orbit" /></td>
<td><img src="image4" alt="p-orbit" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
<td></td>
</tr>
<tr>
<td>n=3</td>
<td><img src="image5" alt="s-orbit" /></td>
<td><img src="image6" alt="p-orbit" /></td>
<td><img src="image7" alt="d-orbit" /></td>
<td><img src="image8" alt="f-orbit" /></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
</tr>
<tr>
<td>n=4</td>
<td><img src="image9" alt="s-orbit" /></td>
<td><img src="image10" alt="p-orbit" /></td>
<td><img src="image11" alt="d-orbit" /></td>
<td><img src="image12" alt="f-orbit" /></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
</tr>
<tr>
<td>n=5</td>
<td><img src="image13" alt="s-orbit" /></td>
<td><img src="image14" alt="p-orbit" /></td>
<td><img src="image15" alt="d-orbit" /></td>
<td><img src="image16" alt="f-orbit" /></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
<td>m=0, m=1</td>
</tr>
<tr>
<td>n=6</td>
<td><img src="image17" alt="s-orbit" /></td>
<td><img src="image18" alt="p-orbit" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td>m=0, m=1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n=7</td>
<td><img src="image19" alt="s-orbit" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>m=0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Probability Density Functions for One and Two Hydrogen Atoms

Example: Hydrogen atom

(a) Probability density function of an isolated hydrogen atom

(b) Overlapping probability density function of two adjacent hydrogen atoms
Energy Level Splitting By Interaction Between Two Atoms

For one H atom

\[-\nabla^2 \psi(r, \theta, \phi) + \frac{2m_0}{\hbar^2} V(r) \psi(r, \theta, \phi) = \frac{2m_0}{\hbar^2} E \psi(r, \theta, \phi)\]

For two H atoms

\[-\nabla^2 \psi'(r, \theta, \phi) + \frac{2m_0}{\hbar^2} (V(r) + V_{\text{int}}(r)) \psi'(r, \theta, \phi) = \frac{2m_0}{\hbar^2} E' \psi'(r, \theta, \phi)\]

Additional potential energy due to interaction
Energy Level Splitting Into A Band of Allowed Energies

When many hydrogen atoms are periodically arranged, the initial quantized energy levels will split into a band of discrete energy levels.
Allowed And Forbidden Energy Bands

Discrete atomic energy levels

Energy

Atomic separation

Allowed and forbidden energy bands at atomic spacing $d$