**Atomic Physics**

**Previous Lecture:**
- Particle in a Box, wave functions and energy levels
- Quantum-mechanical tunneling and the scanning tunneling microscope
- Start Particle in 2D,3D boxes

**This Lecture:**
- More on Particle in 2D,3D boxes
- Other quantum numbers than n: angular momentum
- H-atom wave functions
- Pauli exclusion principle

**From last week: particle in a box**

**Classical:** particle bounces back and forth.
Sometimes velocity is to left, sometimes to right

**Quantum mechanics:**
- Particle is a wave: $p = mv = h/\lambda$
- **Standing wave:** superposition of waves traveling left and right $\rightarrow$ integer number of wavelengths in the tube

$\lambda = 2L$
- One half-wavelength

$\lambda = L$
- Two half-wavelengths

**Energy**

Energy is quantized

$$E_n = \frac{p^2}{2m} = \frac{n^2 \hbar^2}{8mL^2}$$

the larger the box the lower the energy of the particle in the box

A quantum particle in a box cannot be at rest!

Fundamental state energy is not zero: $E_{\text{rest}} = 0.38 \text{ eV}$ for an electron in a quantum well of $L = 1 \text{ nm}$

Consequence of uncertainty principle:

$$\Delta x = L \Rightarrow \Delta p_x = 1/L \neq 0!$$
Classical/Quantum Probability

Similar when $n = 3$
$n = 2$
$n = 1$

Tunneling: nonzero probability of escaping the box. Tunneling Microscope: tunneling electron current from sample to probe sensitive to surface variations.

Probability (2D):
$\frac{\hbar}{\lambda_n} = n \frac{\hbar}{2L}$

With increasing energy...

Quantization of angular momentum

$L = \hbar \sqrt{\ell (\ell + 1)}$

$\ell$ is the orbital quantum number

States with same $n$, have same energy and can have $\ell = 0, 1, 2, \ldots , n-1$ orbital quantum number

$\ell = 0$ orbits are most elliptical
$\ell = n-1$ most circular

The $z$ component of the angular momentum must also be quantized

$L_z = m_{z} \hbar$

$m_{z}$ ranges from $-\ell$, to $\ell$ integer

values $=> (2 \ell +1)$ different values
The experiment: Stern and Gerlach

It is possible to measure the number of possible values of \( L_z \) respect to the axis of the \( B \)-field produced by the electron current

The electron moving on the orbit is like a current that produces a magnetic momentum \( \mu = eA \)

\[
\mu = \frac{e}{2m} r^2 = \frac{e}{2m} (nvr) = \frac{\mu_B}{2m} (\ell + 1)
\]

For a quantum state with \( \ell = 2 \), how many different orientations of the orbital angular momentum respect to the z-axis are there?

- A. 1
- B. 2
- C. 3
- D. 4
- E. 5

For hydrogen atom:

- \( n \) describes energy of orbit
- \( \ell \) describes the magnitude of orbital angular momentum
- \( m \) describes the angle of the orbital angular momentum

\( E_n = -\frac{13.6}{n^2} \text{ eV} \)

Next highest energy: \( n = 2 \)

- \( n = 2, \ell = 0, m_l = 0 \)
- \( n = 2, \ell = 1, m_l = 0 \)
- \( n = 2, \ell = 1, m_l = \pm 1 \)

Same energy, but different probabilities

\( n = 3 \): 2 s-states, 6 p-states and...

- \( n = 3, \ell = 0, m_l = 0 \)
- \( n = 3, \ell = 1, m_l = 0 \)
- \( n = 3, \ell = 1, m_l = \pm 1 \)
Quantum state specified by four quantum numbers:
- Three spatial quantum numbers (3-dimensional)
- One spin quantum number

How many different quantum states exist with n=2?

A. 1
B. 2
C. 4
D. 8

Electrons obey Pauli exclusion principle
- Only one electron per quantum state \((n, \ell, m, m_s)\)

Hydrogen: 1 electron
- One quantum state occupied
  \((n=1, \ell=0, m_s=0, m=+1/2)\)

Helium: 2 electrons
- Two quantum states occupied
  \((n=1, \ell=0, m_s=0, m=+1/2)\)
  \((n=1, \ell=0, m_s=0, m=-1/2)\)

Radial probability
\[
\Psi_{n,\ell,m}(r, \theta, \varphi) = R_n(r) Y_{\ell m}(\theta, \varphi)
\]
- For 1s, 2p, 3d, \(r_{\text{peak}} = a_0, 4a_0, 9a_0\)

- These are the Bohr orbit radii!
- Most probable distance of electron from nucleus!
- They behave like Bohr orbits because for states with same \(E\), larger angular momentum corresponds to more spherical orbitals; orbits are elliptical for small \(\ell\)

Pauli exclusion principle
- Electrons obey Pauli exclusion principle
- Only one electron per quantum state \((n, \ell, m, m_s)\)

Building Atoms

<table>
<thead>
<tr>
<th>Atom</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s(^1)</td>
</tr>
<tr>
<td>He</td>
<td>1s(^2)</td>
</tr>
<tr>
<td>Li</td>
<td>1s(^2)2s(^1)</td>
</tr>
<tr>
<td>Be</td>
<td>1s(^2)2s(^2)</td>
</tr>
<tr>
<td>B</td>
<td>1s(^2)2s(^2)2p(^1)</td>
</tr>
<tr>
<td>Ne</td>
<td>1s(^2)2s(^2)2p(^6)</td>
</tr>
</tbody>
</table>

Electron acts like a bar magnet with N and S pole.
- Magnetic moment fixed...
- ...but 2 possible orientations of magnet: up and down

Described by spin quantum number \(m_s\)
- \(z\)-component of spin angular momentum \(S_z = m_s \hbar\)
Atoms in same column have ‘similar’ chemical properties.
Quantum mechanical explanation:
similar ‘outer’ electron configurations.

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| H | 1s^1 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| Li | 2s^1 | Be | 2s^2 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| Na | 3s^1 | Mg | 3s^2 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| K  | 4s^1 | Ca | 4s^2 | Sc | 3d^1 | Y  | 3d^2 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| Ga | 4p^1 | Ge | 4p^2 | As | 4p^3 | Se | 4p^4 | Br | 4p^5 | Kr | 4p^6 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |

The periodic table