MTE 3 Results

Average 79.75/100
std 12.30/100

A 19.9%
AB 20.8%
B 26.3%
BC 17.4%
C 13.1%
D 2.1%
F 0.4%
Final
Mon. May 12, 12:25-2:25, Ingraham B10

Get prepared for the Final!

Remember Final counts 25% of final grade!
It will contain new material and MTE1-3 material

(no alternate exams!!! but notify SOON any potential and VERY serious problem you have with this time)
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
Biomagnetism deals with the registration and analysis of magnetic fields which are produced by organ systems in the body.
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 => integer number of wavelengths in the tube

\[ \lambda = 2L \]  
One half-wavelength \( n=1 \)

\[ \lambda = L \]  
Two half-wavelengths \( n=2 \)

\[ |p| = \frac{h}{\lambda} = \frac{h}{2L} = p_o \]

\[ |p| = \frac{h}{\lambda} = \frac{h}{L} = 2p_o \]
Summary of quantum information

Energy is quantized

\[ E_n = \frac{p^2}{2m} = n^2 \left( \frac{h^2}{8mL^2} \right) \]

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:

\[ E_{n=1} = 0.38 \text{ eV} \] for an electron in a quantum well of \( L = 1 \) nm

Consequence of uncertainty principle:

\[ \Delta x = L \Rightarrow \Delta p_x \approx \frac{1}{L} \neq 0! \]
Classical/Quantum Probability

n=3

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

Similar when n → ∞

Quantum-mechanical distribution

Classical distribution

\[ P = \frac{1}{L} \quad 0 < x < L \]
Particle in a 2D box

Probability (2D)

Ground state: same wavelength (longest) in both $x$ and $y$
Need two quantum #’s, one for $x$-motion, one for $y$-motion
Use a pair $(n_x, n_y)$
Ground state: (1,1)

Same energy but different probability in space

$(n_x, n_y) = (2,1)$

$(n_x, n_y) = (1,2)$
Particle in 3D box

- Ground state surface of constant probability
- \((n_x, n_y, n_z)=(1,1,1)\)

All these states have the same energy, but different probabilities
With increasing energy...

\[ p_x = \frac{h}{\lambda_{n_x}} = n_x \frac{h}{2L} \]

same for y,z

\[ E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} = E_o (n_x^2 + n_y^2 + n_z^2) \]

quantum states with same \( n_x, n_y, n_z \) have same \( E \)

Eg: how many 3D particle states have \( 18E_0 \)?

\[ (n_x, n_y, n_z) = (4,1,1), (1,4,1), (1,1,4) \]
Bohr model fails describing atoms heavier than H

Does it violate the Heisenberg uncertainty principle?

A) YES
B) No

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

radius and energy of electron cannot be exactly known at the same time!

Schrödinger: Hydrogen atom is 3D structure.
Should have 3 quantum numbers.

Coulomb potential (electron-proton interaction) is spherically symmetric.
x, y, z not as useful as r, θ, φ

Modified H-atom should have 3 quantum numbers
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

\[ L_z = m_\ell \hbar \]

\( m_\ell \) 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 $\mathbf{B}$-field produced by the electron current.

The electron moving on the orbit is like a current that produces a magnetic momentum $\mu=IA$.

$$\mu = \frac{e}{T} \pi r^2 = \frac{e v}{2 \pi r} \pi r^2 = \frac{e}{2m} (mvr) = \frac{e}{2m} L$$

$$|\vec{\mu}| = \mu_B \sqrt{\ell(\ell + 1)}$$
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

\[
\begin{align*}
\text{s: } \ell &= 0 \\
\text{p: } \ell &= 1 \\
\text{d: } \ell &= 2 \\
\text{f: } \ell &= 3 \\
\text{g: } \ell &= 4
\end{align*}
\]

“atomic shells”
Summary of quantum numbers

**TABLE 28.2** Three Quantum Numbers for the Hydrogen Atom

<table>
<thead>
<tr>
<th>Quantum Number</th>
<th>Name</th>
<th>Allowed Values</th>
<th>Number of Allowed States</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )</td>
<td>Principal quantum number</td>
<td>1, 2, 3, \ldots</td>
<td>Any number</td>
</tr>
<tr>
<td>( \ell )</td>
<td>Orbital quantum number</td>
<td>0, 1, 2, \ldots, ( n - 1 )</td>
<td>( n )</td>
</tr>
<tr>
<td>( m_\ell )</td>
<td>Orbital magnetic quantum</td>
<td>( -\ell, -\ell + 1, \ldots )</td>
<td>( 2\ell + 1 )</td>
</tr>
<tr>
<td>number</td>
<td>number</td>
<td>( 0, \ldots, \ell - 1, \ell )</td>
<td></td>
</tr>
</tbody>
</table>

For hydrogen atom:

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

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

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

\[
L_z = m_\ell \hbar
\]
3D Surfaces of constant prob. for H-atom

Electron cloud: probability density in 3D of electron around the nucleus

\[ P(r, \theta, \phi) dV = |\Psi(r, \theta, \phi)|^2 dV \]

- Spherically symmetric.
- Probability decreases exponentially with radius.
- Shown here is a surface of constant probability

\[ n = 1, \quad \ell = 0, \quad m_\ell = 0 \]
Next highest energy: $n = 2$

2$s$-state

$n = 2, \ \ell = 0, \ m_\ell = 0$

2$p$-state

$n = 2, \ \ell = 1, \ m_\ell = 0$

2$p$-state

$n = 2, \ \ell = 1, \ m_\ell = \pm 1$

Same energy, but different probabilities
n = 3: 2 s-states, 6 p-states and...

\[ n = 3, \; \ell = 0, \; m_\ell = 0 \]

\[ n = 3, \; \ell = 1, \; m_\ell = 0 \]

\[ n = 3, \; \ell = 1, \; m_\ell = \pm 1 \]
...10 d-states

$n = 3, \ell = 2, m_\ell = 0$

$n = 3, \ell = 2, m_\ell = \pm 1$

$n = 3, \ell = 2, m_\ell = \pm 2$
Radial probability

\[ \Psi_{n, \ell, m}(r, \theta, \phi) = R_{n, \ell}(r) Y_{\ell, m}(\theta, \phi) \]

- For 1s, 2p, 3d, \( r_{\text{peak}} = a_0, 4a_0, 9a_0 \)
- These are the Bohr orbit radii!
  
  \[ r_n = n^2 a_o \]

- 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 orbits, orbits are elliptical for small \( \ell \)
New electron property: 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 $S_z = m_s \hbar$

Spin up $m_s = +1/2$

Spin down $m_s = -1/2$
All quantum numbers of electrons in atoms

- Quantum state specified by four quantum numbers:
  \( (n, \ell, m_\ell, m_s) \)
  
  - Three spatial quantum numbers (3-dimensional)
  
  - One spin quantum number

How many different quantum states exist with \( n=2 \)?

A. 1

\( \ell = 0 \) : \( 2s^2 \)

B. 2

\( m_\ell = 0 \) : \( m_s = 1/2, -1/2 \) 2 states

C. 4

\( \ell = 1 \) : \( 2p^6 \)

\( m_\ell = +1 \) : \( m_s = 1/2, -1/2 \) 2 states

\( m_\ell = 0 \) : \( m_s = 1/2, -1/2 \) 2 states

\( m_\ell = -1 \) : \( m_s = 1/2, -1/2 \) 2 states
Pauli exclusion principle

- Electrons obey **Pauli exclusion principle**
- Only one electron per quantum state \((n, \ell, m_{\ell}, m_s)\)

**Hydrogen:** 1 electron

- one quantum state occupied
- \((n = 1, \ell = 0, m_{\ell} = 0, m_s = +1/2)\)

**Helium:** 2 electrons

- two quantum states occupied
- \((n = 1, \ell = 0, m_{\ell} = 0, m_s = +1/2)\)
- \((n = 1, \ell = 0, m_{\ell} = 0, m_s = -1/2)\)
<table>
<thead>
<tr>
<th>Atom</th>
<th>Configuration</th>
<th>1s shell filled</th>
<th>2s shell filled</th>
<th>2p shell filled</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s^1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>He</td>
<td>1s^2</td>
<td>1s shell filled</td>
<td>(n=1 shell filled - noble gas)</td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>1s^22s^1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be</td>
<td>1s^22s^2</td>
<td>2s shell filled</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1s^22s^22p^1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ne</td>
<td>1s^22s^22p^6</td>
<td>2p shell filled</td>
<td>(n=2 shell filled - noble gas)</td>
<td></td>
</tr>
</tbody>
</table>
The periodic table

- Atoms in same column have ‘similar’ chemical properties.
- Quantum mechanical explanation: similar ‘outer’ electron configurations.

<table>
<thead>
<tr>
<th></th>
<th>H 1s(^1)</th>
<th>Li 2s(^1)</th>
<th>Be 2s(^2)</th>
<th>Na 3s(^1)</th>
<th>Mg 3s(^2)</th>
<th>K 4s(^1)</th>
<th>Ca 4s(^2)</th>
<th>Sc 3d(^1)</th>
<th>Y 3d(^2)</th>
<th>8 more transition metals</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>2p(^1)</td>
<td>C 2p(^2)</td>
<td>N 2p(^3)</td>
<td>O 2p(^4)</td>
<td>F 2p(^5)</td>
<td>Ne 2p(^6)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al</td>
<td>3p(^1)</td>
<td>Si 3p(^2)</td>
<td>P 3p(^3)</td>
<td>S 3p(^4)</td>
<td>Cl 3p(^5)</td>
<td>Ar 3p(^6)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ga</td>
<td>4p(^1)</td>
<td>Ge 4p(^2)</td>
<td>As 4p(^3)</td>
<td>Se 4p(^4)</td>
<td>Br 4p(^5)</td>
<td>Kr 4p(^6)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>