Physics 228

Today:

Zeeman Effect
Spin
Many-Electron Atoms
Class Average: 68.8 (69%)  Standard Deviation: 15.5 (16%)

Exam 1

Class Average: 52.9 (53%)  Standard Deviation: 17.5 (18%)

Exam 2
Clicker Question

A potential-energy function is shown. If a quantum-mechanical particle has energy $E < U_0$, it is impossible to find the particle in the region.

A) $x < 0$.  
B) $0 < x < L$.  
C) $x > L$.  
D) misleading question — the particle can be found at any $x$.
The first three wave functions for a finite square well are shown. The probability of finding the particle at $x > L$ is

A) least for $n = 1$.

B) least for $n = 2$.

C) least for $n = 3$.

D) the same (and nonzero) for $n = 1, 2, \text{ and } 3$.

E) zero for $n = 1, 2, \text{ and } 3$. 
Shown here is a set of degenerate orbitals belonging to a certain orbital angular momentum quantum number $l$. These orbitals are

- a) s-orbitals
- b) p-orbitals
- c) d-orbitals
- d) f-orbitals
- e) cannot be determined

The degeneracy $2l + 1 = 5$

Thus $l = 2$
Hydrogen Atom in Magnetic Field

- For an object with a magnetic moment $\mu$, there is an interaction energy with the magnetic field $B$:

$$U = -\mu \cdot B.$$ 

- Classically, an electron orbiting around a proton, encircling an area $A$, corresponds to a circular electric current $I$, and thus a magnetic moment: $\mu = IA$.

- The current is given by the electron’s charge $(-e)$, velocity $v$, and orbital radius: $I = -ev/2\pi r$.

- Thus, the magnitude of the magnetic moment is

$$\mu = (-ev/2\pi r)(\pi r^2) = -evr/2 = (-e/2m)L \text{ (L is the angular momentum $rp = rmv$).}$$

$$\mu = (-e/2m)L$$
For a magnetic field in z-direction, the interaction energy thus becomes
\[ U = \frac{e}{2m} L \cdot B = \frac{e}{2m} L_z B. \]

Although this has been derived classically, it is true also in quantum mechanics.

For the H atom, we have \( L_z = m_I \hbar \), thus
\[ U = \frac{e\hbar}{2m} m_I B. \]

The quantity \( \mu_B = \frac{e\hbar}{2m} \) is called the **Bohr magneton** (a quantization unit of magnetic moment):
\[ U = m_I \mu_B B \]

We expect atomic energy levels to split into \((2l + 1)\) magnetic sub-levels when a magnetic field is applied (**Zeeman effect**). Such splitting is indeed observed:
Zeeman effect

\[ U = m_l \mu_B B \]

- A magnetic field removes the \((2l+1)\) - fold degeneracy of each \((n, l)\) level.
- The \((2l+1)\) sub-levels have even separations of \(\mu_B B\). Pieter Zeeman discovered this in 1896.
Because angular momentum is conserved, and the photon carries only one unit of angular momentum, allowed transitions must have

\[ \Delta l = \pm 1 \quad \text{and} \quad \Delta m_l = 0, \pm 1. \]
The Stern-Gerlach Experiment

1. A beam of atoms is directed parallel to the y-axis.

2. Specially shaped magnet poles produce a strongly nonuniform magnetic field that exerts a net force on the magnetic moments of the atoms.

3. Each atom is deflected upward or downward according to the orientation of its magnetic moment.

- If the magnetic field is not constant, there will be a force on the atom $F = -\nabla U = -m_I\mu_B(\text{dB}/\text{dz})$.

- An atom beam will separate into $2l+1$ separate bunches if there is a B field with enough spatial variation.

- This shows the quantization of the z-component of the magnetic moment, and by inference, the quantization of $L_z$. 
The number of “bunches” should be 2l+1, therefore odd.

This is observed for some atoms.

However, in other cases an even number is seen.

If we interpret this as angular momentum quantization, we require half-integer angular momentum quantum numbers \( j = 1/2, 3/2, \) etc.

The number of sublevels 2j+1 is then even.
Electron Spin

• This half-integral angular momentum also shows up in the Zeeman effect (called “anomalous Zeeman effect”).

• Half-integral angular momentum is now understood as “spin” of the electron.

• Spin is an intrinsic angular momentum that the electrons always have, irrespective of orbital motion.

• For electrons, the magnitude of the spin angular momentum is

\[ S = \sqrt{s(s + 1)} \hbar \quad \text{with} \quad s = \frac{1}{2} \quad \text{(spin quantum number)}. \]

• The z-component of the spin angular momentum is

\[ S_z = m_s \hbar \quad \text{with} \quad m_s = \pm \frac{1}{2} \quad \text{(spin magnetic quantum number)}. \]

• For many particles (electrons, protons, neutrons, ...) \( s = \frac{1}{2} \). Such particles are called fermions.

• Other particles have integral spin (\( s = 0 \) for the Higgs boson, \( s = 1 \) for the photon). Such particles are called bosons.
Electron Spin Magnetic Moment

• For a classical spinning body of charge $-e$ and mass $m$ (assuming equal charge and mass distribution), we would expect a magnetic moment of $\mu = (-e/2m)L$, where $L$ would be replaced by the spin angular momentum $S$.

• However, the electron is not a classical spinning body. Its magnetic moment is actually larger than expected classically:

$$\mu = g(e/2m)S$$

• The “quantum mechanics” factor $g$ is called the “$g$-factor” (duh).

• Classical mechanics predicts $g = -1$.

• Experimentally, $g = -2.002319304361$ (the most precisely known fundamental constant in physics!!)

• Nonrelativistic QM (Schroedinger equation) makes no prediction at all. Spin has to be added in an ad-hoc manner (without derivation).

• Relativistic QM (Dirac equation) predicts $g = -2$ (exactly).

• Another refinement of relativistic QM (quantum electrodynamics) predicts $g = -2.002319304361$ (The most accurate theoretical prediction in physics!!)
Anomalous Zeeman Effect

As a result of spin, in each of the H-atom energy levels the electron can be "spin up" or "spin down". Thus, even for s-orbitals, the spin gives rise to a two-fold Zeeman splitting in a magnetic field.

\[ \mathbf{U} = g m_s \mu_B B \text{ (spin)} \]

\[ E_s + (5.795 \times 10^{-5} \text{ eV/T})B \]

\[ E_s - (5.795 \times 10^{-5} \text{ eV/T})B \]

Spin up
\[ m_s = +\frac{1}{2} \]

Spin down
\[ m_s = -\frac{1}{2} \]
What is the magnitude of the spin angular momentum of an electron?

a) 0
b) $\hbar$
c) $\hbar/2$
d) $+\hbar/2$ or $-\hbar/2$, depending on whether spin is “up” or “down”
e) $\frac{3}{4}\hbar$

$$S = \sqrt{s(s+1)}\hbar = \sqrt{\frac{1}{2} \left(\frac{1}{2} + 1\right)}\hbar = \frac{3}{4}\hbar$$
Adding Angular Momenta

If there is both orbital and spin angular momentum, what often matters most is the total angular momentum $J = L + S$. $J$ is characterized by quantum number $j$, with the magnitude of $J$ given by

$$J = \sqrt{j(j + 1)}\hbar.$$

For $l > 0$, $j$ may take on one of two values: $j = l + \frac{1}{2}$, or $j = l - \frac{1}{2}$. For $l = 0$, $j = \frac{1}{2}$. 
The **Dirac equation** predicts the energy of atomic levels to depend on the magnitude of the total angular momentum \( \mathbf{J} = \mathbf{L} + \mathbf{S} \), and thus on the relative orientation of \( \mathbf{L} \) and \( \mathbf{S} \) (there is a term proportional to \( \mathbf{L} \cdot \mathbf{S} \): “spin-orbit coupling”).

Spin-orbit coupling leads to a splitting of spin-up and spin-down electron states even in the absence of a magnetic field! (It is as if there were a magnetic field in the direction of \( \mathbf{L} \)).

Spin-orbit splitting atomic spectra is referred to as “**fine structure**”. The predicted fine structure is experimentally observed to high precision.
Many Electron Atoms

In heavier atoms, the nucleus has charge $Ze$.

The electrons in orbit about the nucleus repel each other.

This leads to “screening” of outer electrons by inner electrons: The potential is no longer $1/r$.

As a consequence, the energy levels of different $l$ quantum numbers (same $n$) are no longer degenerate.

Accurate calculations are much more complicated than for hydrogen (“Coulomb correlations”).

On average, the $2s$ electron is considerably farther from the nucleus than the $1s$ electrons. Therefore, it experiences a net nuclear charge of approximately $+3e - 2e = +e$ (rather than $+3e$).
Pauli Exclusion Principle

• The Pauli exclusion principle states that each single-particle state (characterized by the four quantum numbers $n$, $l$, $m_l$, $m_s$) can accommodate no more than one electron.

• As a consequence, as we add electrons to an atom, the inner shells “fill up” first, then the more weakly bound shells will be populated. (“Aufbau principle”).

• The Pauli exclusion principle applies to all half-integer spin particles, i.e., fermions (incl. protons and neutrons).

• There is no such principle for bosons. For example, a large number of photons may occupy the same quantum state in a laser.