ECE 162A
Mat 162A

Lecture #14:Identical particles, multielectron atoms
E/R: Chapter 9

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Magnetic moments

- CLASSICALLY, an electron moving in a loop produces a current

$$i = \frac{e}{period}$$

$$period = \frac{distance}{velocity} = \frac{2\pi r}{v}$$

$$i = \frac{ev}{2\pi r}$$

- A current in a loop produces a magnetic dipole moment

$$\mu = current \times area = iA = \frac{ev}{2\pi r}\pi r^2 = \frac{evr}{2}$$

Bohr Magneton

- Classically, $L = mrv$

$$\mu = \frac{evr}{2} = \frac{eL}{2m}$$

$$If$$

- (Bohr Magneton) $\mu_b \equiv \frac{e\hbar}{2m} = .927 \times 10^{-23} Am^2$

$$\mu = \frac{\mu_b L}{\hbar}$$

- The correct quantum mechanical result is
- (g_l is the orbital g factor and g_l=1)

$$\vec{\mu} = -\frac{g_l \mu_b}{\hbar} \vec{L}$$

Dipole in a Magnetic Field

- The effect of a magnetic field on a magnetic dipole is to exert a torque

$$\vec{T} = \vec{\mu} \times \vec{B}$$

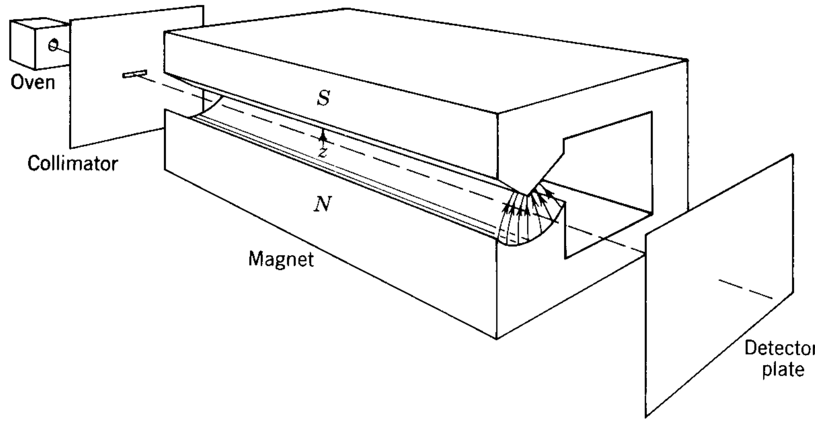
- The potential energy is lowest when the dipole is aligned with the magnetic moment

$$\Delta E = -\vec{\mu} \bullet \vec{B}$$

- Uniform magnetic field: precession, but no translation.
- Converging magnetic field: translational force.

$$F_z = \frac{\partial B}{\partial z} \mu_z$$

Stern Gerlach Experiment



- Stern Gerlach Exp: Pass a beam of silver atoms through a nonuniform magnetic field and record deflections
- Classical prediction: a range of deflections corresponding to μ_z ranging from + μ to - μ.
- Quantum mechanical prediction: discrete deflections corresponding to m_l=–l,…0…l
- Result: 2 discrete components: one positive, one negative.

Phipps/Taylor (1927) Experiment

- Repeat Stern Gerlach Exp with hydrogen atoms in the ground state. $l=0$. $m_l=0$.
- Quantum mechanical prediction: No deflection corresponding to $m_l=0$
- Result: 2 beams, one deflected positive, one negative.
- Something is missing in the theory.

Electron Spin

- Goudsmit and Uhlenbeck (1925), grad students.
- Explain fine splitting of Hydrogen lines by assuming the electron is a small spinning sphere with surface charge i.e. a magnetic moment.

$$Quantum\ numbers\ s = 1/2$$

$$Intrinsic\ angular\ momentum\ S = \sqrt{s(s+1)}\hbar$$

- The z component of spin is quantized:

$$S_z = m_s\hbar$$

$$m_s = -1/2, 1/2$$

$$g_l = 2$$

Spin Orbit Interaction

- The spin orbit interaction is the result of the electron spin magnetic moment and the internal magnetic field of the atom due to the electrons angular momentum.

$$\Delta E = \frac{1}{2m^2c^2 r}\frac{dV}{dr}\vec{S} \bullet \vec{L}$$

- This is typically about 10^{-4} eV. This splitting is called fine structure.

Total Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

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- Due to the spin orbit interaction, L and S are not independent. The spin orbit interaction causes a coupling between L and S and a precession about the axes.
- The total angular momentum is fixed and quantized.
- The z component of total angular momentum is quantized.

Total Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

The total angular momentum in terms of quantum number j

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

The z component of angular momentum is

$$J_z = m_j \hbar$$

Where the quantum number m_j is

$$m_j = -j, \ldots 0 \ldots j$$

How does j relate to l and s?

$$\left|\vec{L}+\vec{S}\right| \geq \left|\vec{J}\right| \geq \left|\vec{L}-\vec{S}\right|$$

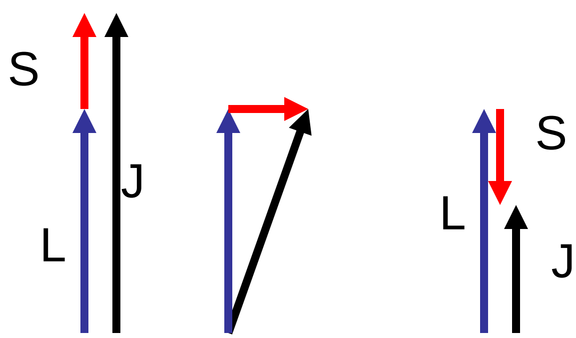
$$\sqrt{l(l+1)}+\sqrt{s(s+1)} \geq \sqrt{j(j+1)} \geq \sqrt{l(l+1)}-\sqrt{s(s+1)}$$

The result of this inequality is that j can have two values:

$$j = l+1/2, l-1/2$$

When l=0, then there is only one value of j:

$$j = 1/2$$



Hydrogen spectra

- The spectra of hydrogen show a fine structure which is well explained by Schroedinger’s equation with spin.
- There is also a hyperfine structure, which is due to the spin of the nucleus.

Identical Particles

- In classical physics, particles can be followed, and hence labels can be attached to each.

- In quantum physics, measurable results obtained from calculations should not depend on the assignment of labels to identical particles.

Example: Two identical particles in a box-no interaction between particles

x_1 The position of particle 1

x_2 The position of particle 2

$$V(x_1, x_2) = 0 \; for \;\; 0 < x_1, x_2 < L; \infty \;\; otherwise$$

$$[-\frac{\hbar^2}{2m}(\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}) + V(x_1, x_2)]\psi(x_1, x_2) = E\psi(x_1, x_2)$$

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This is separable since V depends on only one particle at a time.

$$\psi(x_1, x_2) = \psi_{n1}(x_1)\psi_{n2}(x_2)$$

This can be substituted into SE, and the solution is

$$\psi_{n1}(x_1) = A_1 \sin\frac{n_1 \pi x_1}{L}$$

$$\psi(x_1, x_2) = A_3 \sin\frac{n_1 \pi x_1}{L} \sin\frac{n_2 \pi x_2}{L}$$

But, this is not symmetric under exchange of 1→2

Example: Two identical particles in a box-no interaction between particles

$$\psi(x_1, x_2) = \psi_{n1}(x_1)\psi_{n2}(x_2)$$

This wavefunction is symmetric under exchange 1→2

$$\psi_S(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_{n1}(x_1)\psi_{n2}(x_2) + \psi_{n2}(x_1)\psi_{n1}(x_2))$$

This wavefunction changes sign under exchange, so $\psi*\psi$ is the same under exchange.

$$\psi_A(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_{n1}(x_1)\psi_{n2}(x_2) - \psi_{n2}(x_1)\psi_{n1}(x_2))$$

Pauli Exclusion Principle

- In a multielectron atom, there can never be more than one electron in the same quantum state.
- **Note that this is satisfied automatically by the antisymmetric state:**

$$\psi_{S\,n1n1}(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_{n1}(x_1)\psi_{n1}(x_2) + \psi_{n1}(x_1)\psi_{n1}(x_2)) = \sqrt{2}\psi_{n1}(x_1)\psi_{n1}(x_2)$$

$$\psi_{A\,n1n1}(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_{n1}(x_1)\psi_{n1}(x_2) - \psi_{n1}(x_1)\psi_{n1}(x_2)) = 0$$

- **A system containing several electrons must be described by an antisymmetric total eigenfunction.**

- Fermions: particles with half integral spin (1/2,3/2,…) such as electrons and protons. Fermions obey the Pauli exclusion principle and have antisymmetric wavefunctions.
- Bosons: particles with integral spin (0, 1,…) such as photons, They need not obey the Pauli Exclusion Principle and have symmetric wavefunctions.

How to include spin as a quantum number?

- Spatial variables (x,y,z) are continuous.
- Spin is discrete, either up or down (+1/2 or -1/2).
- Wave function is a product of the spatial wavefunction and the spin wavefunction.
- Antisymmetric wave function can be achieved by:
  - Antisymmetric spin wavefunction, symmetric space wavefunction
  - Symmetric spin wavefunction, antisymmetric space wavefunction

Spin wave functions

- Antisymmetric (singlet state)

$$\frac{1}{\sqrt{2}}(\left|1/2,-1/2\right\rangle - \left|-1/2,+1/2\right\rangle)$$

- Symmetric (triplet state)

$$\left|1/2,1/2\right\rangle$$

$$\frac{1}{\sqrt{2}}(\left|1/2,-1/2\right\rangle + \left|-1/2,1/2\right\rangle)$$

$$\left|-1/2,-1/2\right\rangle$$

Spatial Antisymmetric States

- Wavefunctions goes to zero at the symmetry point.
- Apparent repulsive force (exchange force)

Spatial Symmetric States

- Wavefunctions does not go to zero at the symmetry point.

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Spins aligned: Apparent repulsive force.
Spins opposite: No repulsive force.