Angular Momentum and Spin

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Lecture 26

Motivation from Lecture 10

- A magnetic dipole can have different origins. It can be
  - a current-carrying coil,
  - a permanent magnet,
  - a rotating sphere of charge, such as Earth, or
  - a subatomic particle.
- A complete description of magnetism needs quantum mechanics. In the classical picture, it suffices to model magnetic dipoles by current loops, which help explain some magnetic phenomena.

Motivation from Lecture 25

- According to the Bohr model for a hydrogen atom, the magnitude of the angular momentum $\vec{L}$ of the electron in its orbit is restricted (quantized) to the values

$$L = n\hbar, \text{ for } n = 1, 2, 3, \ldots.$$

- Is this true in Schroedinger's wave picture?
- Is a magnetic dipole momentum quantized? How is it quantized?

- The wave function of a particular quantum state of the hydrogen atom can be labeled by a set of quantum numbers (n, ℓ, m_ℓ).
  - The corresponding energy only depends on the **principal quantum number** $n = 1, 2, 3, \ldots$.
  - The **orbital quantum number** $\ell = 0, 1, 2, \ldots, n-1$ is a measure of the magnitude of the angular momentum of the quantum state. States with $\ell = 0$, 1, 2, 3 are called s, p, d, f.
  - The **orbital magnetic quantum number** $m_\ell = -\ell, -\ell+1, \ldots, \ell-1, \ell$ is related to the space orientation of this angular momentum vector.

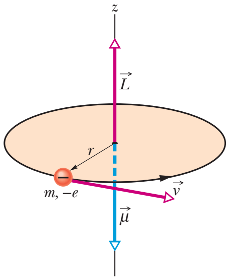
Outline

- Classical Loop Model for Electron Orbits
- Orbital Angular Momentum
- Spin Angular Momentum
- Magnetic Resonance
- Spin-Orbit Coupling

Classical Loop Model for Electron Orbits

- Consider an electron moving along a circular path of radius r at constant speed v. The orbital angular momentum of the electron is

$$L_{\mathrm{orb}} = mrv.$$



- The motion of the negative charge of the electron is equivalent to a current i:

$$i = \frac{\mathrm{charge}}{\mathrm{time}} = \frac{e}{2\pi r/v}.$$

- The magnitude of the orbital magnetic dipole moment of such a current loop is

$$\mu_{\rm orb} = i(\pi r^2) = \frac{evr}{2}.$$

In the vector formulation,

$$\vec{\mu}_{\rm orb} = -\frac{e}{2m}\vec{L}_{\rm orb} \equiv \gamma \vec{L}_{\rm orb}.$$

The minus sign means that $\vec{\mu}$ and $\vec{L}$ have opposite directions. It arises from the negative charge of the electron.

A Lesson from the Vector Notation

- The vector notation for angular momentum is

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

- Heuristically, $\Delta L_x \Delta L_y$ involves $\Delta z \Delta p_z$, therefore cannot vanish due to the uncertainty principle. In other words, one cannot simultaneously measure any two components of $\vec{L}$.
- However, one can simultaneously measure L^2 and L_z.

- In quantum mechanics,

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ -i\hbar\frac{\partial}{\partial x} & -i\hbar\frac{\partial}{\partial y} & -i\hbar\frac{\partial}{\partial z} \end{vmatrix}$$

- Explicitly,

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial \phi}.$$

- Note that $L_z R(r) = 0$. Now, calculate $L_z x$, $L_z y$, and $L_z z$, as well as other combinations.

Orbital Angular Momentum

- Every quantum state of an electron in an atom has an associated **orbital angular momentum** and **orbital magnetic dipole moment**.
- As in the hydrogen atom, the electron has
  - Orbital quantum number $\ell = 0, 1, 2, \ldots, n-1$ is a measure of the magnitude of the angular momentum of the quantum state. States with $\ell = 0$, 1, 2, 3 are called s, p, d, f.
  - Orbital magnetic quantum number $m_\ell = -\ell, -\ell+1, \ldots, \ell-1, \ell$ is related to the space orientation of this angular momentum vector.

- For example, the wave function in an s orbital ($\ell = m_\ell = 0$) is a radial function only.

$$\psi_{n00}(r, \theta, \phi) = f(r).$$

- One can show that

$$L^2\psi_{n00}(r, \theta, \phi) = \left(L_x^2 + L_y^2 + L_z^2\right)\psi_{n00}(r, \theta, \phi) = 0,$$

$$L_z\psi_{n00}(r, \theta, \phi) = 0.$$

- In the second example, the wave functions in p orbitals ($\ell = 1$) are

$$\begin{aligned} p_x + ip_y \ (m_\ell = 1): &\quad g(r)(x+iy) = \tilde{g}(r) \sin\theta e^{i\phi} \\ p_z \ (m_\ell = 0): &\quad g(r)z = \tilde{g}(r) \cos\theta \\ p_x - ip_y \ (m_\ell = -1): &\quad g(r)(x-iy) = \tilde{g}(r) \sin\theta e^{-i\phi} \end{aligned}$$

- One can show that

$$L^2\{p_x + ip_y, p_z, p_x - ip_y\} = 2\hbar^2\{p_x + ip_y, p_z, p_x - ip_y\},$$

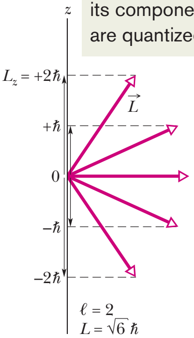
$$L_z\{p_x + ip_y, p_z, p_x - ip_y\} = \hbar\{p_x + ip_y, 0, -(p_x - ip_y)\}.$$

- Therefore, unlike a classical particle, the electron's orbital angular momentum $\vec{L}$ is quantized. The allowed magnitude is given by

$$L = \sqrt{\ell(\ell+1)}\hbar, \text{ for } \ell = 0, 1, 2, \ldots,$$

but its quantum nature does not permit a definite direction.

The vector and its component are quantized.

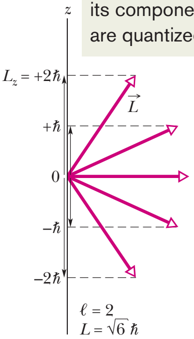


- We can measure definite values of a component L_z along a chosen measurement axis (usually taken to be a z axis) as given by

$$L_z = m_\ell \hbar, \text{ for } m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell.$$

- In general, if the electron has a definite value of L_z it may not have definite values of L_x and L_y. This is a manifestation of Heisenberg's uncertainty principle.

The vector and its component are quantized.



- Therefore, the orbital magnetic dipole moment is also quantized:

$$\mu_{\rm orb} = |\gamma| L = \frac{e}{2m}\sqrt{\ell(\ell+1)}\hbar,$$

$$\mu_{\rm orb,z} = \gamma L_z = -m_\ell \frac{e\hbar}{2m} = -m_\ell \mu_B,$$

where we define the **Bohr magneton**

$$\mu_B = \frac{eh}{4\pi m} = \frac{e\hbar}{2m} = 9.274 \times 10^{-24}\ \mathrm{J/T}.$$

Dynamics in a Uniform Magnetic Field

- Let us recall (from Lecture 8 and 10) that an external magnetic field $\vec{B}$ will rotate a magnetic dipole moment $\vec{\mu}$ with a total torque

$$\vec{\tau} = \vec{\mu} \times \vec{B},$$

or, for an electron with orbital angular momentum $\vec{L}$,

$$\vec{\tau} = \frac{d\vec{L}}{dt} = \gamma \vec{L} \times \vec{B}.$$

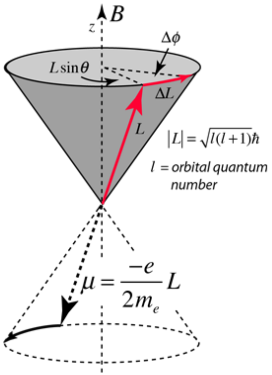
- Since $\vec{L} \times \vec{B}$ is always perpendicular to $\vec{L}$ and $\vec{B}$, the tip of $\vec{L}$ moves in a circle around $\vec{B}$, or processes at a frequency (**Larmor frequency**)

$$\vec{\omega} = -\gamma \vec{B},$$

such that

$$\frac{d\vec{L}}{dt} = \vec{\omega} \times \vec{L}.$$

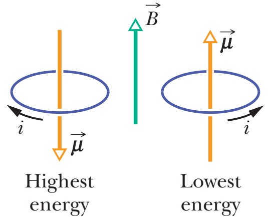
- This is called **Larmor precession**.



- In the quantum mechanical description of the dipole, it is preferable to summarize the interaction between the moment and the magnetic field in terms of the potential energy associated with the torque

$$U_B = -\vec{\mu} \cdot \vec{B} = -\mu B \cos\theta.$$

The magnetic moment vector attempts to align with the magnetic field.



- As we expect, the potential energy is minimized when the dipole moment and the magnetic field are parallel.

Dipole in a Nonuniform Magnetic Field

- The interaction between a nonuniform magnetic field $\vec{B}(z) = B(z)\hat{z}$ and a magnetic dipole $\vec{\mu}$ is

$$U = -\vec{\mu} \cdot \vec{B}(z) = -\mu_z B(z).$$

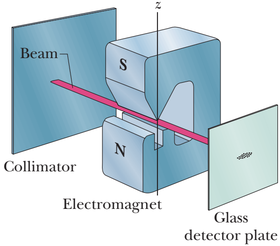
- The force along the z axis is, then,

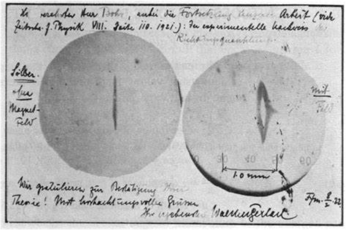
$$F_z = -\frac{dU}{dz} = \mu_z \frac{dB}{dz},$$

as long as the dipole moment μ_z does not change with z.

The Stern-Gerlach Experiment (1922)

- In the Stern-Gerlach experiment, a narrow beam of silver atoms passes through an electromagnet (with a nonuniform magnetic field) and then lands on a glass detector plate.

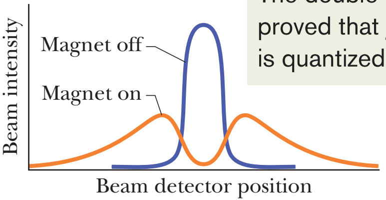




- When the electromagnet was turned on, Stern and Gerlach found that the silver atoms formed two distinct spots on the glass plate.

- If the magnetic moment is a classical vector with a given length μ, the z-component μ_z can be anywhere between $-\mu$ to $+\mu$. One expects to observe a vertical spread of silver on the glass plate, with a maximum in the center.

- However, Stern and Gerlach observed two spots of silver, instead. Therefore, classical physics cannot be right.



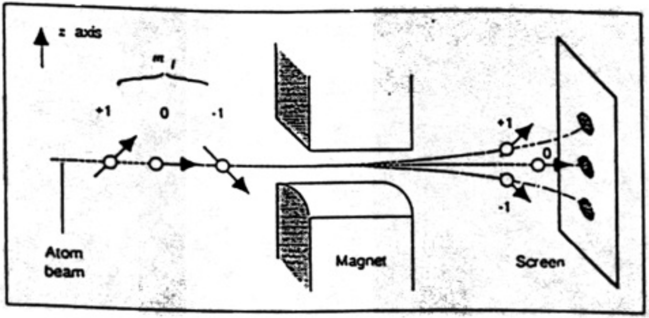
The double peak proved that μ_z is quantized.

In Old Quantum Theory

- In the old quantum theory by Bohr (and Sommerfeld) an atom in a state with angular momentum equal to one ($L = 1$) would have a magnetic moment with two components relative to the direction of the magnetic field.
- In this case the spot on the receiving plate will therefore be split into two, each of them having the same size but half the intensity of the original spot.
- The Stern-Gerlach result seemed to confirm the prediction of spatial quantization. Stern sent a postcard to Bohr: "We congratulate you on the confirmation of your theory." But, there is a serious problem, hence, a challenge.

In (Then) New Quantum Theory

- The later, or new, quantum theory developed by Heisenberg, Schroedinger, and others, predicted that for an $L = 1$ state the beam should split into three components.



- In fact, we now know that a silver atom consists of many electrons ([Kr]$4\mathrm{d}^{10}5\mathrm{s}^{1}$).
- We also know that all those magnetic moments vectorially cancel out except for a single electron (5s^1), and the orbital dipole moment of that electron is *zero*.
- Therefore, the Stern-Gerlach result posed a serious problem for the new quantum theory.
- This was solved when Uhlenbeck and Goudsmit (1925, 1926) proposed that the electron had an intrinsic angular momentum, not associated with its orbital motion.

Spin

- The Stern-Gerlach experiment belongs to a class of quantum phenomena involving a quantum degree of freedom called **spin**, which has no classical counterpart.
- Fortunately, one can describe spin and its dynamics without appealing to any mechanical model (such as that of a spinning top), starting with just the observed fact that it is a form of angular momentum.

Electron Spin

- Every electron, whether trapped in an atom or free, has a **spin angular momentum** and a **spin magnetic dipole moment** that are as intrinsic as its mass and charge.
- The existence of electron spin was postulated on experimental evidence by George Uhlenbeck and Samuel Goudsmit from their studies of atomic spectra.
- For every electron, spin $s = 1/2$ and the electron is said to be a spin-1/2 particle. (Protons and neutrons are also spin-1/2 particles.)

- As with the angular momentum associated with motion, spin angular momentum can have a definite magnitude but does not have a definite direction.
- The best we can do is to measure its component along the z axis (or along any axis), and that component can have only the definite values given by

$$S_z = m_s \hbar, \text{ for } m_s = \pm s = \pm 1/2.$$

- Here m_s is the *spin magnetic quantum number*, which can have only two values: $m_s = +s = +1/2$ (the electron is said to be **spin up**) and $m_s = -s = -1/2$ (the electron is said to be **spin down**).

- The electron is not spinning; the theoretical basis for spin was provided by Paul Dirac, who developed a relativistic quantum theory of the electron.
- As with the orbital angular momentum, a magnetic dipole moment is associated with the spin angular momentum. Let us write

$$\vec{\mu}_s = g\gamma\vec{S},$$

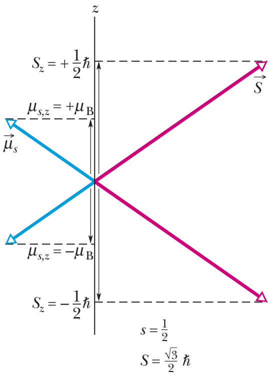
where $\gamma = -e/(2m)$ and the constant g is referred to as the g-factor.
- It turns out that the spin angular momentum generates a magnetic moment twice as large as the orbital angular momentum does, i.e. $g = 2$.

- Therefore, the spin magnetic dipole moment is also quantized:

$$\mu_s = g|\gamma|S = \frac{e}{m}\sqrt{s(s+1)}\hbar,$$

$$\mu_{s,z} = -g m_s \mu_B,$$

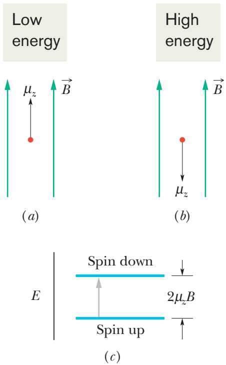
where $g = 2$ is used.



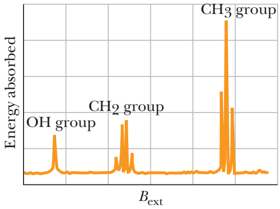
- In fact, there is a small correction in quantum electrodynamics corresponding to $g = 2.00232$. But for most purposes, it is sufficient to use $g = 2$.

Nuclear Spin and Magnetic Resonance

- A hydrogen ion (proton) has a spin magnetic dipole moment $\vec{\mu}$ that is associated with the proton's intrinsic spin angular momentum $\vec{S}$.
- In a magnetic field $\vec{B} = B\hat{z}$, $\vec{\mu}$ has two possible quantized components along that axis with different energy (the Zeeman effect).
- A proton can *flip* its spin from up to down by absorbing a photon with energy
$$\hbar\omega = \Delta E = 2\mu_z B.$$



- Such absorption is called **magnetic resonance** or, as originally, **nuclear magnetic resonance (NMR)**.
- In practice, the photons required for magnetic resonance have an associated frequency in the radio-frequency (RF) range.
- NMR is usually detected by sweeping the magnitude B_{ext} through a range of values while the frequency ω of the RF source is kept at a predetermined value and the energy loss of the RF source is monitored.

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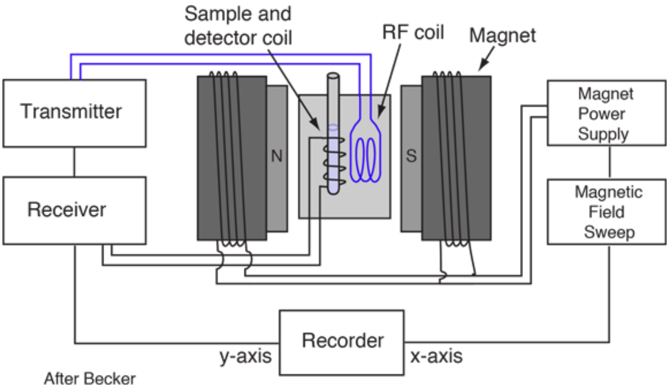
- Proton NMR, which studies the precession of the proton spin in the magnetic field, is a practical medical imaging technique.
  - A strong magnetic field produces partial polarization of the protons (hydrogen nuclei) in a human body.
  - A strong RF field is also imposed to excite some of the nuclear spins into their higher energy state.
  - When this strong RF signal is switched off, the spins tend to return to their lower state, producing a small amount of radiation at the Larmor frequency associated with that field.
  - The emission of radiation is associated with the "spin relaxation" of the protons from their excited state.
  - It induces a radio frequency (RF) signal in a detector coil which is amplified to display the NMR signal.



- Since the Larmor frequency depends on the applied magnetic field, placing a magnetic field gradient across the human body allows you to locate the source of the MRI signal (hence the name *Magnetic Resonance Imaging*).

Spin-Orbit Coupling

- So far, the spin has played a rather trivial role. It is decoupled from the orbital motion of electrons.
- This is not true in reality, where we know spin plays an important role
  - in the behavior of electronic devices at low temperatures, and
  - in generating the nontrivial band structures in topological insulators.
- However, the spin-orbit interaction is difficult to derive classically. Crudely speaking, to the electron the nucleus appears to rotate around it and the moving nuclear charge or current creates a magnetic field $B^* \propto L$.

- The spin–orbit interaction Hamiltonian is given by

$$H_{\mathrm{SO}} = \xi_{n\ell} \vec{L} \cdot \vec{S},$$

where the **spin-orbit coupling constant** $\xi_{n\ell}$, which is positive, is essentially the averaged gradient of the Coulomb interaction.

- To solve the Hamiltonian with such an interaction, we need to introduce the total angular momentum $\vec{J} = \vec{L} + \vec{S}$ and and use the expression

$$\vec{J} \cdot \vec{J} = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S}) = \vec{S} \cdot \vec{S} + 2\vec{L} \cdot \vec{S} + \vec{L} \cdot \vec{L}.$$

Summary

- Understand orbital and spin angular momentum, in particular the quantized values of the magnitude of angular momentum, the z component, the magnitude of the magnetic moment and its z component.
- Understand Stern-Gerlach experiment and its application in measuring spin components.
- Understand the working principle of nuclear magnetic resonance.

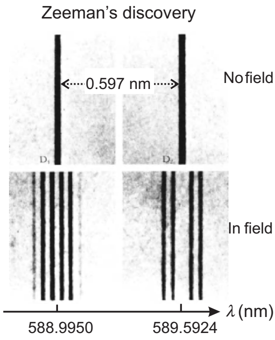
Reading

Halliday, Resnick & Krane:

- Chapter 48: Properties of Atoms

Appendix 26A: The Emission Spectrum of Na

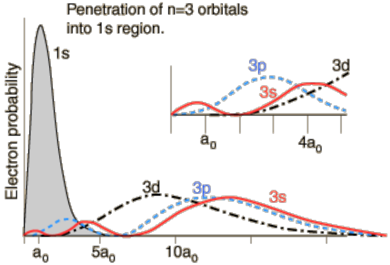
- Pieter Zeeman examined the emission spectrum of a flame that contained sodium (Na). In the absence of a magnetic field the Na spectrum consists of a bright spin–orbit split doublet in the yellow part of the spectrum, the so-called Na D-lines at 588.9950 and 589.5924 nm wavelength.



- Zeeman (1896) discovered that the doublet splits into a characteristic pattern in the presence of a magnetic field.

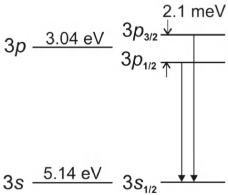
- A full explanation has several ingredients, including the spin-orbit interaction and the Zeeman interaction.
- First of all, the strong yellow emission line of Na is due to an electronic transition from the first excited $3p$ state to the $3s$ ground state. Why are they not degenerate as in a hydrogen atom?

- The sodium $3s$ level is significantly lower than the $3p$ because of greater penetration past the shielding of the $1s$ electron.
- What causes fine structure?



Spin-Orbit Coupling in Sodium

- Both $3s$ and $3p$ levels penetrate enough to be significantly lower than the $n = 3$ hydrogen energy ($E_R/3^2 \approx 1.5$ eV) which they would have if the shielding were perfect.



- The **spin-orbit coupling**, which is a relativistic effect, in sodium lifts the degeneracy of $3p$ orbit by creating two states $3p_j$ with $j = 1 \pm 1/2$.
- Crudely speaking, to the electron the nucleus appears to rotate around it and the moving nuclear charge or current creates a magnetic field $B^* \propto L$.

- The spin–orbit interaction Hamiltonian is given by

$$H_{\mathrm{SO}} = \xi_{n\ell} \vec{L} \cdot \vec{S},$$

where the **spin-orbit coupling constant** $\xi_{n\ell}$, which is positive, is essentially the averaged gradient of the Coulomb interaction. Now, can you extract the value of $\xi_{n\ell}$ for the sodium $3p$ orbit?

- The energy of these two states are obtained by writing $\vec{J} = \vec{L} + \vec{S}$ and using the expression

$$\vec{J} \cdot \vec{J} = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S}) = \vec{S} \cdot \vec{S} + 2\vec{L} \cdot \vec{S} + \vec{L} \cdot \vec{L}$$

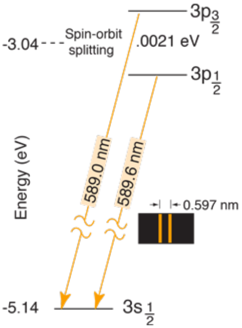
to rewrite the spin–orbit Hamiltonian.

- Notice $S^2 = s(s+1) = 3/4$ and $L^2 = l(l+1) = 2$.
- For $j = 3/2$, $J^2 = j(j+1) = 15/4$.

$$\vec{L} \cdot \vec{S} = (J^2 - S^2 - L^2)/2 = 1/2.$$

- For $j = 1/2$, $J^2 = j(j+1) = 3/4$.

$$\vec{L} \cdot \vec{S} = -1.$$



- Therefore, the energy difference of the $3p_{3/2}$ and $3p_{1/2}$ states is $3\xi_{n\ell}/2 = 2.1$ meV. Hence, $\xi_{n\ell} = 1.4$ meV.

- The further splits are due to the Zeeman interaction between a magnetic dipole and an external magnetic field, as well as the corresponding *selection rules*.