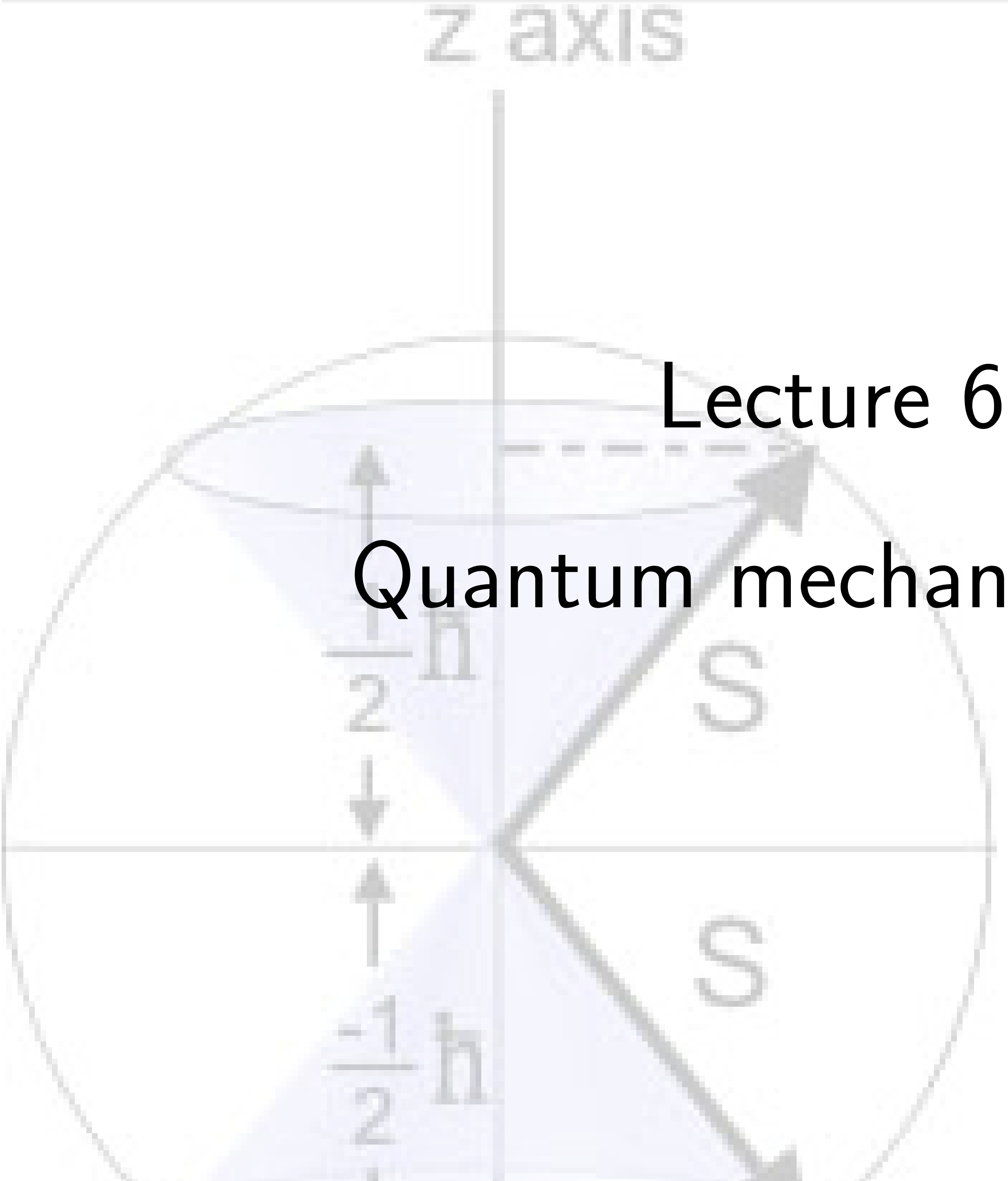
Lecture 6

Quantum mechanical spin



Background

- Until now, we have focused on quantum mechanics of particles which are "featureless" – carrying no internal degrees of freedom.
- A relativistic formulation of quantum mechanics (due to Dirac and covered later in course) reveals that quantum particles can exhibit an intrinsic angular momentum component known as spin.
- However, the discovery of quantum mechanical spin predates its theoretical understanding, and appeared as a result of an ingeneous experiment due to Stern and Gerlach.

Spin: outline

1. Stern-Gerlach and the discovery of spin
2. Spinors, spin operators, and Pauli matrices
3. Spin precession in a magnetic field
4. Paramagnetic resonance and NMR

Background: expectations pre-Stern-Gerlach

- Previously, we have seen that an electron bound to a proton carries an orbital magnetic moment,

$$\boxed{\boldsymbol{\mu} = -\frac{e}{2m_e}\hat{\mathbf{L}} \equiv -\mu_{\mathrm{B}}\hat{\mathbf{L}}/\hbar, \qquad H_{\mathrm{int}} = -\boldsymbol{\mu}\cdot\mathbf{B}}$$

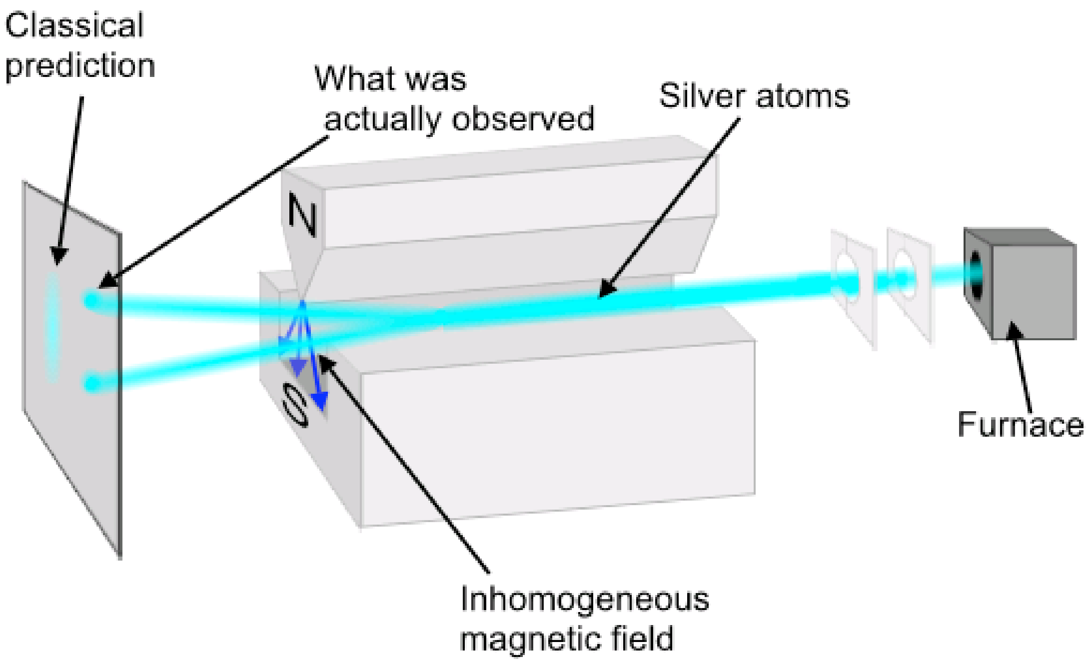
- For the azimuthal component of the wavefunction, $e^{im\phi}$, to remain single-valued, we further require that the angular momentum ℓ takes only integer values (recall that $-\ell \leq m \leq \ell$).
- When a beam of atoms are passed through an inhomogeneous (but aligned) magnetic field, where they experience a force,

$$\boxed{\mathbf{F} = \nabla(\boldsymbol{\mu}\cdot\mathbf{B}) \simeq \mu_z(\partial_z B_z)\hat{\mathbf{e}}_z}$$

we expect a splitting into an **odd integer** $(2\ell+1)$ number of beams.

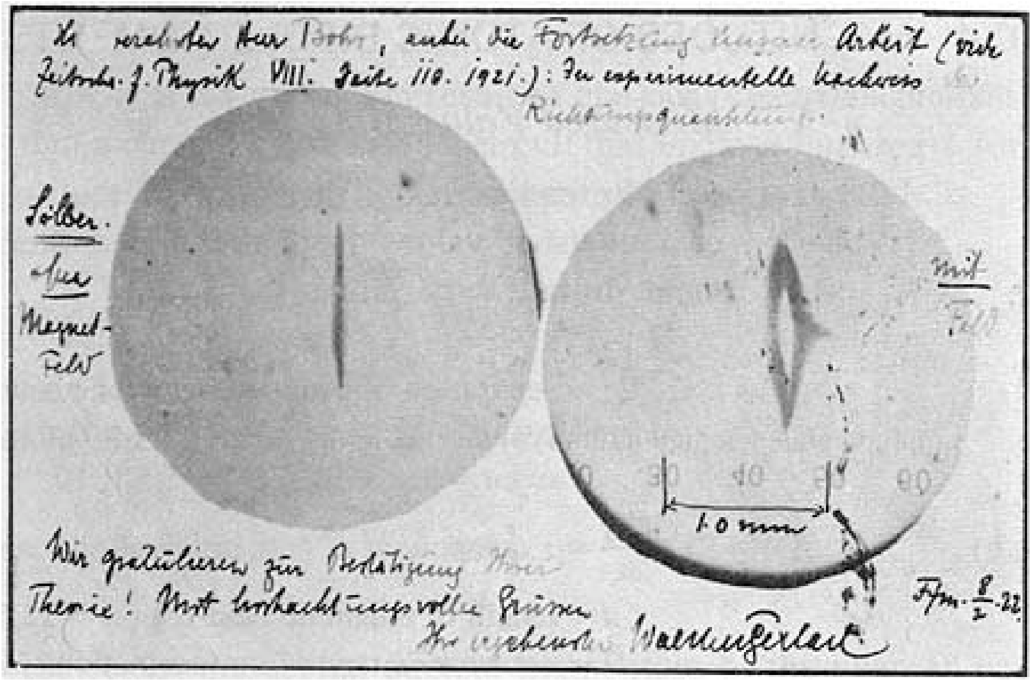
Stern-Gerlach experiment

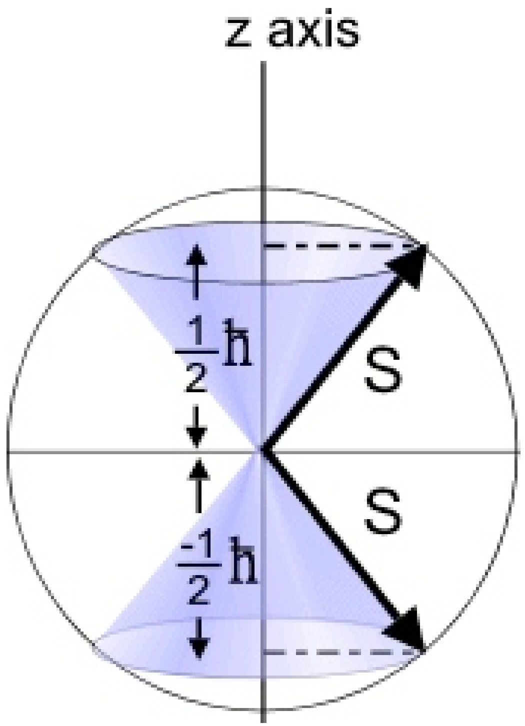
- In experiment, a beam of silver atoms were passed through inhomogeneous magnetic field and collected on photographic plate.
- Since silver involves spherically symmetric charge distribution plus one $5s$ electron, total angular momentum of ground state has $L = 0$.
- If outer electron in $5p$ state, $L = 1$ and the beam should split in 3.



Stern-Gerlach experiment

- However, experiment showed a bifurcation of beam!





Gerlach's postcard, dated 8th February 1922, to Niels Bohr

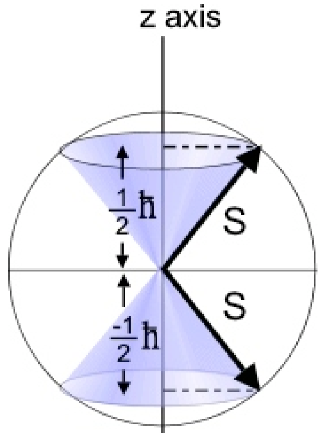
- Since orbital angular momentum can take only integer values, this observation suggests electron possesses an additional intrinsic "$\ell = 1/2$" component known as **spin**.

Quantum mechanical spin

- Later, it was understood that elementary quantum particles can be divided into two classes, **fermions** and **bosons**.
- Fermions (e.g. electron, proton, neutron) possess half-integer spin.
- Bosons (e.g. mesons, photon) possess integral spin (including zero).

Spinors

- Space of angular momentum states for spin $s = 1/2$ is two-dimensional:



$$\boxed{|s = 1/2, m_s = 1/2\rangle = |\uparrow\rangle, \qquad |1/2, -1/2\rangle = |\downarrow\rangle}$$

- General **spinor** state of spin can be written as linear combination,

$$\alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \qquad |\alpha|^2 + |\beta|^2 = 1$$

- Operators acting on spinors are 2×2 matrices. From definition of spinor, z-component of spin represented as,

$$\boxed{S_z = \frac{1}{2}\hbar\sigma_z, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

i.e. S_z has eigenvalues $\pm\hbar/2$ corresponding to $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Spin operators and Pauli matrices

- From general formulae for raising/lowering operators,

$$\hat{J}_+|j,m\rangle = \sqrt{j(j+1)-m(m+1)}\hbar\,|j,m+1\rangle,$$
$$\hat{J}_-|j,m\rangle = \sqrt{j(j+1)-m(m-1)}\hbar\,|j,m-1\rangle$$

with $S_\pm = S_x \pm iS_y$ and $s = 1/2$, we have

$$S_+|1/2,-1/2\rangle = \hbar|1/2,1/2\rangle, \qquad S_-|1/2,1/2\rangle = \hbar|1/2,-1/2\rangle$$

- i.e., in matrix form,

$$S_x + iS_y = S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad S_x - iS_y = S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

- Leads to **Pauli matrix** representation for spin $1/2$, $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Pauli spin matrices are Hermitian, traceless, and obey defining relations (cf. general angular momentum operators):

$$\sigma_i^2 = \mathbb{I}, \qquad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

- Total spin

$$\mathbf{S}^2 = \frac{1}{4}\hbar^2\boldsymbol{\sigma}^2 = \frac{1}{4}\hbar^2\sum_i \sigma_i^2 = \frac{3}{4}\hbar^2\,\mathbb{I} = \frac{1}{2}(\frac{1}{2}+1)\hbar^2\,\mathbb{I}$$

i.e. $s(s+1)\hbar^2$, as expected for spin $s = 1/2$.

Spatial degrees of freedom and spin

- Spin represents additional internal degree of freedom, independent of spatial degrees of freedom, i.e. $[\hat{\mathbf{S}}, \mathbf{x}] = [\hat{\mathbf{S}}, \hat{\mathbf{p}}] = [\hat{\mathbf{S}}, \hat{\mathbf{L}}] = 0$.
- Total state is constructed from **direct product**,

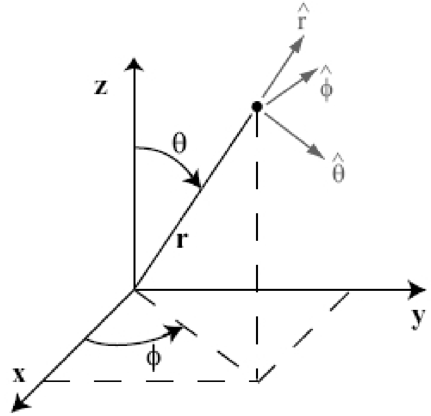
$$\boxed{|\psi\rangle = \int d^3x \, (\psi_+(\mathbf{x})|\mathbf{x}\rangle \otimes |\uparrow\rangle + \psi_-(\mathbf{x})|\mathbf{x}\rangle \otimes |\downarrow\rangle) \equiv \begin{pmatrix} |\psi_+\rangle \\ |\psi_-\rangle \end{pmatrix}}$$

- In a weak magnetic field, the electron Hamiltonian can then be written as

$$\boxed{\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(r) + \mu_{\mathrm{B}} \left(\hat{\mathbf{L}}/\hbar + \boldsymbol{\sigma} \right) \cdot \mathbf{B}}$$

Relating spinor to spin direction

For a general state $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$, how do α, β relate to orientation of spin?



- Let us assume that spin is pointing along the unit vector $\hat{\mathbf{n}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, i.e. in direction (θ, φ).
- Spin must be eigenstate of $\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ with eigenvalue unity, i.e.

$$\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

- With normalization, $|\alpha|^2 + |\beta|^2 = 1$, (up to arbitrary phase),

$$\boxed{\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}}$$

Spin symmetry

$$\boxed{\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}}$$

- Note that under 2π rotation,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \mapsto -\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

- In order to make a transformation that returns spin to starting point, necessary to make two complete revolutions, (cf. spin 1 which requires 2π and spin 2 which requires only π!).

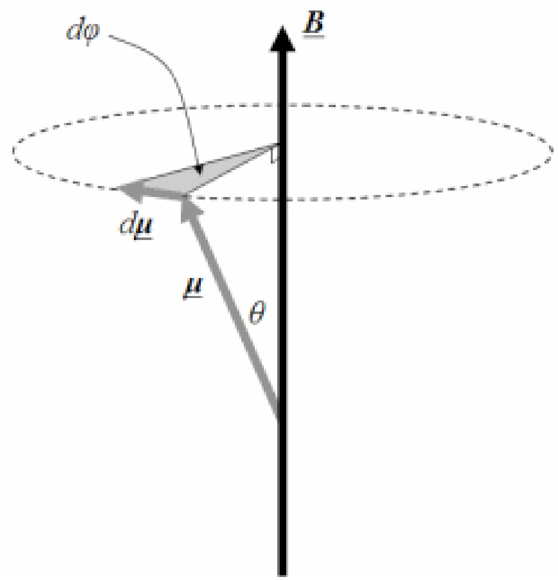
(Classical) spin precession in a magnetic field

Consider magnetized object spinning about centre of mass, with angular momentum $\mathbf{L}$ and magnetic moment $\boldsymbol{\mu} = \gamma \mathbf{L}$ with γ gyromagnetic ratio.

- A magnetic field $\mathbf{B}$ will then impose a torque

$$\boxed{\mathbf{T} = \boldsymbol{\mu} \times \mathbf{B} = \gamma \mathbf{L} \times \mathbf{B} = \partial_t \mathbf{L}}$$

- With $\mathbf{B} = B\hat{\mathbf{e}}_z$, and $L_+ = L_x + iL_y$, $\partial_t L_+ = -i\gamma B L_+$, with the solution $L_+ = L_+^0 e^{-i\gamma Bt}$ while $\partial_t L_z = 0$.



  - Angular momentum vector $\mathbf{L}$ precesses about magnetic field direction with angular velocity $\boldsymbol{\omega}_0 = -\gamma \mathbf{B}$ (independent of angle).
  - We will now show that precisely the same result appears in the study of the quantum mechanics of an electron spin in a magnetic field.

(Quantum) spin precession in a magnetic field

- Last lecture, we saw that the electron had a magnetic moment, $\boldsymbol{\mu}_{\text{orbit}} = -\frac{e}{2m_e}\hat{\mathbf{L}}$, due to orbital degrees of freedom.
- The intrinsic electron spin imparts an additional contribution, $\boldsymbol{\mu}_{\text{spin}} = \gamma\hat{\mathbf{S}}$, where the **gyromagnetic ratio**,

$$\boxed{\gamma = -g\frac{e}{2m_e}}$$

  and g (known as the **Landé g-factor**) is very close to 2.
- These components combine to give the total magnetic moment,

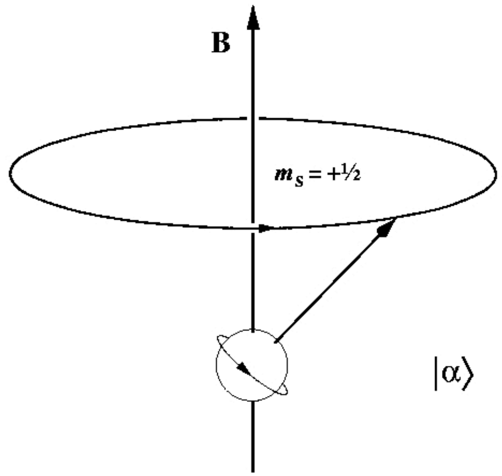
$$\boxed{\boldsymbol{\mu} = -\frac{e}{2m_e}(\hat{\mathbf{L}} + g\hat{\mathbf{S}})}$$

- In a magnetic field, the interaction of the dipole moment is given by

$$\boxed{\hat{H}_{\text{int}} = -\boldsymbol{\mu}\cdot\mathbf{B}}$$

(Quantum) spin precession in a magnetic field

- Focusing on the spin contribution alone,



$$\boxed{\hat{H}_{\rm int} = -\gamma\hat{\mathbf{S}}\cdot\mathbf{B} = -\frac{\gamma}{2}\hbar\boldsymbol{\sigma}\cdot\mathbf{B}}$$

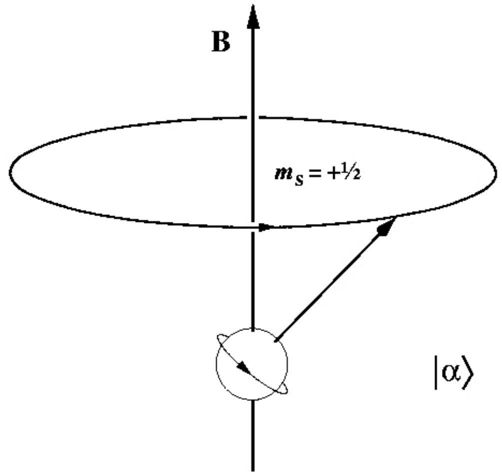
- The spin dynamics can then be inferred from the time-evolution operator, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$, where

$$\boxed{\hat{U}(t) = e^{-i\hat{H}_{\rm int}t/\hbar} = \exp\left[\frac{i}{2}\gamma\boldsymbol{\sigma}\cdot\mathbf{B}t\right]}$$

- However, we have seen that the operator $\hat{U}(\theta) = \exp[-\frac{i}{\hbar}\theta\hat{\mathbf{e}}_n\cdot\hat{\mathbf{L}}]$ generates spatial rotations by an angle θ about $\hat{\mathbf{e}}_n$.
- In the same way, $\hat{U}(t)$ effects a spin rotation by an angle $-\gamma Bt$ about the direction of $\mathbf{B}$!

(Quantum) spin precession in a magnetic field

$$\boxed{\hat{U}(t) = e^{-i\hat{H}_{\rm int}t/\hbar} = \exp\left[\frac{i}{2}\gamma\boldsymbol{\sigma}\cdot\mathbf{B}t\right]}$$



- Therefore, for initial spin configuration,

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2)\\ e^{i\varphi/2}\sin(\theta/2)\end{pmatrix}$$

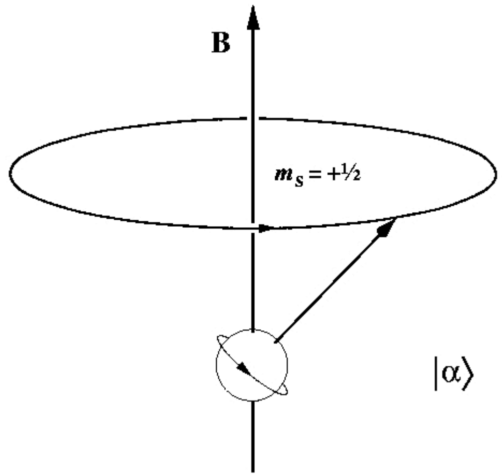
- With $\mathbf{B} = B\hat{\mathbf{e}}_z$, $\hat{U}(t) = \exp[\frac{i}{2}\gamma Bt\sigma_z]$, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$,

$$\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} = \begin{pmatrix} e^{-\frac{i}{2}\omega_0 t} & 0\\ 0 & e^{\frac{i}{2}\omega_0 t}\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix} e^{-\frac{i}{2}(\varphi+\omega_0 t)}\cos(\theta/2)\\ e^{\frac{i}{2}(\varphi+\omega_0 t)}\sin(\theta/2)\end{pmatrix}$$

- i.e. spin precesses with angular frequency $\boldsymbol{\omega}_0 = -\gamma\mathbf{B} = -g\omega_c\hat{\mathbf{e}}_z$, where $\omega_c = \frac{eB}{2m_e}$ is **cyclotron frequency**, $(\frac{\omega_c}{B} \simeq 10^{11}\,\mathrm{rad\,s^{-1}T^{-1}})$.

Paramagnetic resonance

- This result shows that spin precession frequency is independent of spin orientation.
- Consider a frame of reference which is itself rotating with angular velocity $\boldsymbol{\omega}$ about $\hat{\mathbf{e}}_z$.

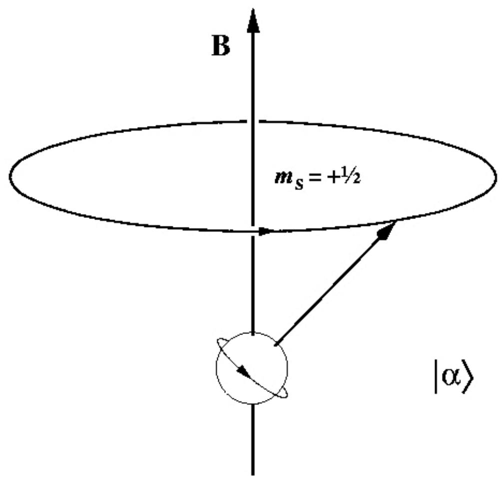


- If we impose a magnetic field $\mathbf{B}_0 = B_0\hat{\mathbf{e}}_z$, in the rotating frame, the observed precession frequency is $\boldsymbol{\omega}_r = -\gamma(\mathbf{B}_0 + \boldsymbol{\omega}/\gamma)$, i.e. an effective field $\mathbf{B}_r = \mathbf{B}_0 + \boldsymbol{\omega}/\gamma$ acts in rotating frame.
- If frame rotates exactly at precession frequency, $\boldsymbol{\omega} = \boldsymbol{\omega}_0 = -\gamma\mathbf{B}_0$, spins pointing in any direction will remain at rest in that frame.
- Suppose we now add a small additional component of the magnetic field which is rotating with angular frequency $\boldsymbol{\omega}$ in the xy plane,

$$\boxed{\mathbf{B} = B_0\hat{\mathbf{e}}_z + B_1(\hat{\mathbf{e}}_x \cos(\omega t) - \hat{\mathbf{e}}_y \sin(\omega t))}$$

Paramagnetic resonance

$$\boxed{\mathbf{B} = B_0\hat{\mathbf{e}}_z + B_1(\hat{\mathbf{e}}_x \cos(\omega t) - \hat{\mathbf{e}}_y \sin(\omega t))}$$



- Effective magnetic field in a frame rotating with same frequency ω as the small added field is $\mathbf{B}_r = (B_0 + \omega/\gamma)\hat{\mathbf{e}}_z + B_1\hat{\mathbf{e}}_x$
- If we tune ω so that it exactly matches the precession frequency in the original magnetic field, $\boldsymbol{\omega} = \boldsymbol{\omega}_0 = -\gamma\mathbf{B}_0$, in the rotating frame, the magnetic moment will only see the small field in the x-direction.
- Spin will therefore precess about x-direction at slow angular frequency γB_1 – matching of small field rotation frequency with large field spin precession frequency is **"resonance"**.

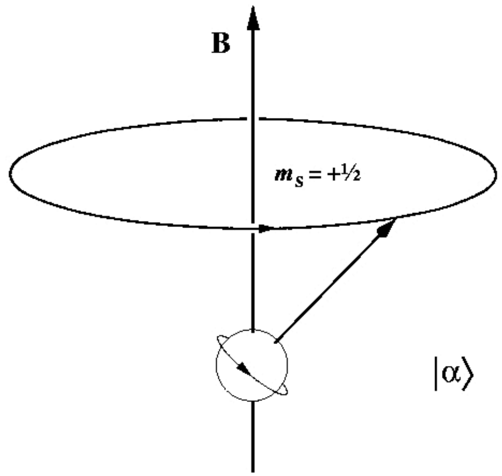
Nuclear magnetic resonance

- The general principles exemplified by paramagnetic resonance underpin methodology of **Nuclear magnetic resonance (NMR)**.
- NMR principally used to determine structure of molecules in chemistry and biology, and for studying condensed matter in solid or liquid state.
- Method relies on nuclear magnetic moment of atomic nucleus,

$$\boxed{\boldsymbol{\mu} = \gamma \hat{\mathbf{S}}}$$

e.g. for proton $\gamma = g_P \frac{e}{2m_p}$ where $g_p = 5.59$.

Nuclear magnetic resonance



- In uniform field, $\mathbf{B}_0$, nuclear spins occupy equilibrium thermal distibution with

$$\boxed{\frac{P_\uparrow}{P_\downarrow} = \exp\left[\frac{\hbar\omega_0}{k_\mathrm{B} T}\right], \qquad \omega_0 = \gamma B_0}$$

i.e. (typically small) population imbalance.

- Application of additional oscillating resonant in-plane magnetic field $\mathbf{B}_1(t)$ for a time, t, such that

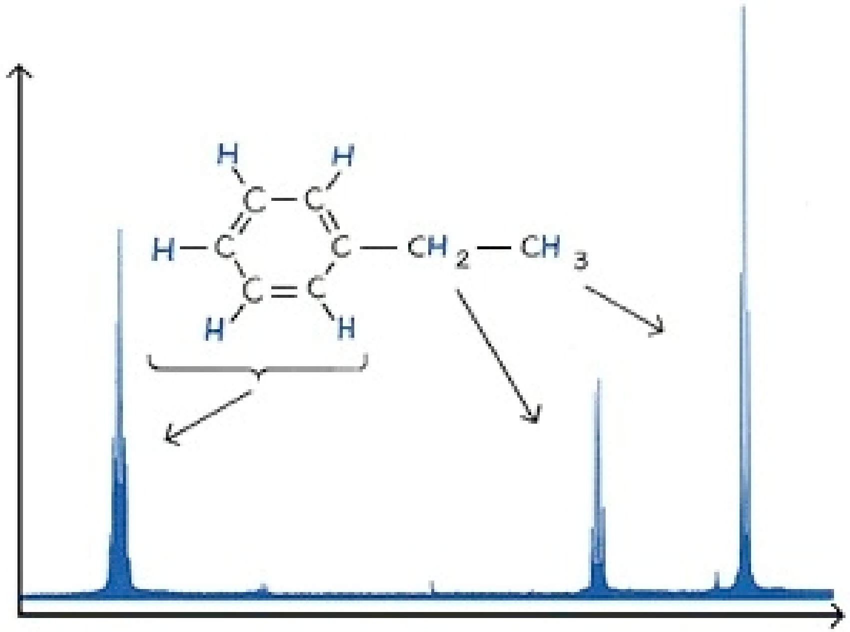
$$\boxed{\omega_1 t = \frac{\pi}{2}, \qquad \omega_1 = \gamma B_1}$$

(“$\pi/2$ pulse”) orients majority spin in xy-plane where it precesses at resonant frequency allowing a coil to detect a.c. signal from induced e.m.f.

- Return to equilibrium set by transverse relaxation time, T_2.

Nuclear magnetic resonance

- Resonance frequency depends on nucleus (through γ) and is slightly modified by environment $\rightsquigarrow$ splitting.



- In **magnetic resonance imaging (MRI)**, focus is on proton in water and fats. By using non-uniform field, $\mathbf{B}_0$, resonance frequency can be made position dependent – allows spatial structures to be recovered.

Summary: quantum mechanical spin

- In addition to orbital angular momentum, $\hat{\mathbf{L}}$, quantum particles possess an intrinsic angular momentum known as spin, $\hat{\mathbf{S}}$.
- For fermions, spin is half-integer while, for bosons, it is integer.
- Wavefunction of electron expressed as a two-component spinor,

$$\boxed{|\psi\rangle = \int d^3x \left(\psi_+(\mathbf{x})|\mathbf{x}\rangle \otimes |\uparrow\rangle + \psi_-(\mathbf{x})|\mathbf{x}\rangle \otimes |\downarrow\rangle\right) \equiv \begin{pmatrix} |\psi_+\rangle \\ |\psi_-\rangle \end{pmatrix}}$$

- In a weak magnetic field,

$$\boxed{\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(r) + \mu_{\mathrm{B}}\left(\hat{\mathbf{L}}/\hbar + \frac{g}{2}\boldsymbol{\sigma}\right) \cdot \mathbf{B}}$$

- Spin precession in a uniform field provides basis of paramagnetic resonance and NMR.