Lecture 5: continued

- But what happens when **free** (i.e. unbound) charged particles experience a magnetic field which influences orbital motion?

e.g. electrons in a metal.

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{x}, t))^2 + q\varphi(\mathbf{x}, t), \qquad q = -e$$

- In this case, classical orbits can be macroscopic in extent, and there is no reason to neglect the diamagnetic contribution.
- Here it is convenient (but not essential – see PS1) to adopt **Landau gauge**, $\mathbf{A}(\mathbf{x}) = (-By, 0, 0)$, $\mathbf{B} = \nabla \times \mathbf{A} = B\hat{\mathbf{e}}_z$, where

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Free electrons in a magnetic field: Landau levels

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Free electrons in a magnetic field: Landau levels

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$$\left[\frac{\hat{p}_y{}^2}{2m} + \frac{1}{2}m\omega^2(y - y_0)^2\right]\chi(y) = \left(E - \frac{p_z^2}{2m}\right)\chi(y)$$

where $y_0 = \frac{p_x}{eB}$ and $\omega = \frac{eB}{m}$ is classical **cyclotron frequency**

- p_x defines centre of harmonic oscillator in y with frequency ω, i.e.

$$E_{n,p_z} = (n + 1/2)\hbar\omega + \frac{p_z^2}{2m}$$

- The quantum numbers, n, index infinite set of **Landau levels**.

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- Taking $p_z = 0$ (for simplicity), for lowest Landau level, $n = 0$, $E_0 = \frac{\hbar\omega}{2}$; what is level degeneracy?

- Consider periodic rectangular geometry of area $A = L_x \times L_y$. Centre of oscillator wavefunction, $y_0 = \frac{p_x}{eB}$, lies in $[0, L_y]$.
- With periodic boundary conditions $e^{ip_x L_x/\hbar} = 1$, $p_x = 2\pi n \frac{\hbar}{L_x}$, i.e. y_0 set by evenly-spaced discrete values separated by $\Delta y_0 = \frac{\Delta p_x}{eB} = \frac{h}{eBL_x}$.
- $\therefore$ degeneracy of lowest Landau level $N = \frac{L_y}{|\Delta y_0|} = \frac{L_y}{h/eBL_x} = \frac{BA}{\Phi_0}$, where $\Phi_0 = \frac{e}{h}$ denotes **"flux quantum"**, ($\frac{N}{BA} \simeq 10^{14}\,\mathrm{m}^{-2}\mathrm{T}^{-1}$).

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Quantum Hall effect

The existence of Landau levels leads to the remarkable phenomenon of the Quantum Hall Effect, discovered in 1980 by von Kiltzing, Dorda and Pepper (formerly of the Cavendish).

- **Classically**, in a crossed electric $\mathbf{E} = \mathcal{E}\hat{\mathbf{e}}_y$ and magnetic field $\mathbf{B} = B\hat{\mathbf{e}}_z$, electron drifts in direction $\hat{\mathbf{e}}_x$ with speed $v = \mathcal{E}/B$.

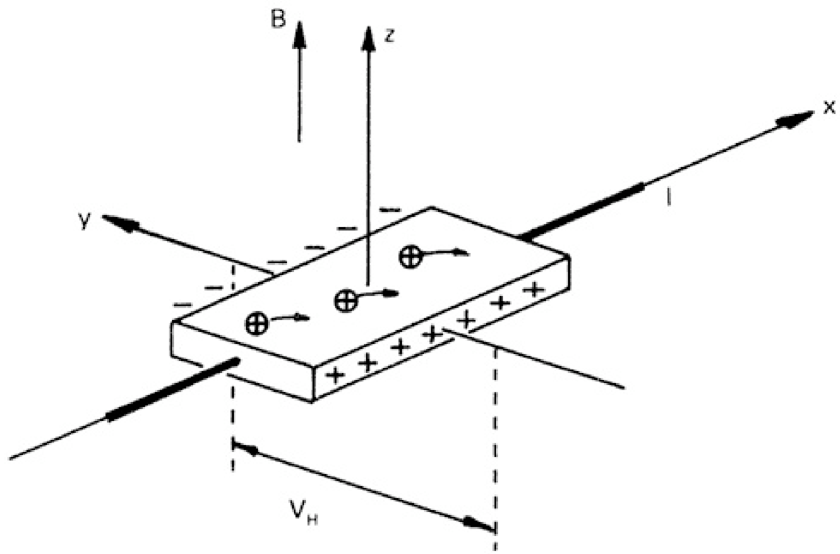
$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

- With current density $j_x = -nev$, Hall resistivity,

$$\rho_{xy} = -\frac{E_y}{j_x} = \frac{\mathcal{E}}{nev} = \frac{B}{en}$$

where n is charge density.

Experiment: linear increase in ρ_{xy} with B punctuated by plateaus at which $\rho_{xx} = 0$ – dissipationless flow!



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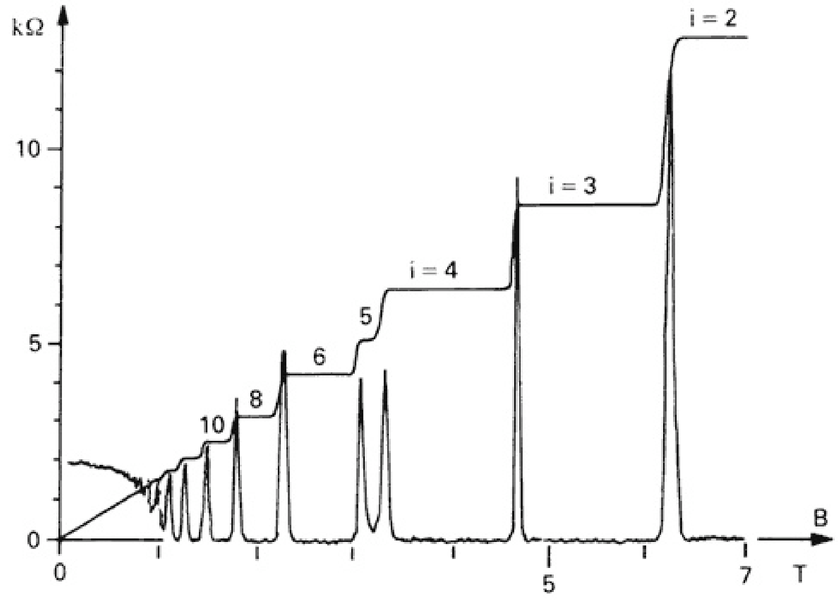

Quantum Hall Effect

- Origin of phenomenon lies in Landau level quantization: For a state of the lowest Landau level,

$$\psi_{p_x}(y) = \frac{e^{ip_x x/\hbar}}{\sqrt{L_x}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}(y-y_0)^2}$$

current $j_x = \frac{1}{2m}(\psi^*(\hat{p}_x + eA_x)\psi + \psi((\hat{p}_x + eA_x)\psi)^*)$, i.e.

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is non-vanishing. (Note that current operator also gauge invariant.)

- However, if we compute total current along x by integrating along y, sum vanishes, $I_x = \int_0^{L_y} dy\, j_x(y) = 0$.

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- If electric field now imposed along y, $-e\varphi(y) = -e\mathcal{E}y$, symmetry is broken; but wavefunction still harmonic oscillator-like,

$$\left[\frac{\hat{p}_y{}^2}{2m} + \frac{1}{2}m\omega^2(y - y_0)^2 - e\mathcal{E}y\right]\chi(y) = E\chi(y)$$

but now centered around $y_0 = \frac{p_x}{eB} + \frac{m\mathcal{E}}{eB^2}$.

- However, the current is still given by

$$j_x(y) = \sqrt{\frac{m\omega}{\pi\hbar}}\frac{1}{L_x}e^{-\frac{m\omega}{\hbar}(y-y_0)^2}$$

- Integrating, we now obtain a non-vanishing current flow

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- To obtain total current flow from all electrons, we must multiply I_x by the total number of occupied states.
- If Fermi energy lies between two Landau levels with n occupied,

$$I_{\rm tot} = nN \times I_x = -n\frac{eB}{h}L_xL_y \times \frac{e\mathcal{E}}{BL_x} = -n\frac{e^2}{h}\mathcal{E}L_y$$

- With $V = -\mathcal{E}L_y$, voltage drop across y, **Hall conductance** (equal to conductivity in two-dimensions),

$$\sigma_{\rm xy} = -\frac{I_{\rm tot}}{V} = n\frac{e^2}{h}$$

- Since no current flow in direction of applied field, longitudinal conductivity σ_{yy} vanishes.

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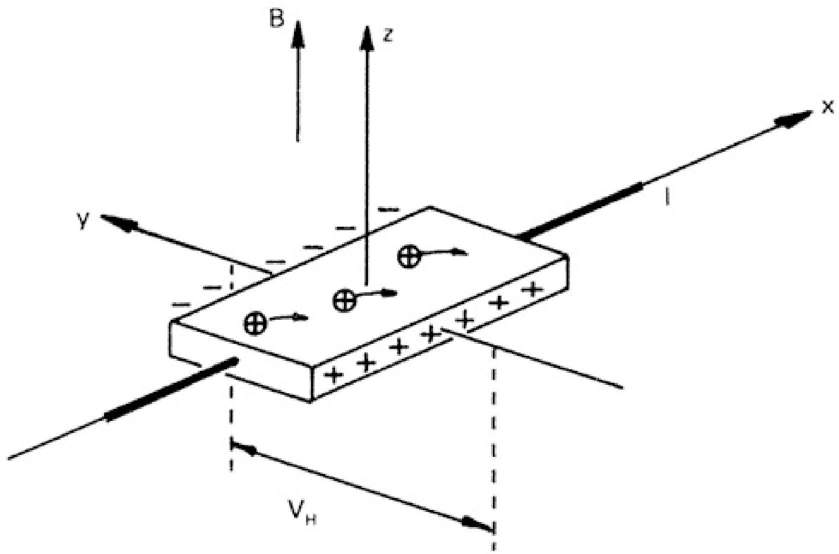
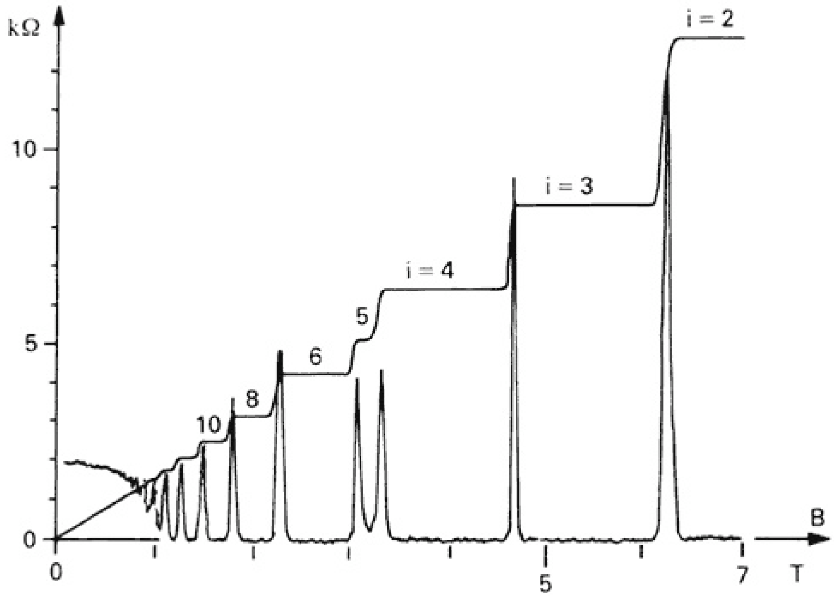
Quantum Hall Effect

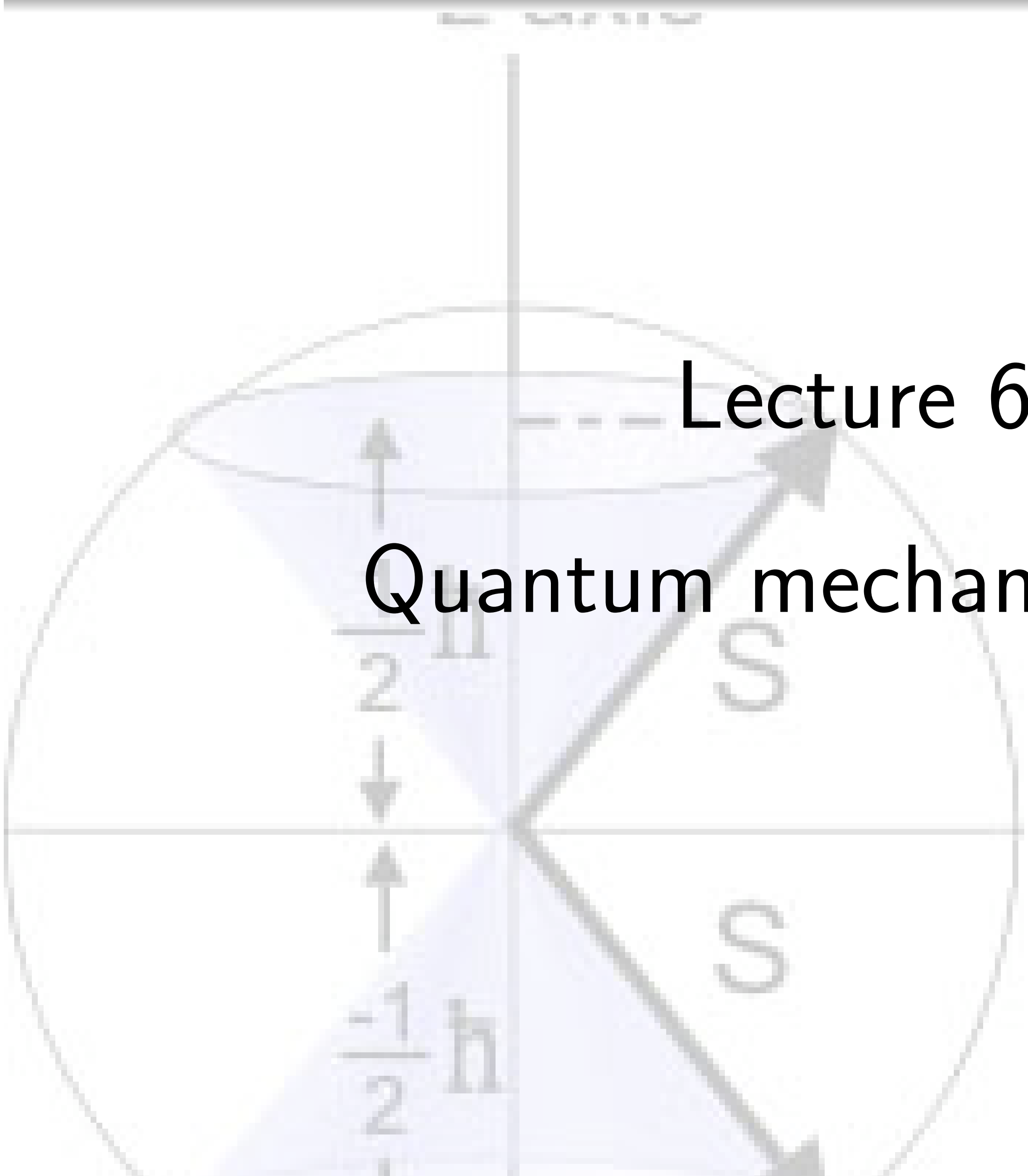
- Since there is no potential drop in the direction of current flow, the longitudinal resistivity ρ_{xx} also vanishes, while

$$\rho_{yx} = \frac{1}{n}\frac{h}{e^2}$$

- Experimental measurements of these values provides the best determination of fundamental ratio e^2/h, better than 1 part in 10^8.







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,

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

- 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,

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

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

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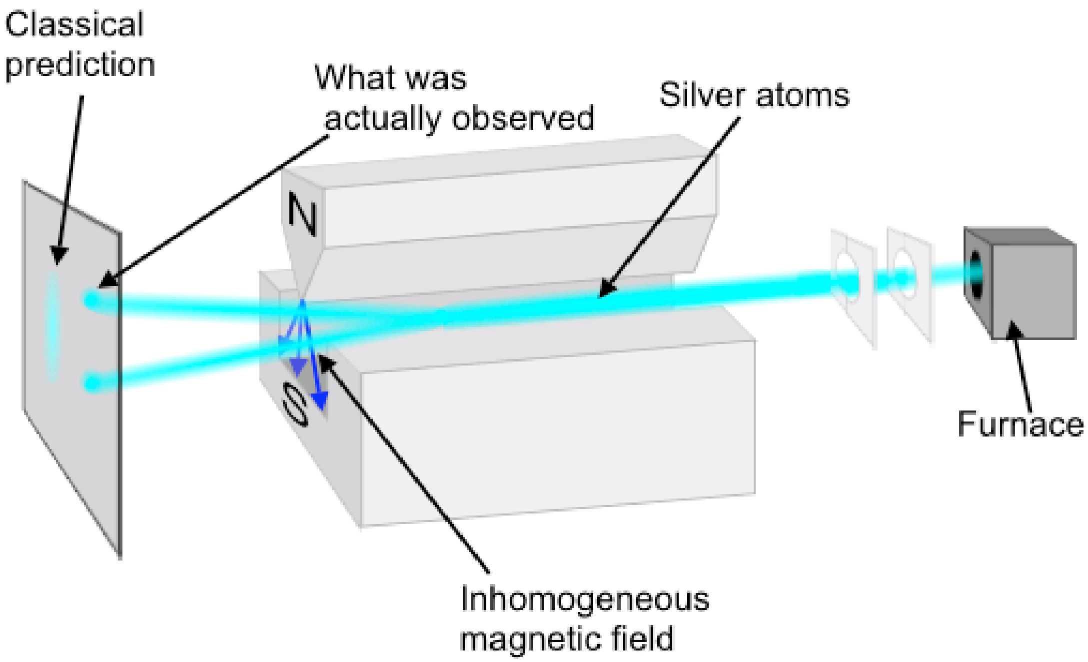
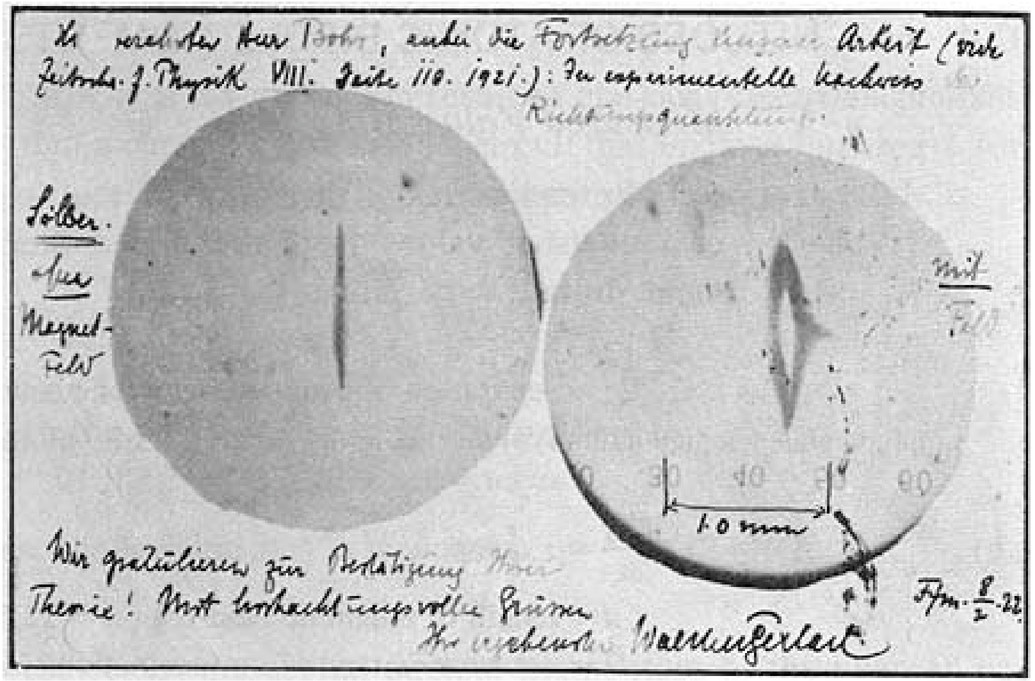
Stern-Gerlach experiment

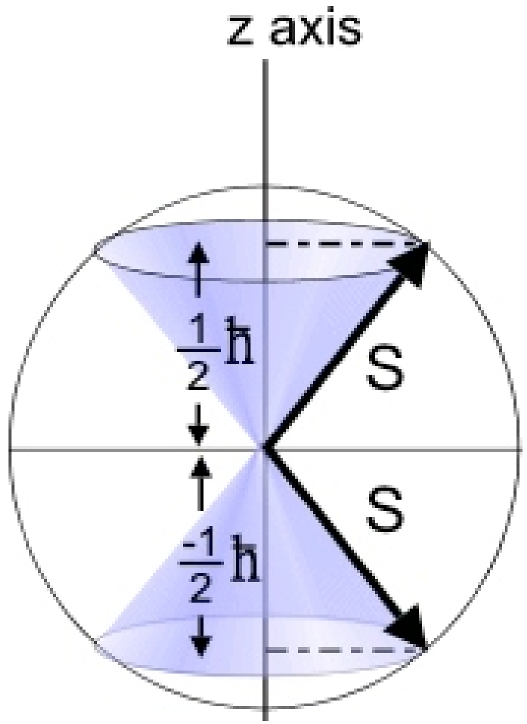
- In experiment, a beam of silver atoms were passed through inhomogeneous magnetic field and collected on photographic plate.
- Since silver involves spherically symmetric charge distribution plus one 5s electron, total angular momentum of ground state has $L = 0$.
- If outer electron in 5p state, $L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



Stern-Gerlach experiment

- However, experiment showed a bifurcation of beam!





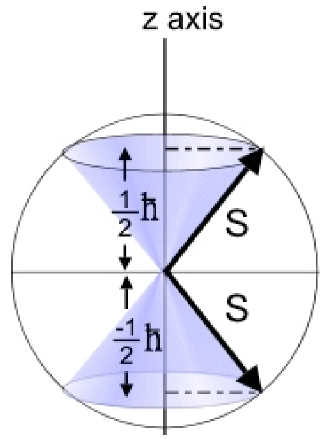
Gerlach's postcard, dated 8th February 1922, to Niels Bohr

- 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:

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

- 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,

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

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

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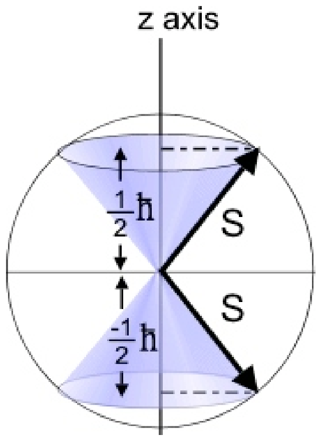

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Spin operators and Pauli matrices

- 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, $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$

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

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- 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, $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$

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

Spin operators and Pauli matrices

- From general formulae for raising/lowering operators,

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

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

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

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

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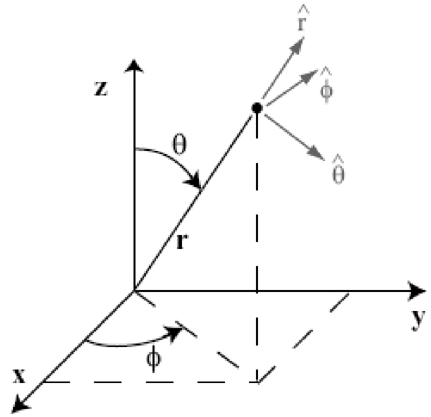
Relating spinor to spin direction



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.

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

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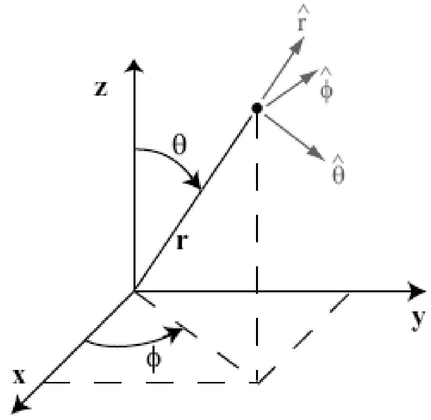

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Spin symmetry

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

- 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!).

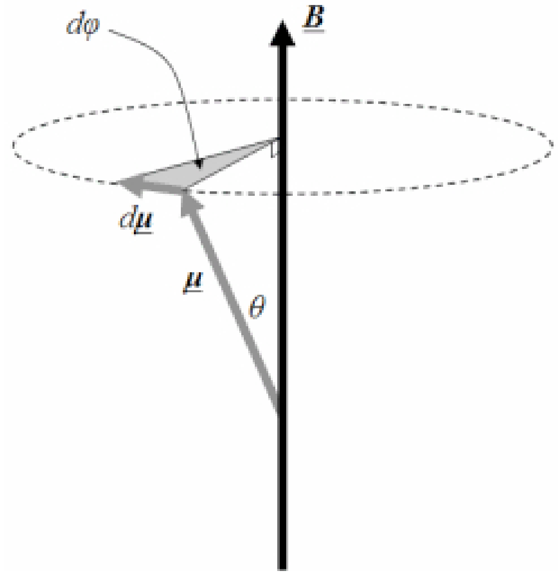
(Classical) spin precession in a magnetic field

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

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

- 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 $\omega_0 = -\gamma \mathbf{B}$ (independent of angle).
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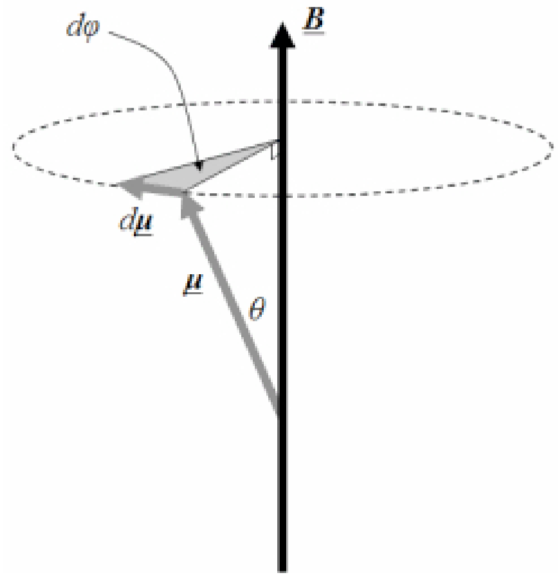

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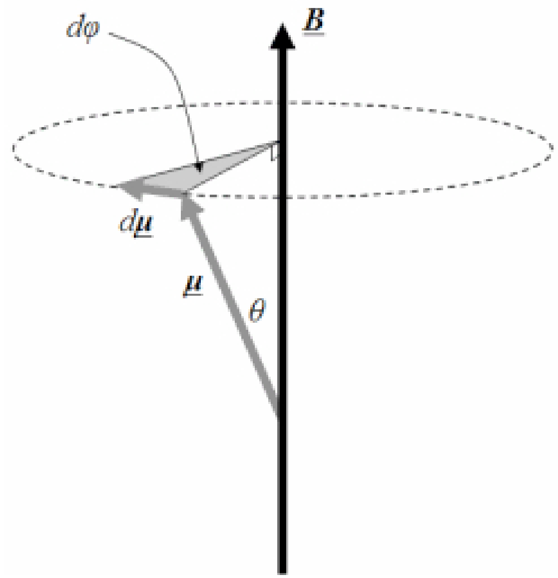

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(Quantum) spin precession in a magnetic field

- 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**,

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

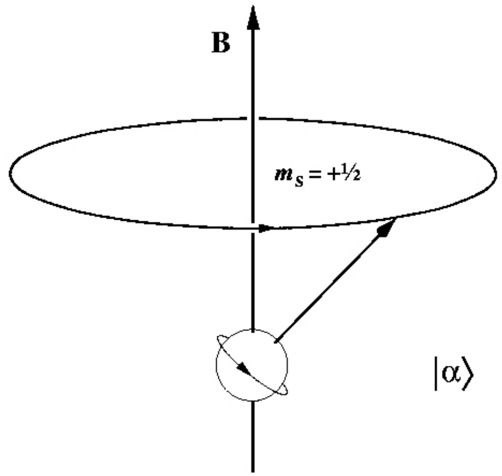
  and g (known as the **Landé g-factor**) is very close to 2.
- These components combine to give the total magnetic moment,

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

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

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

(Quantum) spin precession in a magnetic field



- Focusing on the spin contribution alone,

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

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

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

- 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 $-\gamma B t$ about the direction of $\mathbf{B}$!

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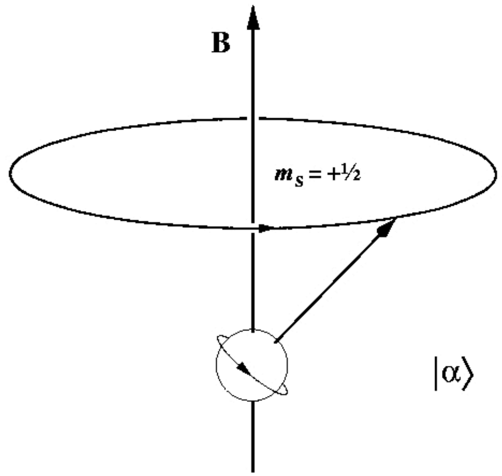

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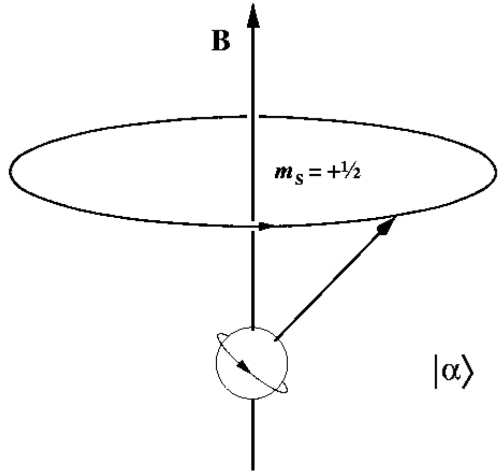


- Therefore, for initial spin configuration,

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

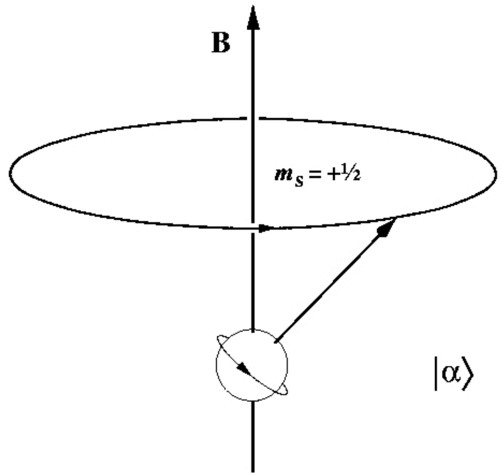
- With $\mathbf{B} = B\hat{\mathbf{e}}_z$, $\hat{U}(t) = \exp[\frac{i}{2}\gamma Bt\sigma_z]$, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$,

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

- 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**, ($\frac{\omega_c}{B} \simeq 10^{11}\,\text{rad}\,\text{s}^{-1}\text{T}^{-1}$).

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 ω in the xy plane,

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

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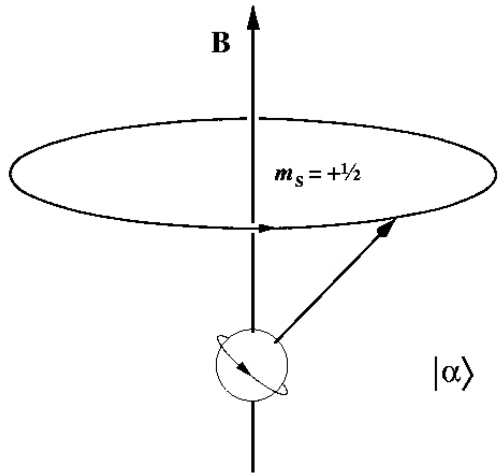

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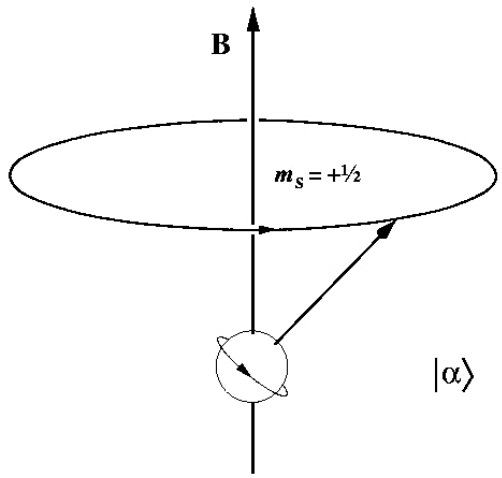

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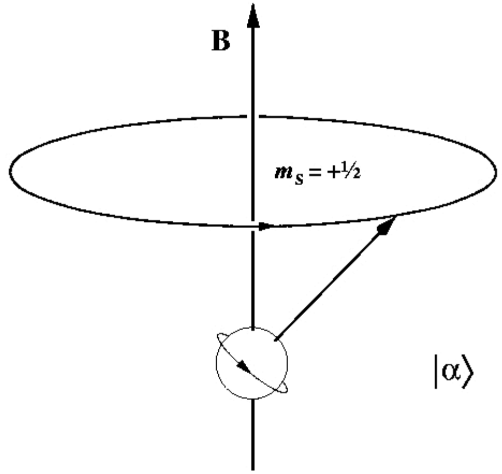

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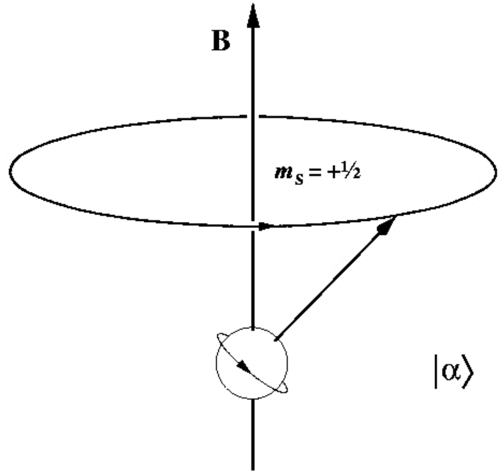

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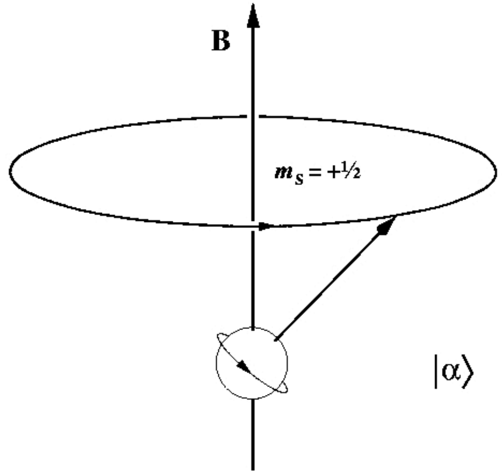

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Nuclear magnetic resonance

- 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,

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

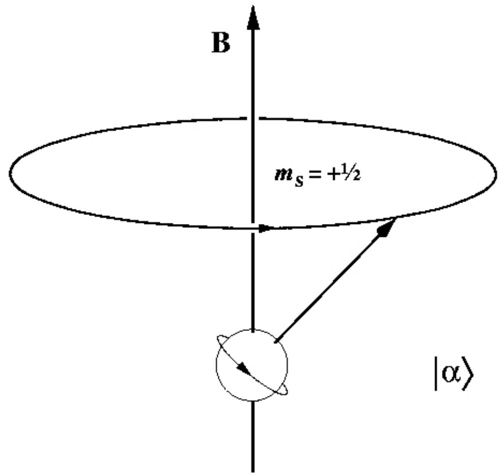
e.g. for proton $\gamma = g_P \frac{e}{2m_p}$ where $g_p = 5.59$.

Nuclear magnetic resonance

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

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

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

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

("$\pi/2$ 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.

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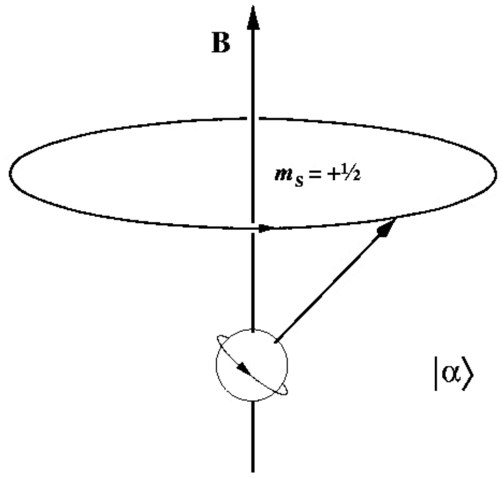

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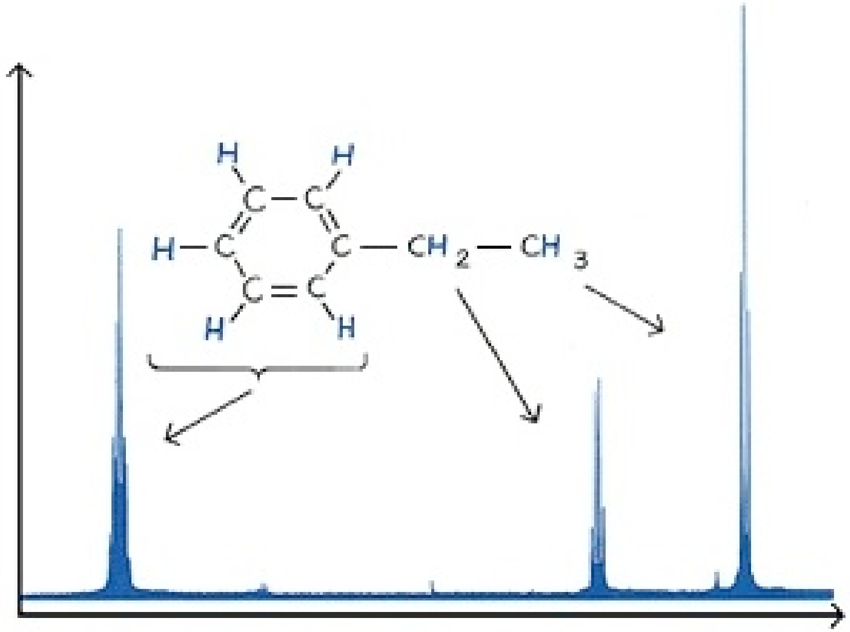

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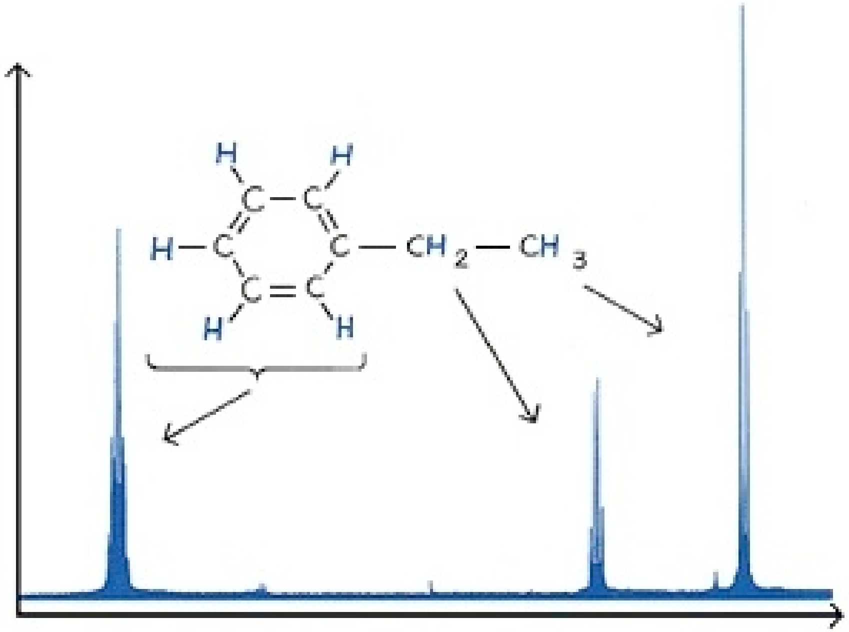

- In **magnetic resonance imaging (MRI)**, focus is on proton in water and fats. By using non-uniform field, $\mathbf{B}_0$, resonance frequency can be made position dependent – allows spatial structures to be recovered.

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,

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

- In a weak magnetic field,

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

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