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Intrinsic Spin of an Electron

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References

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Angular Momentum

In Cartesian coordinates the three components of the angular momentum vector $\vec{L}$ are

$$L_x = yp_z - zp_y,$$
$$L_y = zp_x - xp_z,$$
$$L_z = xp_y - yp_x.$$

The corresponding quantum mechanical operators have

$$[L_x, L_y] = i\hbar L_z,$$
$$[L_y, L_z] = i\hbar L_x,$$
$$[L_z, L_x] = i\hbar L_y,$$

so only one component of $\vec{L}$ can be diagonal in any given basis set. If

$$L^2 = L_x^2 + L_y^2 + L_z^2,$$

then

$$0 = [L_x, L^2] = [L_y, L^2] = [L_z, L^2].$$

Thus a basis set can simultaneously diagonalize one *component* of $\vec{L}$ and L^2. Let $\Psi_{\lambda\mu}$ be a basis set with

$$L^2\Psi_{\lambda\mu} = \lambda\Psi_{\lambda\mu},$$
$$L_z\Psi_{\lambda\mu} = \mu\Psi_{\lambda\mu}.$$

If

$$\Phi = (L_x \pm iL_y)\Psi_{\lambda\mu},$$

The spin of the electron

Dirac constructed a relativistic theory for the electron in 1932. To do so, however, he had to replace Schrödinger's wave function with a *spinor* field, i.e.,

$$\psi(r) \rightarrow \psi = \begin{bmatrix} \psi_1(r) \\ \psi_2(r) \\ \psi_3(r) \\ \psi_4(r) \end{bmatrix}.$$

The matrix index corresponds to a discrete observable with no classical analogue. A two component spinor provides a good representation of the states in the non-relativistic limit and the discrete observable corresponds to the electronic spin.

If $\ell = 1/2$, there are just two possible 'spin' states. To construct a non-relativistic matrix representation for the states, we introduce two basis vectors,

$$\alpha = \Psi_{\frac{1}{2},\frac{1}{2}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$
$$\beta = \Psi_{\frac{1}{2},-\frac{1}{2}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

In the $\{\alpha, \beta\}$ basis set,

$$L_z = \frac{1}{2}\hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{1a}$$

If $c\alpha = L_+\beta$,

$$|c^2| = \langle L_+\beta | L_+\beta \rangle = \langle \beta | L_- L_+ \beta \rangle$$
$$= \langle \beta | (L^2 - L_z^2 - \hbar L_z)\beta \rangle = \hbar^2$$

Choose the relative phases of α and β so that $c = \hbar$. Then $L_+\beta = \hbar\alpha$, or

$$L_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

L_- is just the Hermitian conjugate of L_+,

$$L_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

Thus

$$L_x = \frac{1}{2}(L_+ + L_-) = \frac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{1b}$$
$$L_y = \frac{1}{2i}(L_+ - L_-) = \frac{1}{2}\hbar \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}. \tag{1c}$$

These matrices (1a-c) are the Pauli spin matrices.

Proton magnetic resonance spectroscopy

Associated with the intrinsic spin ($\ell = \frac{1}{2}$) of a proton is a magnetic moment $\boldsymbol{\mu}$. For the proton

$$\boldsymbol{\mu} = \gamma \boldsymbol{L},$$

with the gyromagnetic ratio

$$\begin{aligned}\gamma =& 2.67519 \times 10^8 \text{ rad } s^{-1}T^{-1} \\ =& 1.52103 \times 10^{-20} \quad \text{atomic units.}\end{aligned}$$

The interaction of this magnetic moment with a magnetic field $\boldsymbol{B}$ is governed by the Zeeman Hamiltonian

$$\hat{H} = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\gamma \boldsymbol{L} \cdot \boldsymbol{B} = -\gamma \hat{\boldsymbol{s}} \cdot \boldsymbol{B},$$

with $\hat{\boldsymbol{s}} = \hat{s}_x \boldsymbol{i} + \hat{s}_y \boldsymbol{j} + \hat{s}_z \boldsymbol{k}$, a vector operator with the Pauli spin matrices (1a-c) for components.

For a constant field $\boldsymbol{B}$ the solution to the dynamical equation is

$$\psi(t) = e^{i\gamma \boldsymbol{B}\cdot\hat{\boldsymbol{s}}t/\hbar}\psi(0). \tag{2}$$

Now a rotation by an angle $\delta\phi$ about an axis $\hat{\boldsymbol{n}}$ (a unit vector) moves points

$$\boldsymbol{r} \rightarrow \boldsymbol{r} + \delta\phi\, \hat{\boldsymbol{n}} \times \boldsymbol{r}$$

and transforms functions

$$\psi(\boldsymbol{r}) \rightarrow \psi(\boldsymbol{r} - \delta\phi\, \hat{\boldsymbol{n}} \times \boldsymbol{r}).$$

For small $\delta\phi$,

$$\begin{aligned}\psi(\boldsymbol{r}) &\rightarrow \psi(\boldsymbol{r}) - \delta\phi\, \hat{\boldsymbol{n}} \times \boldsymbol{r} \cdot \nabla\psi(\boldsymbol{r}) \\ &= \psi(\boldsymbol{r}) - \delta\phi\, \hat{\boldsymbol{n}} \cdot \boldsymbol{r} \times \nabla\psi(\boldsymbol{r}) \\ &= \psi(\boldsymbol{r}) - \frac{i}{\hbar}\delta\phi\, \hat{\boldsymbol{n}} \cdot \boldsymbol{r} \times \hat{\boldsymbol{p}}\, \psi(\boldsymbol{r})\end{aligned}$$

Thus

$$\frac{d\psi(\boldsymbol{r})}{d\phi} = -\frac{i}{\hbar}\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{L}}\psi(\boldsymbol{r})$$

and

$$\psi(\boldsymbol{r}, \phi) = e^{-\frac{i}{\hbar}\phi\, \hat{n}\cdot\hat{\boldsymbol{L}}}\psi(\boldsymbol{r}, 0).$$

Comparison with (2) shows that in a constant magnetic field $\boldsymbol{B}$ the spin of the proton rotates about the axis of $\boldsymbol{B}$ with rate $-\gamma|\boldsymbol{B}|$.

This (Larmor) precession of a spin leads to an oscillating magnetic moment which can be observed by a detection coil. Hence 'magnetic resonance spectroscopy'. In a real experiment, however, the magnetic field $\boldsymbol{B}$ is not simply the field produced by an external electromagnet. In a sample of many spins each spin will see a slightly different $\boldsymbol{B}$ because of local environmental effects.

Problem Set #8

1. All spin states of a proton are of the form

$$\psi = \begin{bmatrix} a(t) \\ b(t) \end{bmatrix}.$$

We can associate with each state ψ a spin operator

$$\hat{s} = \hat{\boldsymbol{s}} \cdot \hat{\boldsymbol{n}} = \hat{s}_x \cos\phi \sin\theta + \hat{s}_y \sin\phi \sin\theta + \hat{s}_z \cos\theta,$$

with the unit vector $\hat{\boldsymbol{n}}$ oriented in direction ϕ, θ in spherical coordinates, by requiring that $\hat{s}\psi = \frac{1}{2}\hbar\psi$.

If

$$b/a = re^{i\chi},$$

relate θ, ϕ to r, χ. Conclusion: we can always describe a proton's spin state (up to a phase factor) by giving an orientation 'θ, ϕ' for the spin.

2. Suppose that $\boldsymbol{B} = B_0\hat{\boldsymbol{k}}$. Show that

$$e^{i\omega_0 \hat{s}_z t/\hbar} = \begin{bmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{bmatrix}.$$

If the spin is initially oriented along (a) $\hat{\imath}$, (b) $\hat{\boldsymbol{k}}$, and (c) $\frac{1}{\sqrt{2}}[\hat{\imath} + \hat{\boldsymbol{k}}]$, how will ϕ and θ vary with time? Construct an animated exhibit of the motion of the spin orientation.

Show[Graphics3D[Line[{{0,0,0}, {x,y,z}}]],PlotRange→{{-1,1}, {-1,1}, {-1,1}}] will plot a line from the origin to the point x, y, z in a 3D frame.

3. Consider the motion of $\psi(t)$ induced by

$$\begin{aligned} \hat{H} &= -\gamma B_1 \cos\Omega t \;\; \hat{s}_x + \gamma B_1 \sin\Omega t \;\; \hat{s}_y - \gamma B_0 \hat{s}_z \\ &= -\omega_1\Big(\cos\Omega t \;\; \hat{s}_x - \sin\Omega t \;\; \hat{s}_y\Big) - \omega_0 \hat{s}_z. \end{aligned}$$

How could this Hamiltonian be realized in the laboratory?

If $\psi_1(t) = e^{-i\omega_0 t\hat{s}_z/\hbar}\psi(t)$, then

$$i\hbar\frac{\partial\psi_1(t)}{\partial t} = e^{-i\omega_0 t\hat{s}_z/\hbar}[-\omega_1(\cos\Omega t\ \ \hat{s}_x - \sin\Omega t\ \ \hat{s}_y)]e^{i\omega_0 t\hat{s}_z/\hbar}\ \psi_1(t).$$

$\psi_1(t)$ is referred to colloquially as the 'spin state in the rotating frame.' Why? Why must $\hat{s}_x^2 = \hat{s}_y^2 = \hat{s}_z^2 = \hbar^2\hat{1}/4$? Show that

$$e^{i\Omega t\hat{s}_z/\hbar}\hat{s}_x e^{-i\Omega t\hat{s}_z/\hbar} = \cos\Omega t\ \ \hat{s}_x - \sin\Omega t\ \ \hat{s}_y.$$

Thus

$$i\hbar\frac{\partial\psi_1(t)}{\partial t} = e^{-i(\omega_0-\Omega)t\hat{s}_z/\hbar}(-\omega_1\ \hat{s}_x)e^{i(\omega_0-\Omega)t\hat{s}_z/\hbar}\ \psi_1(t).$$

If $\psi_2(t) = e^{i(\omega_0-\Omega)t\hat{s}_z/\hbar}\ \psi_1(t)$,

$$i\hbar\frac{\partial\psi_2(t)}{\partial t} = [(\Omega-\omega_0)\hat{s}_z - \omega_1\hat{s}_x]\ \psi_2(t).$$

Suppose $\psi(0) = \alpha$. Make an animation showing the time evolution of $\psi(t)$ if $\Omega = \omega_0 = 0.1\omega_1$. If $\Omega = 0.9\omega_0 = 0.1\omega_1$?

4. Suppose that

$$\hat{H} = -\omega_1\Big(\cos\Omega t\ \ \hat{s}_x - \sin\Omega t\ \ \hat{s}_y\Big) - \omega_0\hat{s}_z$$

again and $B_1 \gg B_0$ in the time interval $0 \le \gamma B_1 t \le \pi/2$ (a '$\pi/2$ pulse'). Into what state will this pulse transform $\psi(0) = \alpha$? If B_1 is then turned off, how will (give an analytic expressions) $\langle\hat{s}_x\rangle$ subsequently evolve in time?

5. Suppose that this 'pulse-observe $\hat{s}_x$' experiment is performed on an *ensemble* of protons in which, because of differing local environments, the field B_0 felt at each spin is a little different. Let the distribution on ω_0 values be

$$\frac{1}{\sqrt{2\pi}\,\sigma}\,e^{-(\omega_0-\bar{\omega})^2/2\sigma^2}.$$

How will the resulting magnetic moment appear to the spectrometer?

then

$$\begin{aligned}\hat{L}_z\Phi &= [L_z, L_x \pm iL_y]\Psi_{\lambda\mu} + \mu\Phi \\ &= i\hbar(L_y \mp iL_x)\Psi_{\lambda\mu} + \mu\Phi \\ &= \pm\hbar(L_x \pm iL_y)\Psi_{\lambda\mu} + \mu\Phi \\ &= (\mu \pm \hbar)\Phi.\end{aligned}$$

Thus the operators

$$L_\pm = L_x \pm iL_y$$

raise/lower μ by $\hbar$. Since $[L_\pm, L^2] = 0$, the L^2 eigenvalue is unaltered,

$$L^2\Phi = \lambda\Phi.$$

impact of Z component on total angular momentum = None

Of course $-\sqrt{\lambda} \leq \mu \leq \sqrt{\lambda}$, so, for any given λ, there is a maximum and a minimum value for μ. Denoting these by $\mu_\pm$,

Limits of raising a lowering Z component of L_z angular moment

$$L_+\Phi_{\lambda\mu_+} = 0 \qquad \text{and} \qquad L_-\Phi_{\lambda\mu_-} = 0.$$

Since $L_\pm L_\mp = L_x^2 + L_y^2 \mp i[L_x, L_y] = L_x^2 + L_y^2 \pm \hbar L_z$,

$$0 = (L_x^2 + L_y^2 \mp \hbar L_z)\Psi_{\lambda\mu_\pm}$$

whence

$$L^2\Psi_{\lambda\mu_\pm} = (L_z^2 \pm \hbar L_z)\Psi_{\lambda\mu_\pm}.$$

Thus $\lambda = \mu_\pm^2 \pm \hbar\mu_\pm$ from which it follows that $\mu_- = -\mu_+$. If $\mu_+ = \ell\hbar$, then

$$\begin{aligned}-\ell\hbar = \mu &\leq \ell\hbar, \\ \lambda &= \ell(\ell+1)\hbar^2.\end{aligned}$$

Let us relabel the states with $\lambda \to \ell$, $\mu \to m\hbar$. Thus we have states $\Psi_{\ell m}$ with, for each ℓ, $-\ell \leq m \leq \ell$.

$$\begin{aligned}L_z\Psi_{\ell m} &= m\hbar\Psi_{\ell m}, \\ L^2\Psi_{\ell m} &= \ell(\ell+1)\hbar^2\Psi_{\ell m}.\end{aligned}$$

The number of such states, $2\ell + 1$, must be an integer. Thus ℓ is restricted to $\ell = 0, 1/2, 1, 3/2, \ldots$.

— different spin states allowed values for angular momentum