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Angular Momentum

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Angular Momentum

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Rotating Vectors

If $\boldsymbol{r}$ is a vector in 3D with components $x, y, z,$, a rotation by an angle ϕ about the z-axis transforms

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} \to \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

That is,

$$\frac{d}{d\phi}\begin{bmatrix} x \\ y \\ z \end{bmatrix}\Bigg|_{\phi=0} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix} \tag{1}$$

Space is Isotropic

If the Hamiltonian for a system is invariant under rotations about the z-axis,

$$\begin{aligned} 0 = \frac{d}{d\phi} H(\boldsymbol{p}, \boldsymbol{r})\Big|_{\phi=0} &= \frac{\partial H(\boldsymbol{p}, \boldsymbol{r})}{\partial \boldsymbol{p}} \, \frac{d\boldsymbol{p}}{d\phi}\Big|_{\phi=0} + \frac{\partial H(\boldsymbol{p}, \boldsymbol{r})}{\partial \boldsymbol{r}} \, \frac{d\boldsymbol{r}}{d\phi}\Big|_{\phi=0} \\ &= -\frac{\partial H}{\partial p_x} p_y + \frac{\partial H}{\partial p_y} p_x - \frac{\partial H}{\partial x} y + \frac{\partial H}{\partial y} x \\ &= -\dot{x}\, p_y + \dot{y}\, p_x + \dot{p}_x\, y - \dot{p}_y\, x = -\frac{d}{dt}\left(x\, p_y - y\, p_x\right) \end{aligned}$$

The corresponding (E. Nöther) conserved quantity is the z-component of the *angular momentum.*

Indicial notation

Rather than labeling coordinates x, y and z, let the coordinates be x_i, $i = 1, 2, 3$. A vector (first rank tensor) is a quantity with a single index. Standard vector notation is simplified if we adopt the rule that a *repeated* index is summed over $1, 2, 3$. Thus

$$x_i\, p_i = \sum_{i=1}^{3} x_i\, p_i = \boldsymbol{r} \cdot \boldsymbol{p}.$$

To represent the vector *cross* product in indicial notation, let

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if } i, j, k = 1,2,3 \text{ or } 2,3,1 \text{ or } 3,1,2 \\ -1 & \text{if } i, j, k = 2,1,3 \text{ or } 3,2,1 \text{ or } 1,3,2 \\ 0 & \text{otherwise} \end{cases}$$

The angular momentum is a vector $\boldsymbol{L}$ with components

$$L_x = y p_z - z p_y,$$
$$L_y = z p_x - x p_z,$$
$$L_z = x p_y - y p_x.$$

That is,

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}, \qquad L_i = \epsilon_{ijk} x_j\, p_k$$

Rotations in quantum mechanics

If the rotation (1) is applied to $\psi(x, y, z)$,

$$\frac{d}{d\phi}\psi(x,y,z) = -\frac{\partial\psi}{\partial x}\, y + \frac{\partial\psi}{\partial y}\, x = \frac{i}{\hbar}\left(\hat{x}\, \hat{p}_y - \hat{y}\, \hat{p}_x\right)\, \psi(x,y,z) = \frac{i}{\hbar}\hat{L}_z\, \psi(x,y,z)$$

The physical rotation of the system corresponds to a coordinate shift in the opposite direction, so we say that $-i\, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{n}}/\hbar$ generates a rotation about an axis $\hat{\boldsymbol{n}}$.

Let us denote the components of the angular momentum operator by L_x, L_y, L_z (i.e., drop the $\hat{}$ symbols). The quantum mechanical operators then have the following commutators,

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

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

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

then

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

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,

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

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 $\mu_\pm$,

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

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

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

Thus

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

This gives

$$\lambda = \mu_\pm^2 \pm \hbar\mu_\pm$$

from which it follows that $\mu_- = -\mu_+$. If $\mu_+ = \ell\hbar$, then

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

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

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

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

While $L_\pm$ shifts the L_z eigenvalue $\mu \to \mu \pm \hbar$, it does not produce a normalized state (the dimensions are wrong!). To see this, suppose that $\langle \Psi_{\ell m} | \Psi_{\ell m} \rangle = 1$. Then

$$\begin{aligned} \langle L_\pm \Psi_{\ell m} | L_\pm \Psi_{\ell m} \rangle &= \langle L_x \Psi_{\ell m} | L_\pm \Psi_{\ell m} \rangle \mp i \left\langle L_y \Psi_{\ell m} | L_\pm \Psi_{\ell m} \right\rangle \\ &= \langle \Psi_{\ell m} | L_x L_\pm \Psi_{\ell m} \rangle \mp i \left\langle \Psi_{\ell m} | L_y L_\pm \Psi_{\ell m} \right\rangle \\ &= \langle \Psi_{\ell m} | L_\mp L_\pm \Psi_{\ell m} \rangle = \left\langle \Psi_{\ell m} | (L^2 - L_z^2 \mp \hbar L_z) \Psi_{\ell m} \right\rangle \\ &= \ell(\ell+1)\hbar^2 - m^2\hbar^2 \mp m\hbar^2 \\ &= (\ell \mp m)(\ell \pm m + 1)\hbar^2 \end{aligned}$$

We may thus identify

$$L_\pm \Psi_{\ell m} = \sqrt{(\ell \mp m)(\ell \pm m + 1)}\, \hbar\, \Psi_{\ell, m\pm 1}$$

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.,

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

that describes the electron-positron system. In the non-relativistic limit, a two component spinor provides a good representation of the states of an electron. The discrete variable that labels the components of the spinor corresponds to the electronic spin variable.

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,

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

and

$$L^2 = \frac{3}{4}\hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Since

$$L_+\alpha = 0, \qquad L_-\alpha = \hbar\beta,$$
$$L_+\beta = \hbar\alpha, \qquad L_-\beta = 0,$$

we deduce

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

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

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

and transforms functions

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

For small $\delta\phi$,

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

Thus

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

and

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

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 #7

1. Show that the only state that can simultaneously be an eigenstate of L_x, L_y, and L_z is the $\ell = 0$ state.

2. Show that

$$L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$$

3. Construct a matrix representation for a system with $\ell = 1$.

4. The hydrogen atom has two spin-$\frac{1}{2}$ particles, the electron and the proton. In the electronic ground state all the angular momentum of the atom is associated with these spins. If $\vec{S}_e$ and $\vec{S}_p$ are the angular momenta of the electron and the proton, the total angular momentum is

$$\vec{S} = \vec{S}_e + \vec{S}_p.$$

Since each spin can be represented in terms of an α, β basis set, the atom's spin state can be represented in terms of

$$\psi_{\uparrow\uparrow} = \alpha_e\,\alpha_p, \quad \psi_{\uparrow\downarrow} = \alpha_e\,\beta_p, \quad \psi_{\downarrow\uparrow} = \beta_e\,\alpha_p, \quad \psi_{\downarrow\downarrow} = \beta_e\,\beta_p$$

In what basis set are S_z and $\vec{S}^2$ both diagonal?

5. Show that

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

is the solution to the dynamical equation for an electron in a constant magnetic field $\boldsymbol{B}$. In what basis set is $e^{i\gamma \boldsymbol{B}\cdot\hat{\boldsymbol{s}}t/\hbar}$ diagonal? If $\psi(0) = \alpha$, deduce an equation for $\langle\psi(t)|L_z\psi(t)\rangle$.

6. Sketch a demonstration that a rotation by an angle $\delta\phi$ about an axis $\hat{\boldsymbol{n}}$ (a unit vector) moves points

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

7. 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.

8. Use the results of question #7 to construct an animated exhibit of the motion of a spin that is started in $\psi(0) = \alpha$ and then moves in an external field that is oriented in the direction (a) $\hat{\boldsymbol{\imath}}$, (b) $\hat{\boldsymbol{k}}$, and (c) $\frac{1}{\sqrt{2}}[\hat{\boldsymbol{\imath}} + \hat{\boldsymbol{k}}]$.

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.

9. 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 $\hat{s}_x^2 = \hat{s}_y^2 = \hat{s}_z^2 = \hbar^2\hat{\mathtt{1}}/4$? 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 $\Omega = 0.9\omega_0 = 0.1\omega_1$?

10. 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?

11. 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?