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Spring 3-9-2015

Angular Momentum

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Recommended Citation

Lovett, Ronald, "Angular Momentum" (2015). *Topics in Quantum Mechanics*. 38.
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Angular Momentum

References

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Rotating Vectors

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

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

That is,

$$\left. \frac{d}{d\phi} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \right|_{\phi=0} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix} \quad (1)$$

Space is Isotropic

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

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

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

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

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 \mathbf{L} with components

$$L_x = yp_z - zp_y,$$

$$L_y = zp_x - xp_z,$$

$$L_z = xp_y - yp_x.$$

That is,

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad L_i = \epsilon_{ijk} x_j p_k$$

Rotations in quantum mechanics

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

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

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

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 μ_{\pm} ,

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

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

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

Let us relabel the states with $\lambda \rightarrow \ell$, $\mu \rightarrow m\hbar$. 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 $\ell = 0, 1/2, 1, 3/2, \dots$

While L_{\pm} shifts the L_z eigenvalue $\mu \rightarrow \mu \pm \hbar$, 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

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

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.,

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

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,

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

and

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

Since

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

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

we deduce

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

Thus

$$L_x = \frac{1}{2}(L_+ + L_-) = \frac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (1b)$$

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

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 μ . For the proton

$$\mu = \gamma L,$$

with the gyromagnetic ratio

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

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

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

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

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

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

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

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

and transforms functions

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

For small $\delta\phi$,

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

Thus

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

and

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

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

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 \mathbf{B} is not simply the field produced by an external

electromagnet. In a sample of many spins each spin will see a slightly different 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

$$L^2 = L_+L_- + L_-L_+ + L_z^2 + \hbar L_z$$

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

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

is the solution to the dynamical equation for an electron in a constant magnetic field \mathbf{B} .

In what basis set is $e^{i\gamma \mathbf{B} \cdot \hat{s} t / \hbar}$ 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{n} (a unit vector) moves points

$$\mathbf{r} \rightarrow \mathbf{r} + \delta\phi \hat{n} \times \mathbf{r}.$$

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

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

with the unit vector \hat{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{i} , (b) \hat{k} , and (c) $\frac{1}{\sqrt{2}}[\hat{i} + \hat{k}]$.

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

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

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

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

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

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

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

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

again and $B_1 \gg B_0$ in the time interval $0 \leq \gamma B_1 t \leq \pi/2$ (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?