Orbital angular momentum

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Outline

Spherical harmonics

We construct the operators and the eigenfunctions of orbital angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, in the Hilbert space of position eigenstates. Then the usual differential operator for $\mathbf{p}$ can be used. Under the scaling $\mathbf{r} \to \xi\mathbf{r}$, one has $\mathbf{p} \to \mathbf{p}/\xi$, so that $\mathbf{L}$ is independent of the scale of the radius, ξ. Hence in this problem one can set $|\mathbf{r}| = 1$, *i.e.*, use the unit vector $\hat{\mathbf{r}}$. We will use $\hat{r}_z = \cos\theta$ and $\hat{r}_\pm = \hat{r}_x \pm i\hat{r}_y = \exp(\pm i\phi)\sin\theta$.

The spherical harmonics are defined as

$$Y^l_m(\hat{\mathbf{r}}) = \langle\hat{\mathbf{r}}|lm\rangle, \quad L^2 Y^l_m(\hat{\mathbf{r}}) = \hbar^2 l(l+1) Y^l_m(\hat{\mathbf{r}}), \quad L_z Y^l_m(\hat{\mathbf{r}}) = \hbar m Y^l_m(\hat{\mathbf{r}}).$$

These have completeness and orthonormality

$$|lm\rangle = \int d\Omega |\hat{\mathbf{r}}\rangle\langle\hat{\mathbf{r}}|lm\rangle, \qquad \int d\Omega [Y^{l'}_{m'}(\hat{\mathbf{r}})]^* Y^l_m(\hat{\mathbf{r}}) = \delta_{ll'}\delta_{mm'}.$$

Since $Y^l_m(\theta,\phi) = Y^l_m(\theta,\phi+2\pi)$, one has integer values of m, and hence also of l.

The highest weight eigenfunction

We use the raising and lowering operators

$$L_\pm = \pm\hbar z\left(\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y}\right) \mp \hbar(x \pm iy)\frac{\partial}{\partial z}.$$

The scalar representation must have $L_i Y_0^0 = 0$, *i.e.*, Y_0^0 must be a constant. The normalization condition gives $Y_0^0 = 1/\sqrt{4\pi}$. Since $\hat{\mathbf{r}}$ is a vector operator, one has

$$Y_{\pm l}^l \propto r_\pm^l Y_0^0 = c_l(\hat{r}_x \pm i\hat{r}_y)^l = c_l \mathrm{e}^{\pm il}(\sin\theta)^l.$$

The normalization condition is

$$1 = |c_l|^2 \int \frac{d\phi d(\cos\theta)}{4\pi}(\sin\theta)^{2l} = |c_l|^2 \frac{1}{2}\int_{-1}^{1} dz(1-z^2)^l.$$

A recursion can be used to evaluate the integral. The normalized function is

$$Y_l^l(\theta,\phi) = \frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}(\sin\theta)^l \mathrm{e}^{il\phi}.$$

Using the ladder

Note that

$$\frac{\partial f(\hat{r}_z)}{\partial x_i} = \frac{1}{r^3}(-x_i z + r^2\delta_{i3})\frac{df(\hat{r}_z)}{d\hat{r}_z}, \quad \text{hence} \quad L_- f(\hat{r}_z) = \hbar\hat{r}_- \frac{df(\hat{r}_z)}{d\hat{r}_z}.$$

Also, note that $[L_, \hat{r}_-] = 0$. Now starting from

$$\hat{r}_-^l Y_l^l = c_l(1-\hat{r}_z)^l, \quad \text{one finds} \quad \hat{r}_-^l L_-^N Y_l^l = c_l(\hbar\hat{r}_-^N)\frac{d^N}{d\hat{r}_z^N}(1-\hat{r}_z)^l,$$

by applying L_-^N on both sides. Then, since

$$L_-^N Y_l^l = \hbar^N \sqrt{\frac{(2l)!N!}{(2l-N)!}} Y_{l-N}^l,$$

one finds all the spherical harmonics by the above recursion. This can also be done starting from the lowest weight representation and using L_+^N. Comparing these two gives

$$Y_m^l(-\hat{\mathbf{r}}) = (-1)^l Y_m^l(\hat{\mathbf{r}}), \qquad Y_{-m}^l(\hat{\mathbf{r}}) = (-1)^m [Y_m^l(\hat{\mathbf{r}})]^*.$$

Some spherical harmonics

Y^0_0	$\frac{1}{\sqrt{4\pi}}$	
$Y^1_{\pm 1}$	$\sqrt{\left(\frac{3}{8\pi}\right)\mathrm{e}^{\pm i\phi}}\sin\theta$	$\sqrt{\left(\frac{3}{8\pi}\right)}(x \pm iy)$
Y^1_0	$\sqrt{\left(\frac{3}{4\pi}\right)}\cos\theta$	$\sqrt{\left(\frac{3}{4\pi}\right)}z$
$Y^2_{\pm 2}$	$\sqrt{\left(\frac{15}{32\pi}\right)\mathrm{e}^{\pm 2i\phi}}\sin^2\theta$	$\sqrt{\left(\frac{15}{32\pi}\right)}(x^2 \pm iy^2)$
$Y^2_{\pm 1}$	$\mp\sqrt{\left(\frac{15}{8\pi}\right)\mathrm{e}^{\pm i\phi}}\sin\theta\cos\theta$	$\mp\sqrt{\left(\frac{15}{8\pi}\right)}z(x \pm iy)$
Y^2_0	$\sqrt{\left(\frac{15}{16\pi}\right)}(3\cos^2\theta - 1)$	$\sqrt{\left(\frac{15}{16\pi}\right)}(3z^2 - 1)$

$$\text{Complex conjugation}: \quad [Y^l_m(\theta,\phi)]^* = (-1)^m Y^l_{-m}(\theta,\phi),$$

$$\text{Completeness}: \quad f(\theta,\phi) = \sum_{lm} f_{lm} Y^l_m(\theta,\phi), \quad \text{where}$$

$$f_{lm} = \int d\cos\theta d\phi [Y^l_m(\theta,\phi)]^* f(\theta,\phi).$$

Legendre and Associated Legendre Polynomials

One often writes the spherical harmonics in the form

$$Y^l_m(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\,\frac{(l-m)!}{(l+m)!}}\,\mathrm{e}^{im\phi} P^m_l(\cos\theta),$$

where $P^m_l(z)$ are called associated Legendre polynomials. From the recursion relations used before, one can find

$$P^m_l(z) = \frac{(-1)^l}{2^l l!}(1-z^2)^{m/2}\left(\frac{d}{dz}\right)^{l+m}(1-z^2)^l.$$

The Legendre polynomials are $P_l(z) = P^0_l(z)$. One can check that the Legendre polynomials are a complete set of orthogonal functions in the interval $-1 \le z \le 1$.

A problem

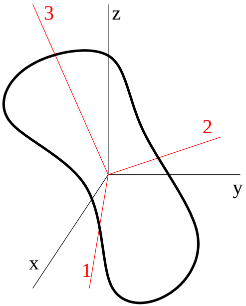
1. Starting from the trivial polynomial $p_0(z) = 1/2$, construct successively polynomials of successively higher orders which are orthogonal to all previously constructed polynomials. Does this process give the Legendre polynomials?
2. Use Mathematica to construct arbitrary Legendre polynomials using the derivative expression given before.
3. Check that they are orthonormal using Mathematica, and then prove that they are orthonormal.
4. Plot successive $P_l(z)$ and check that the zeroes of each P_l is bracketed by the zeroes of P_{l-1}.
5. If the inner product on the Hilbert space of polynomials is changed to

$$\langle f|g\rangle = \int_{-1}^{1} dz w(z) f(z) g(z),$$

then the set of orthogonal polynomials changes. What weight function needs to be used to obtain the associated Legendre polynomials?

Outline

Operators and the Hamiltonian



The angular momentum of a top around its center of mass can be resolved into components along space fixed axes or along the principal axes of the body (body fixed axes),

$$\mathbf{L} = L_x\hat{x} + L_y\hat{y} + L_z\hat{z} = L_1\hat{n}_1 + L_2\hat{n}_2 + L_3\hat{n}_3.$$

The Hamiltonian of the top is

$$H = \frac{L_1^2}{2I_1} + \frac{L_2^2}{2I_2} + \frac{L_3^2}{2I_3},$$

where I_j are the principal moments of inertia. The commutation relations of the space-fixed components of $\mathbf{L}$ are $[L_x, L_y] = i\hbar L_z$, *etc.*. However, the commutation relations of the body-fixed components are $[L_1, L_2] = -i\hbar L_3$,

The meaning of commutators

Rotations about two different axes do not commute. One finds—

$$\begin{aligned}
&R_x(\phi_x)R_y(\phi_y) - R_y(\phi_y)R_x(\phi_x) \\
&\quad \simeq (1 + i\phi_x L_x/\hbar + \cdots)(1 + i\phi_y L_y/\hbar + \cdots) - \\
&\qquad\qquad (1 + i\phi_y L_y/\hbar + \cdots)(1 + i\phi_x L_x/\hbar + \cdots) \\
&\quad \simeq -i\phi_x\phi_y(L_xL_y - L_yL_x)/\hbar + \cdots \\
&\quad = 1 - R_z(\phi_x\phi_y) + \mathcal{O}(\phi^3).
\end{aligned}$$

These manipulations start from the effect of rotations on quantum states. However, the fact that the difference of two rotations about different axes in opposite orders can be written as a third rotation can be seen even in classical mechanics (Goldstein).

Rotations in body fixed axes

Now examine the commutator

$$R_1(\phi_1)R_2(\phi_2) - R_2(\phi_2)R_1(\phi_1),$$

in the configuration where the body fixed and space fixed axes coincide before the rotations are made. The first rotation can then be replaced by a space fixed rotation. So, for example, the first term above can be written as

$$R_1(\phi_1)R_y(\phi_2) = R_{x'}(\phi_1)R_y(\phi_2),$$

where we have used the fact that the axis about which the second rotation is performed changes as a result of the first. But a rotation about a changed axis can be related to that about the original axis through

$$R_{x'}(\phi_1) = R(\hat{x} \to \hat{x}')R_x(\phi_1)R^{-1}(\hat{x} \to \hat{x}').$$

By the argument above, one sees that $R(\hat{x} \to \hat{x}') = R_y(\phi_2)$.

Commutation relations in body fixed axes

The previous arguments show that

$$R_1(\phi_1)R_y(\phi_2) = R_y(\phi_2)R_x(\phi_1)R_y^{-1}(\phi_2)R_y(\phi_2) = R_y(\phi_2)R_x(\phi_1).$$

The reversal of order also occurs in the second term, as a result of which the commutator reverses sign, and

$$R_1(\phi_1)R_2(\phi_2) - R_2(\phi_2)R_1(\phi_1) = R_3(\phi_1\phi_2) - 1 + \mathcal{O}(\phi^3).$$

One has $R_3 = R_z$ in this formula, since the rotation R_3 is applied in the original unrotated frame, *i.e.*, when the body fixed axes coincide with the space fixed axes. This shows that the commutation relations in the body fixed axes become

$$[L_j, L_k] = -i\hbar\epsilon_{jkl}L_l.$$

However, this change of sign in the commutator does not affect the spectrum of L_3 and L^2. (**Check**)

Spectrum of a rigid rotor

When $I_1 = I_2 = I_3$, the Hamiltonian is

$$H = \frac{L^2}{2I}.$$

The eigenfunctions of this Hamiltonian are $|j, m\rangle$, and the eigenvalues are exatly those of L^2, *i.e.*, $l(l+1)\hbar^2/2I$. In the context of atomic spectra it is customary to introduce a *rotational constant*, $B = \hbar/(4\pi I)$ and write $E = Bhl(l+1)$. There is a $(2l+1)$-fold degeneracy for each eigenstate. Successive energy levels are separated by $\Delta E = 2Bh$. Transitions between levels which are separated by $\Delta l > 1$ are not allowed by *selection rules*. For a typical diatomic molecule, the reduced mass $m \simeq (A/2)$ GeV, where A is the mass number of each atom. The separation between the nuclei is of the order of 0.1 nm. In these units $\hbar \simeq 200$ eV nm. Hence, $\Delta E \simeq (40000/10^8)$ eV, *i.e.*, $\Delta E \simeq 10^{-4}$ eV.

The symmetric quantum top

When $I_1 = I_2 \neq I_3$, one has a symmetric top. In this case,

$$H = \frac{L^2}{2I_1} + \left(\frac{1}{2I_3} - \frac{1}{2I_1}\right) L_3^2.$$

The Hamiltonian is no longer spherically symmetric, since $[H, \mathbf{L}] \neq 0$. However, the two terms can be simultaneously diagonalized, and the eigenfunctions of the Hamiltonian are precisely $|l, m\rangle$ and that

$$E(l, m) = \hbar^2 \left[\frac{l(l+1)}{2I_1} + \left(\frac{1}{2I_3} - \frac{1}{2I_1}\right) m^2\right].$$

When $I_1 < I_3$, there are l doubly degenerate energy levels below a single level which coincides with that of the rigid rotor. For the case of $I_1 > I_3$, the $m \neq 0$ levels all lie above that of the rigid rotor. Note also that the states $|j, m\rangle$ and $|j, -m\rangle$ can mix.

Asymmetric quantum tops

For the asymmetric top, in which all three principal components of the inertia tensor are unequal, a general formula for the energy is not possible. However, since $[H, L^2] = 0$, one can diagonalize the Hamiltonian for each l separately. For $l = 0$, one finds that $E = 0$. For $l = 1$, the 3×3 matrix to be diagonalized is

$$H = \frac{\hbar^2}{4} \begin{pmatrix} \frac{1}{I_1} + \frac{1}{I_2} + \frac{2}{I_3} & 0 & \frac{1}{I_1} - \frac{1}{I_2} \\ 0 & \frac{2}{I_1} + \frac{2}{I_2} & 0 \\ \frac{1}{I_1} - \frac{1}{I_2} & 0 & \frac{1}{I_1} + \frac{1}{I_2} + \frac{2}{I_3} \end{pmatrix}.$$

The eigenvalues of this matrix are easily found to be

$$E = \frac{\hbar^2}{2}\left(\frac{1}{I_1} + \frac{1}{I_2}\right), \quad \frac{\hbar^2}{2}\left(\frac{1}{I_1} + \frac{1}{I_3}\right), \quad \frac{\hbar^2}{2}\left(\frac{1}{I_2} + \frac{1}{I_3}\right),$$

with eigenvectors $|1, 0\rangle$, $|1, 1\rangle + |1, -1\rangle$ and $|1, 1\rangle - |1, -1\rangle$ respectively.

A problem

1. Construct the matrices which represent **L** in the $l = 2$ representation.
2. Solve the asymmetric top problem for $l = 2$.
3. The classical motion of a top can be described in terms of precession and nutation. Are such motions inherent in the solutions of the quantum asymmetric top problem?
4. Set up and solve the asymmetric top problem for $j = 1/2$. Interpret the results.
5. Does your interpretation correctly predict the behaviour of the asymmetric top for $j = 3/2$.

Outline

References

1. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture are scattered through chapters 4, 8 and 14 of this book.
2. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 6 of this book discusses angular momentum. The presentation in these lectures follow this chapter sometimes.
3. Classical Mechanics, J. Goldstein. The material on rotations in this book is a pre-requisite for understanding angular momenta in quantum mechanics.
4. Discussion of the Rigid Rotator Problem, N. I. Greenberg, *Am. J. Phys.*, 45 (1977) 199–204. This article has a nice detailed and self-contained discussion of the quantum top.
5. A Handbook of Mathematical Functions, by M. Abramowicz and I. A. Stegun. This is a handy place to look up useful things about various classes of functions.