Quantum Mechanics 2

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Spherical Harmonics

Part 1 (Lowest State)

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L_z States

In [angular momentum], we have evaluated the eigenvalues of the operators L^2 and L_z

$$L^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle$$

$$L_z|l,m\rangle = m\hbar|l,m\rangle$$

Let us now evaluate the eigenfunctions. For orbital angular momentum,

$$L_z = -i\hbar\frac{\partial}{\partial\varphi}$$

Thus, if we separate the eigenfunctions as

$$\langle\theta,\varphi|l,m\rangle = Y_{lm}(\theta,\varphi) = P_{lm}(\theta)\Phi(\varphi)$$

we have

$$-i\hbar\frac{d\Phi}{d\varphi} = m\hbar\Phi$$

which yields

$$\Phi(\varphi) = e^{im\varphi}$$

Angular Momentum Quantum Numbers

As we will see later in this course, the quantum number m manifests itself in the presence of magnetic fields. It is therefore called the **magnetic quantum number.** It was shown previously that it may take on values

$$m = -j, -j+1, -j+2, \cdots, j-1, j$$

In the case of orbital angular momentum, we write $j = l$. Now, the **angular momentum quantum number** j was shown to be either a positive definite half-integer, or a positive definite integer.

For orbital angular momentum, the φ – dependent part of eigenfunction is

$$\Phi(\varphi) = e^{im\varphi}$$

Orbital angular momenta are generators of rotation. A rotation of 2π will result in

$$\Phi(\varphi + 2\pi) = e^{im\varphi}e^{i2m\pi}$$

If l is a half-integer, so will m. Thus, $e^{i2m\pi} = -1$, leading to a non-single valued eigenfunction as $\Phi(\varphi + 2\pi) = -\Phi(\varphi)$. This suggests that for orbital angular momentum, ***l* must be a positive-definite integer**.

Ladder Operators

Now let us look for the $\theta -$ dependent part of the eigenfunctions. For this, we will need the ladder operators

$$J_{\pm} = J_x \pm iJ_y$$

which operates on the $J^2$and J_z eigenkets as follows

$$J_{\pm} \left| j, m \right\rangle = \sqrt{j(j+1) - m(m \pm 1)}\hbar \left| j, m \pm 1 \right\rangle$$

For orbital angular momentum,

$$L_{\pm} = -i\hbar e^{\pm i\varphi} \left[\pm i \frac{\partial}{\partial \theta} - \cot\theta \frac{\partial}{\partial \varphi} \right]$$

The Lowest m −State

We begin with the eigenket with the lowest value of m. Since it cannot go any lower,

$$L_{-}|l,-l\rangle = 0$$

This translates to

$$L_{-}Y_{l,-l}(\theta,\varphi) = -i\hbar e^{i\varphi}\left[-i\frac{\partial}{\partial\theta} - \cot\theta\,\frac{\partial}{\partial\varphi}\right]P_{l,-l}(\theta)e^{-il\varphi} = 0$$

which gives us

$$\frac{dP_{l,-l}(\theta)}{d\theta} = l\cot\theta\,P_{l,-l}(\theta)$$

This separable ODE yields

$$\ln P_{l,-l} = l\ln|\sin\theta| + \ln C_l$$

and so

$$P_{l,-l}(\theta) = C_l \sin^l\theta$$

Normalization

We may evaluate C_l through normalization of the eigenfuction

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$$\int Y_{lm}^{*}(\theta,\varphi)Y_{lm}(\theta,\varphi)d\Omega = \int_0^{\pi} \left|P_{l,-l}(\theta)\right|^2 \sin\theta \, d\theta \int_0^{2\pi} \left|e^{-il\varphi}\right|^2 d\varphi$$

$$= 2\pi \int_0^{\pi} |C_l|^2 \sin^{2l}\theta \sin\theta \, d\theta = 1$$

Integrating by parts,

$1 - (\sin\theta)^2$

$$\int_0^{\pi} (\sin\theta)^{2l} \sin\theta \, d\theta = -(\sin\theta)^{2l}\cos\theta\Big|_0^{\pi} + 2l\int_0^{\pi} (\sin\theta)^{2l-1}(\cos\theta)^2 d\theta$$

$$= 2l\left[\int_0^{\pi} (\sin\theta)^{2l-1} d\theta - \int_0^{\pi} (\sin\theta)^{2l+1} d\theta\right]$$

Thus,

$$[2l+1]\int_0^{\pi} (\sin\theta)^{2l+1} d\theta = 2l\int_0^{\pi} (\sin\theta)^{2l-1} d\theta$$

Normalization

If we apply

$$\int_0^{\pi} (\sin\theta)^{2l+1} d\theta = \frac{2l}{2l+1} \int_0^{\pi} (\sin\theta)^{2l-1} d\theta$$

successively,

$$\int_0^{\pi} (\sin\theta)^{2l+1} d\theta = \frac{2l}{2l+1} \int_0^{\pi} (\sin\theta)^{2l-1} d\theta = \frac{(2l)(2l-2)}{(2l+1)(2l-1)} \int_0^{\pi} (\sin\theta)^{2l-3} d\theta$$

$$= \cdots = \frac{(2l)(2l-2)\cdots 2}{(2l+1)(2l-1)\cdots 3} \int_0^{\pi} \sin\theta \, d\theta = \frac{2l!!\,(2)}{(2l+1)!!}$$

The double factorials may be recast as follows

$$\frac{2l!!}{(2l+1)!!} = \frac{(2l)(2l-2)\cdots 2}{(2l+1)(2l-1)\cdots(3)(1)} = \frac{[(2l)(2l-2)\cdots 2]^2}{(2l+1)(2l)(2l-1)(2l-2)\cdots(3)(2)(1)}$$

$$= \frac{[2^l(l)(l-1)\cdots 1]^2}{(2l+1)!} = \frac{[2^l l!]^2}{(2l+1)!}$$

Normalization

We thus have

$$1 = 2\pi \int_0^{\pi} |C_l|^2 \sin^{2l}\theta \, \sin\theta \, d\theta = |C_l|^2 4\pi \frac{[2^l l!]^2}{(2l+1)!}$$

and

$$C_l = [2^l l!]^{-1} \sqrt{\frac{(2l+1)!}{4\pi}}$$

We then have

$$Y_{l,-l} = [2^l l!]^{-1} \sqrt{\frac{(2l+1)!}{4\pi}} \ \sin^l\theta \ \ e^{-il\varphi}$$

Verification

We now verify that

$$Y_{l,-l} = (-1)^l [2^l l!]^{-1} \sqrt{\frac{(2l+1)!}{4\pi}} \ \sin^l\theta \ e^{-il\varphi}$$

is indeed an eigenfunction of L^2

$$L^2 Y_{l,-l} = -\hbar^2 C_l \left[\frac{e^{-il\varphi}}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial (\sin\theta)^l}{\partial\theta} \right) + \frac{(\sin\theta)^l}{\sin^2\theta} \frac{\partial^2 e^{-il\varphi}}{\partial\varphi^2} \right]$$

$$= -\hbar^2 C_l \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(l(\sin\theta)^l \cos\theta \right) - l^2 (\sin\theta)^{l-2} \right] e^{-il\varphi}$$

$$= -\hbar^2 C_l [l^2 (\sin\theta)^{l-2} (\cos\theta)^2 - l(\sin\theta)^l - l^2 (\sin\theta)^{l-2}] e^{-il\varphi}$$

$$= \hbar^2 C_l [l^2 (\sin\theta)^{l-2} (\sin\theta)^2 + l(\sin\theta)^l] e^{-il\varphi}$$

$$= l(l+1)\hbar^2 C_l (\sin\theta)^l e^{-il\varphi} = l(l+1)\hbar^2 Y_{l,-l}$$