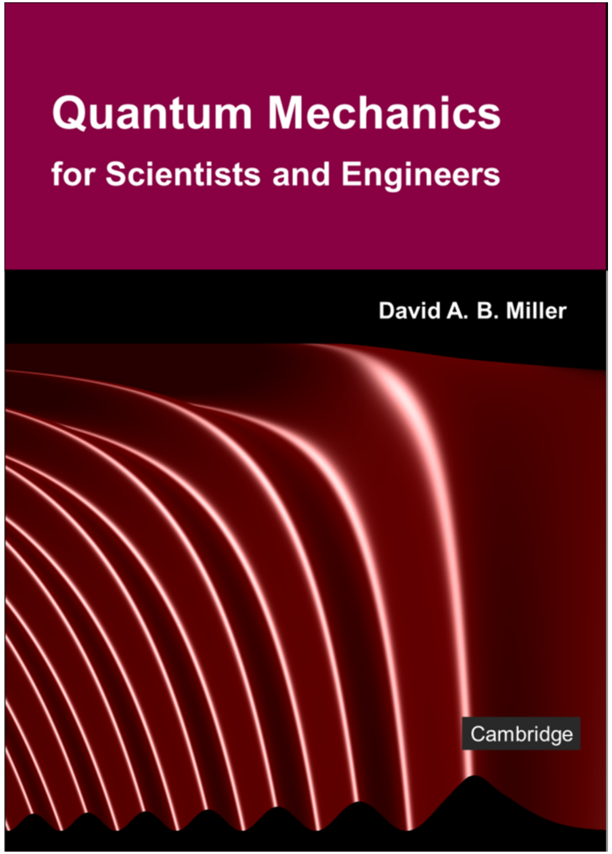
7.2 The L squared operator

Slides: Video 7.2.1 Separating the L squared operator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 9.2



The L squared operator

Separating the L squared operator

Quantum mechanics for scientists and engineers

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The L^2 operator

In quantum mechanics

we also consider another operator

associated with angular momentum

the operator $\hat{L}^2$

This should be thought of as

the "dot" product of $\hat{\mathbf{L}}$ with itself

and is defined as

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

The L^2 operator

It is straightforward to show then that

$$\hat{L}^2 = -\hbar^2 \nabla^2_{\theta,\phi}$$

where the operator $\nabla^2_{\theta,\phi}$ is given by

$$\nabla^2_{\theta,\phi} = \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

which is actually the θ and ϕ part of

the Laplacian (∇^2) operator in spherical polar coordinates

hence the notation

Commutation of L^2

$\hat{L}^2$ commutes with each of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$

It is easy to see from

$$\nabla^2_{\theta,\phi} = \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

and the form of $\hat{L}_z = -i\hbar \dfrac{\partial}{\partial\phi}$

that at least $\hat{L}^2$ and $\hat{L}_z$ commute

The operation $\partial / \partial\phi$ has no effect

on functions or operators depending on θ alone

Commutation of L²

Of course, the choice of the z direction is arbitrary

We could equally well have chosen the polar axis

along the x or y directions

Then it would similarly be obvious that

$\hat{L}^2$ commutes with $\hat{L}_x$ or $\hat{L}_y$

How can $\hat{L}^2$ commute with each of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$

but $\hat{L}_x, \hat{L}_y$, and $\hat{L}_z$ do not commute with each other?

Answer

we can choose the eigenfunctions of $\hat{L}^2$ to be

the same as those of any *one* of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$

Eigenfunctions of L^2

We want eigenfunctions of $\hat{L}^2$ or, equivalently, $\nabla^2_{\theta,\phi}$

and so the equation we hope to solve is of the form

$$\nabla^2_{\theta,\phi} Y_{lm}(\theta,\phi) = -l(l+1) Y_{lm}(\theta,\phi)$$

We anticipate the answer

by writing the eigenvalue in the form $-l(l+1)$

but it is just an arbitrary number to be determined

The notation $Y_{lm}(\theta,\phi)$

also anticipates the final answer

but it is just an arbitrary function to be determined

Separation of variables

We presume that the final eigenfunctions can be separated in the form

$$Y_{lm}(\theta,\phi)=\Theta(\theta)\Phi(\phi)$$

where

$\Theta(\theta)$ only depends on θ and

$\Phi(\phi)$ only depends on ϕ

Substituting this form in $\nabla^2_{\theta,\phi}Y_{lm}(\theta,\phi)=-l(l+1)Y_{lm}(\theta,\phi)$

gives

$$\frac{\Phi(\phi)}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta(\theta)+\frac{\Theta(\theta)}{\sin^2\theta}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}=-l(l+1)\Theta(\theta)\Phi(\phi)$$

Separation of variables

Multiplying by $\sin^2\theta / \Theta(\theta)\Phi(\phi)$ and rearranging, gives

$$\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = -l(l+1)\sin^2\theta - \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta(\theta)$$

The left hand side depends only on ϕ

whereas the right hand side depends only on θ

so these must both equal a ("separation") constant

Anticipating the answer

we choose a separation constant of $-m^2$

where m is still to be determined

ϕ equation

Taking the left hand side of

$$\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = -l(l+1)\sin^2\theta - \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta(\theta) = -m^2$$

we now have an equation

$$\frac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi)$$

The solutions to an equation like this are of the form

$\sin m\phi$, $\cos m\phi$ or $\exp im\phi$

ϕ equation

For the solutions of $\dfrac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi)$

we choose the exponential form $\exp im\phi$

so Φ is also a solution of the $\hat{L}_z$ eigen equation

$$\hat{L}_z\Phi(\phi) = m\hbar\Phi(\phi)$$

We expect that Φ and its derivative are continuous

so this wavefunction must repeat every 2π of angle ϕ

Hence, m must be an integer

θ equation

Taking the right hand side of the separation equation

$$-l(l+1)\sin^2\theta - \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta(\theta) = -m^2$$

Multiplying by $\Theta(\theta)/\sin^2\theta$ and rearranging gives

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)\Theta(\theta) - \frac{m^2}{\sin^2\theta}\Theta(\theta) + l(l+1)\Theta(\theta) = 0$$

This is the associated Legendre equation

whose solutions are the associated Legendre functions

$$\Theta(\theta) = P_l^m(\cos\theta)$$

θ equation

The solutions $\Theta(\theta) = P_l^m(\cos\theta)$ to this equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)\Theta(\theta) - \frac{m^2}{\sin^2\theta}\Theta(\theta) + l(l+1)\Theta(\theta) = 0$$

require that

$$l = 0, 1, 2, 3, \ldots$$

$-l \le m \le l$ (m integer)

The associated Legendre functions can conveniently be defined using Rodrigues' formula

$$P_l^m(x) = \frac{1}{2^l l!}\left(1-x^2\right)^{m/2}\frac{d^{l+m}}{dx^{l+m}}\left(x^2-1\right)^l$$

Associated Legendre functions

For example

$l = 0$

$$P_0^0(x) = 1$$

$l = 1$

$$P_1^0(x) = x$$

$$P_1^1(x) = \left(1 - x^2\right)^{1/2}$$

$$P_1^{-1}(x) = -\frac{1}{2}\left(1 - x^2\right)^{1/2}$$

$l = 2$

$$P_2^0(x) = \frac{1}{2}\left(3x^2 - 1\right)$$

$$P_2^1(x) = 3x\left(1 - x^2\right)^{1/2}$$

$$P_2^{-1}(x) = -\frac{1}{2}x\left(1 - x^2\right)^{1/2}$$

$$P_2^2(x) = 3\left(1 - x^2\right)$$

$$P_2^{-2}(x) = \frac{1}{8}\left(1 - x^2\right)$$

Associated Legendre functions

We see that these functions $P_l^m(x)$ have the following properties

- The highest power of the argument x is always x^l
- The functions for a given l for $+m$ and $-m$ are identical other than for numerical prefactors
- Less obviously

  between -1 and $+1$

    and not including the values at those end points

      the functions have $l-|m|$ zeros

Eigenfunctions of L^2

Putting this all together, the eigen equation is

$$\hat{L}^2 Y_{lm}(\theta,\phi) = \hbar^2 l(l+1) Y_{lm}(\theta,\phi)$$

with **spherical harmonics** $Y_{lm}(\theta,\phi)$ as the eigenfunctions

which, after normalization, can be written

$$Y_{lm}(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)\exp(im\phi)$$

where $l = 0,1,2,3,\ldots$, where m is an integer, $-l \le m \le l$

and the eigenvalues are $\hbar^2 l(l+1)$

Eigenfunctions of L^2 and L_z

As is easily verified

these spherical harmonics

are also eigenfunctions of the $\hat{L}_z$ operator

Explicitly, we have the eigen equation

$$\hat{L}_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

with eigenvalues of $\hat{L}_z$ being $m\hbar$

It makes no difference to the $\hat{L}_z$ eigenfunctions

if we multiply them by a function of θ