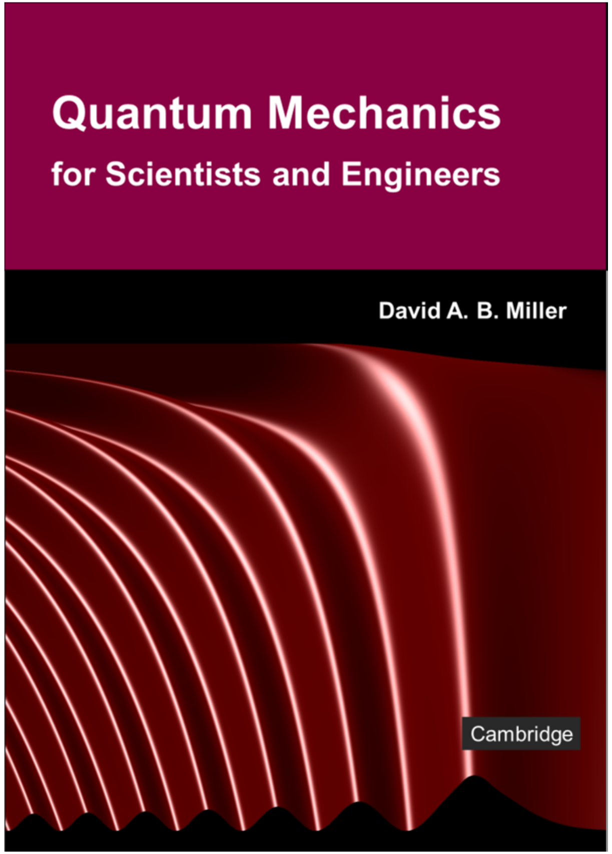
7.2 The L squared operator

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

David Miller

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

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

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 L^2

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

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

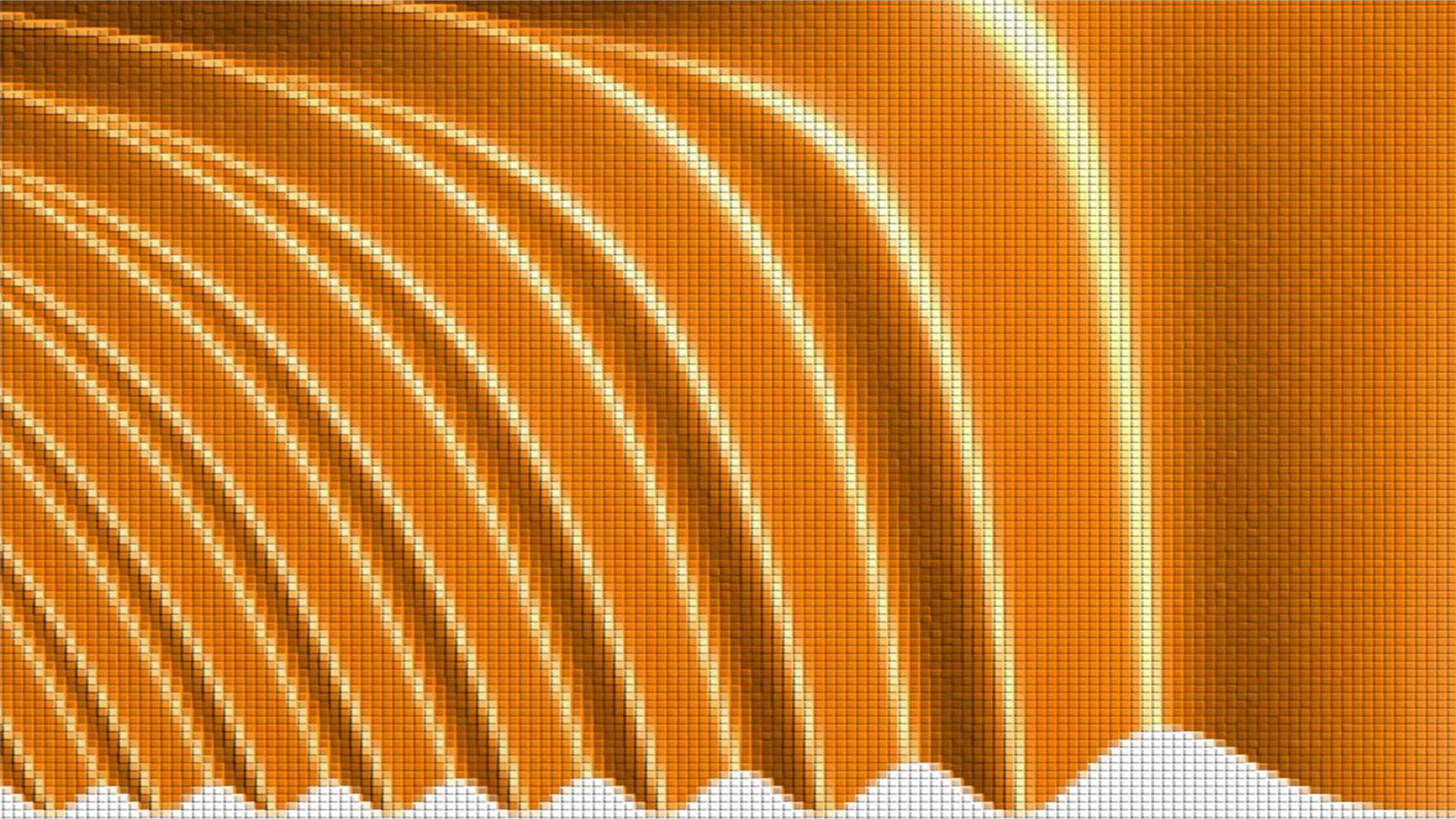
Explicitly, we have the eigen equation

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

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

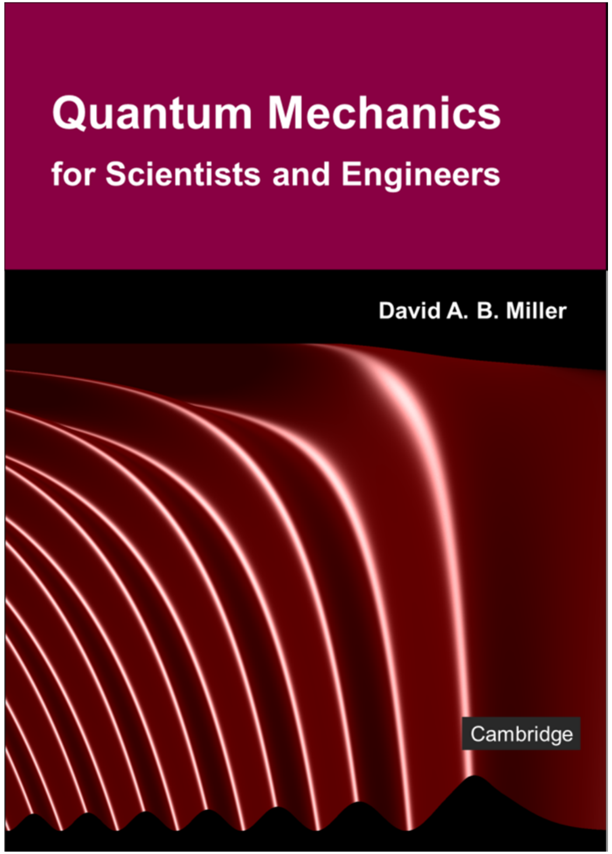


7.2 The L squared operator

Slides: Video 7.2.3 Visualizing spherical harmonics

Text reference: Quantum Mechanics for Scientists and Engineers

Section 9.3



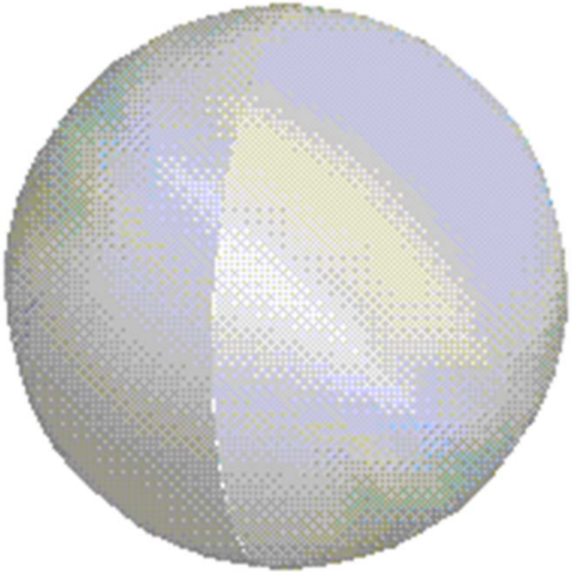
The L squared operator

Visualizing spherical harmonics

Quantum mechanics for scientists and engineers

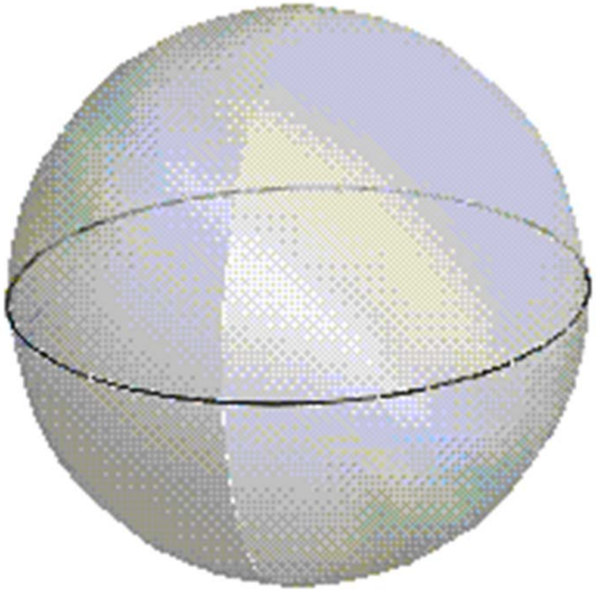
David Miller

Oscillating modes for spherical shell



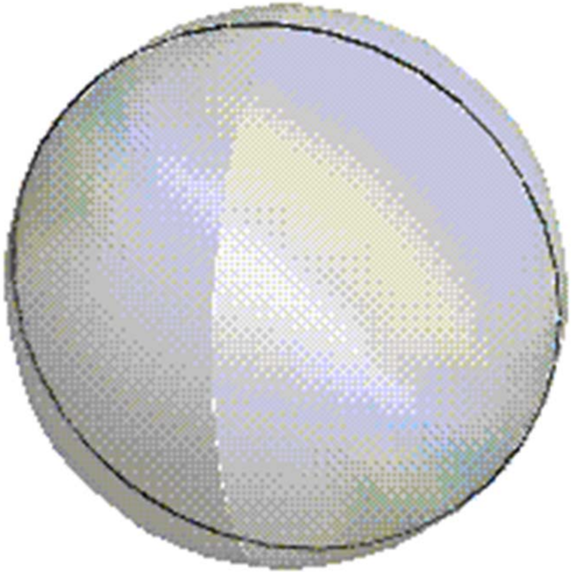
$l = 0$
$m = 0$

Oscillating modes for spherical shell



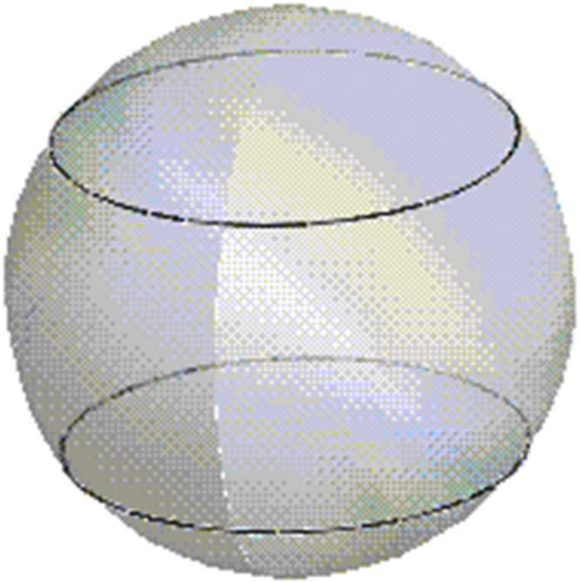
$$l = 1$$
$$m = 0$$

Oscillating modes for spherical shell



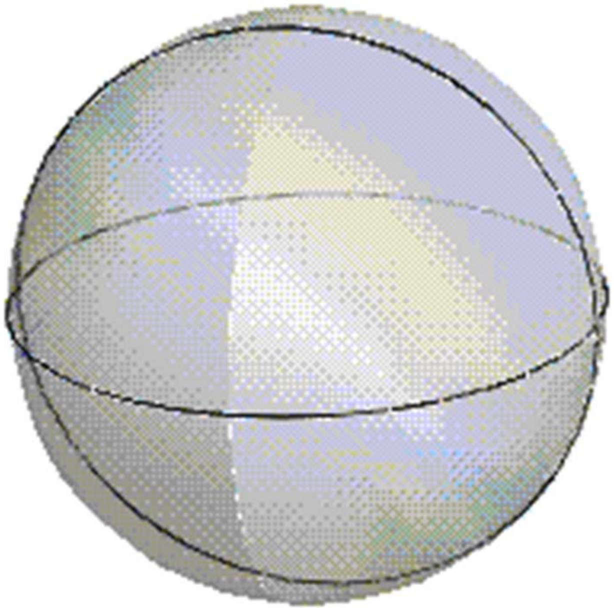
$l = 1$
$m = 1$

Oscillating modes for spherical shell



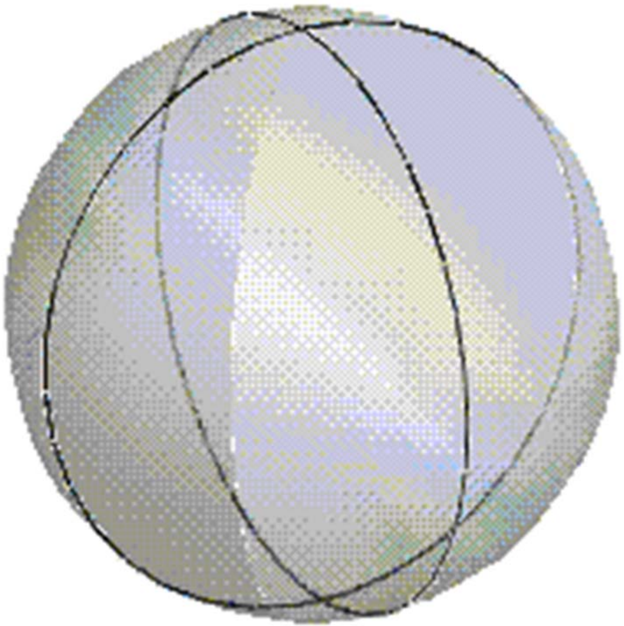
$l = 2$
$m = 0$

Oscillating modes for spherical shell



$l = 2$
$m = 1$

Oscillating modes for spherical shell



$l = 2$
$m = 2$

Constructing spherical harmonics for a shell

The lowest solution

$$l = 0, m = 0$$

- is the "breathing" mode
  - The spherical shell expands and contracts periodically

For all other solutions

- there are one or more nodal circles on the sphere
  - A nodal circle is one that is unchanged in that particular oscillating mode

Constructing spherical harmonics for a shell

Note the following rules for the spherical shell modes

- the surfaces on opposite sides of a nodal circle oscillate in opposite directions
- the total number of nodal circles is equal to l
- the number of nodal circles passing through the poles is m, and they divide the sphere equally in the azimuthal angle ϕ
- the remaining nodal circles are either equatorial or parallel to the equator

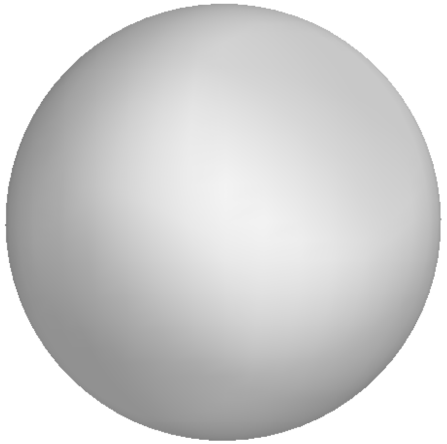
  symmetrically distributed between the top and bottom halves of the sphere

Spherical harmonics

We can formally also plot the spherical harmonic in a parametric plot

where the distance from the center at a given angle

represents the magnitude of amplitude of the spherical harmonic



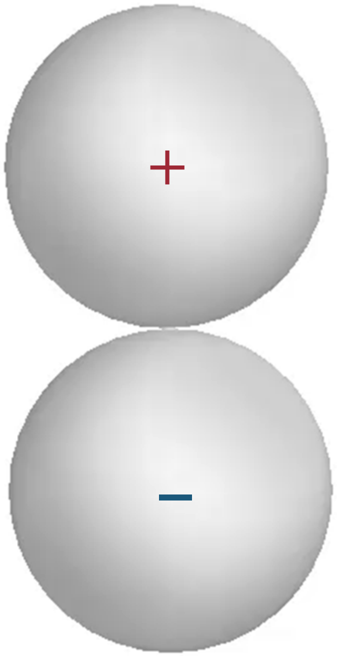
$$l = 0$$
$$m = 0$$

Spherical harmonics

We can formally also plot the spherical harmonic in a parametric plot

- where the distance from the center at a given angle
  - represents the magnitude of amplitude of the spherical harmonic
    - Adjacent “lobes” have opposite signs

$l = 1$
$m = 0$



Spherical harmonics

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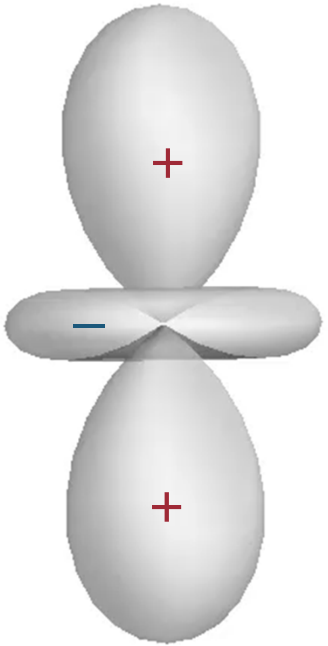
$l = 2$
$m = 0$



Spherical harmonics

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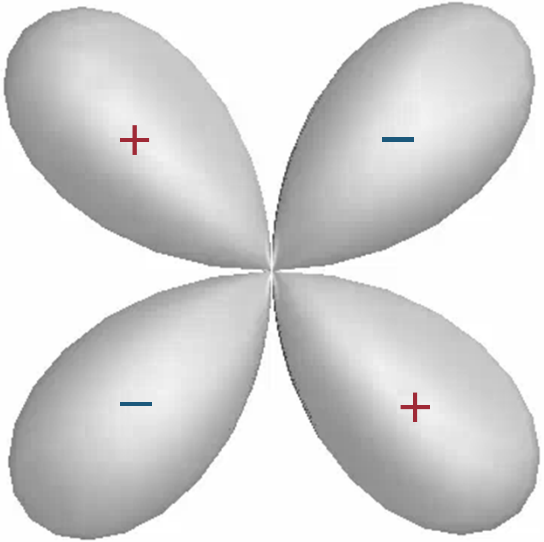
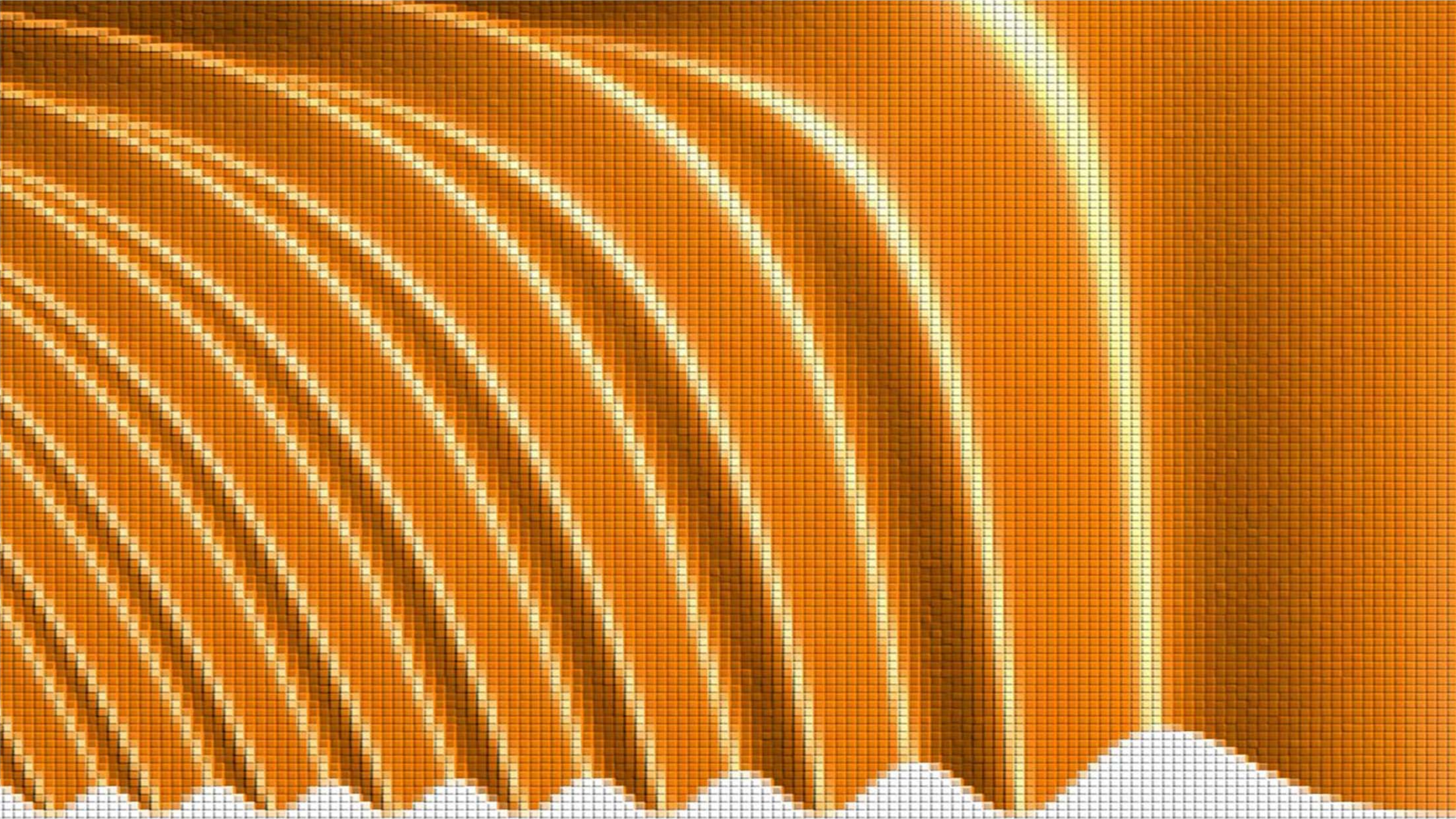


$l = 2$

$m = 1$

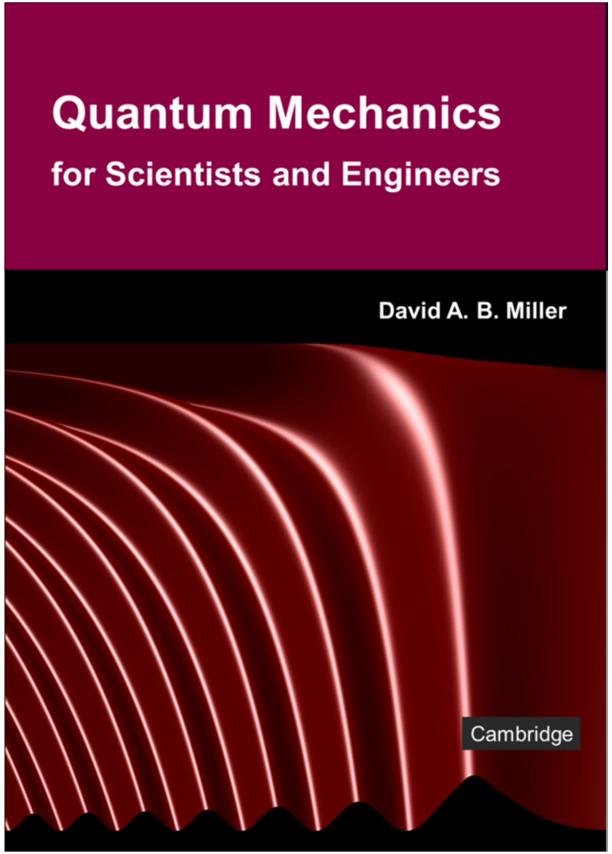


7.2 The L squared operator

Slides: Video 7.2.5 Notations for spherical harmonics

Text reference: Quantum Mechanics for Scientists and Engineers

Section 9.4



The L squared operator

Notations for spherical harmonics

Quantum mechanics for scientists and engineers

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Dirac notation

We often use Dirac notation

in writing equations associated with angular momentum

It is common to write

$$\hat{L}^2 \left| l,m \right\rangle = \hbar^2 l \left(l+1 \right) \left| l,m \right\rangle$$

instead of

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

and

$$\hat{L}_z \left| l,m \right\rangle = m\hbar \left| l,m \right\rangle$$

instead of

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

"s, p, d, f" notation

The spherical harmonics arise in the solution of the hydrogen atom problem

- Different values of l give rise to
  - different sets of spectral lines from hydrogen
    - identified empirically in the 19th century

Spectroscopists identified groups of lines called

- "sharp" (s)
- "principal" (p)
- "diffuse" (d), and
- "fundamental" (f)

“s, p, d, f” notation

Each of these is now identified with the specific values of l

Now we also alphabetically extend to higher l values

l	0	1	2	3	4	5
notation	s	p	d	f	g	h

It is convenient that

the “s” wavefunctions are all spherically symmetric

even though the “s” of the notation originally

had nothing to do with spherical symmetry