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Angular Momentum

(1) Leaping from 1d QM to 3d QM

(2) The separation of variables method

(3) Separating the radial and angular variables in spherical coordinates

(4) Separating the angular variables in spherical coordinates

(5) Other coordinate systems

WHERE WE ARE GOING

SOLVE ev, e$\hat{v}$ PROBLEM FOR ANGULAR MOMENTUM

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

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

$$L_\pm \, | \ell, m \rangle = \sqrt{\ell(\ell+1) - m(m \pm 1)} \; \hbar \, | \ell, m \pm 1 \rangle$$

THREE REPRESENTATIONS

DIRAC REP (IN THE HILBERT SPACE)

MATRIX REP (IN ANG MOMENTUM SPACE)

FUNCTION REP (IN POSITION SPACE θ, φ)

LECTURE ANGULAR MOMENTUM

TODAY: MOTIVATION

BACKGROUND

LADDER OP

NEXT TIME:

DIFF EQ SOLN

SPHERICAL HARMONICS

LEGENDRE POLYNOMIALS

MOTIVATION: We want to solve hydrogen problem

1d → 3d

classical analogue: planetary motion

$\vec{L}$ conserved

SHO $H = p^2 + x^2$

$a = x - ip$

$a^+ = x + ip$

$H = p_x^2 + p_y^2 + p_z^2 + V(\vec{x})$

$= \left[\frac{p_r^2}{2m} + V(\vec{r}) \right] + \frac{L^2}{2I}$

L^2 L_z

Analogy with SHO

Ladder Operators

$L_\pm = L_x \pm i L_y$

CLASSICALLY $\vec{L} = \vec{r} \times \vec{p}$

$$\vec{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

$$= (y p_z - z p_y)\hat{i} - (x p_z - z p_x)\hat{j} + (x p_y - y p_x)\hat{k}$$

QM

$$\boxed{\begin{aligned} L_{x\,op} &= y_{op} p_{z\,op} - z_{op} p_{y\,op} \\ L_{y\,op} &= -(x_{op} p_{z\,op} - z_{op} p_{x\,op}) \\ L_{z\,op} &= x_{op} p_{y\,op} - y_{op} p_{x\,op} \end{aligned}}$$

POSITION SPACE

$$x_{op} \to x \qquad p_{x\,op} \to -i\hbar\frac{\partial}{\partial x}$$

$$y_{op} \to y \qquad p_{y\,op} \to -i\hbar\frac{\partial}{\partial y}$$

$$z_{op} \to z \qquad p_{z\,op} \to -i\hbar\frac{\partial}{\partial z}$$

MOMENTUM SPACE

$$x_{op} \to i\hbar\frac{\partial}{\partial p_x} \qquad p_{x\,op} \to p_x$$

$$y_{op} \to i\hbar\frac{\partial}{\partial p_y} \qquad p_{y\,op} \to p_y$$

$$z_{op} \to i\hbar\frac{\partial}{\partial p_z} \qquad p_{z\,op} \to p_z$$

DEEP IDEA HERE

SYMMETRY $\longrightarrow$ CONSERVATION LAW

TRANSLATIONAL INVARIANCE $\longrightarrow$ LINEAR MOMENTUM CONSERVATION

ROTATIONAL INVARIANCE $\longrightarrow$ ANGULAR MOMENTUM CONSERVATION

TIME TRANSLATION INVARIANCE $\longrightarrow$ ENERGY CONSERVATION

UNITARY OPERATORS

TRANSLATION BY $\vec{a} = (a_x, a_y, a_z)$

$$T(\vec{a}) = e^{-i\vec{p}\cdot\vec{a}/\hbar}$$

$$T(\vec{b})\, T(\vec{a}) = T(\vec{a}+\vec{b})$$

$$[p_i, p_j] = 0$$

ROTATIONS

$$R(\vec{\theta}) = e^{-i\vec{L}\cdot\vec{\theta}/\hbar}$$

$$R(\theta_z) = e^{-iL_z\cdot\theta_z/\hbar}$$

in coordinates

$$L_z = x_{op}\, p_{y\,op} - y_{op}\, p_{x\,op}$$

$$= -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]$$

very messy to calculate ...

TIME TRANSLATION

$$U(t) = e^{-iHt/\hbar}$$

ROTATIONAL SYMMETRY $\Rightarrow$ WORK IN SPHERICAL COORDINATES

$$(x, y, z) \longrightarrow (r, \theta, \varphi)$$

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

$$L_x = i\hbar \left[\sin\varphi \frac{\partial}{\partial \theta} + \cos\varphi \cot\theta \frac{\partial}{\partial \varphi} \right]$$

$$L_y = i\hbar \left[-\cos\varphi \frac{\partial}{\partial \theta} + \sin\varphi \cot\theta \frac{\partial}{\partial \varphi} \right]$$

$$L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

$$L^2 = -\hbar^2 \left[\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan\theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

LADDER OPERATORS $L_\pm = L_x \pm i L_y$

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

Simultaneous Eigenvalue Problem

EIGENVALUE PROBLEM

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

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

IF H IS ROTATIONALLY INVARIANT

$$\boxed{\begin{aligned} [H, L_i] &= 0 \\ [H, L^2] &= 0 \\ [H, L_z] &= 0 \end{aligned}}$$

Complete Set of Commuting Observables

(H eigenfcns) = (radial eigenfcn)(spherical harmonic)

LADDER OPERATOR SOLUTION

$$L^2 = \vec{L} \cdot \vec{L} = L_x^2 + L_y^2 + L_z^2$$

$$[L_i, L_j] = i\hbar \, \epsilon_{ijk} L_k$$

EINSTEIN SUMMATION OVER K.

$\boxed{\text{SEPARATION OF VARIABLES}}$

DIFF EQN (x, y, z)

TRY PRODUCT SOLUTION $\psi(\vec{r}) = X(x)\, Y(y)\, Z(z)$

Cartesian Ansatz

PUT IN DIFF EQN

REARRANGE TERMS SO ONLY ONE VARIABLE ON RHS

IF POSSIBLE, THEN THAT VARIABLE SEPARATES

$$\text{FCN}(x, y) = \text{FCN}'(z)$$

ONLY POSSIBLE IF CONSTANT

$$\text{FCN}(x, y) = \text{FCN}'(z) = \text{CONSTANT}$$

CALLED SEPARATION CONSTANT

$$\boxed{TDSE \Rightarrow TISE}$$

$$\boxed{H\,\psi(\vec{r},t) = i\hbar \frac{d}{dt}\,\psi(\vec{r},t)}$$

Start with TDSE

$$\psi(\vec{r},t) = \varphi(\vec{r})\;T(t)$$

Space Time Ansatz

$$H\Big(\varphi(\vec{r})\;T(t)\Big) = i\hbar \frac{d}{dt}\Big(\varphi(\vec{r})\;T(t)\Big)$$

$$T(t)\;H\,\varphi(\vec{r}) = \varphi(\vec{r})\left(i\hbar\,\frac{dT}{dt}\right)$$

MULTIPLY BOTH SIDES BY (PRODUCT ANSATZ)$^{-1}$

$$\frac{\cancel{T(t)}\big(H\,\varphi(\vec{r})\big)}{\varphi(\vec{r})\;\cancel{T(t)}} = \frac{\cancel{\varphi(\vec{r})}\left(i\hbar\,\frac{dT}{dt}\right)}{\cancel{\varphi(\vec{r})}\;T(t)} = \text{CONSTANT}$$

out comes the TISE ...

$$H\,\varphi(\vec{r}) = E\,\varphi(\vec{r}) \qquad\qquad i\hbar\,\frac{dT}{dt} = E\;T(t)$$

... and the time-dependent phase factors

$$e^{-iEt/\hbar}$$

position of the proton and the position of the electron

separate into center-of-mass and relative coordinates

SOLVING H ATOM DIFF EQ

SEPARATE TDSE => TISE

$\psi(r, \theta, \varphi, t) \Rightarrow \psi(r, \theta, \varphi)\, T(t)$

SEPARATE TISE

$\psi(r, \theta, \varphi) \Rightarrow R_{n\ell}(r)$ RADIAL EQN

RADIAL WAVEFCNS

$\Rightarrow Y_{\ell m}(\theta, \varphi)$ ANGULAR EQN

SPHERICAL HARMONICS

SEPARATE $Y_{\ell m}(\theta, \varphi) \Rightarrow e^{im\varphi}$ PHI DEPENDENCE

$P_{\ell m}(\theta)$ ASSOCIATED LEGENDRE FCNS

$P_{\ell}(\theta)$ LEGENDRE POLYNOMIALS

TISE FOR $\psi_m(\vec{r})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi_m(r) = E_m(r)$$

$$-\frac{\hbar^2}{2m}\left[\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial\psi_m}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_m}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi_m}{\partial\varphi^2}\right)\right.$$

$$\left. + V(r)\right]\psi_m(r) = E_m\psi_m(r)$$

ANSATZ $\quad \psi_m(r) = R(r)\,Y(\theta,\varphi)$

$\qquad\qquad R_n \qquad Y_{lm}$

SEPARATES $\rightarrow R_n$ RADIAL EQN

$\qquad\searrow Y_{lm}$ ANGULAR EQN

product ansatz for relative coordinate TISE separates it into radial and angular components

Chapter 10 The Hydrogen Atom

There are many good reasons to address the hydrogen atom beyond its historical significance. Though hydrogen spectra motivated much of the early quantum theory, research involving the hydrogen remains at the cutting edge of science and technology. For instance, transitions in hydrogen are being used in 1997 and 1998 to examine the constancy of the fine structure constant over a cosmological time scale[2]. From the view point of pedagogy, the hydrogen atom merges many of the concepts and techniques previously developed into one package. It is a particle in a box with spherical, soft walls. Finally, the hydrogen atom is one of the precious few realistic systems which can actually be solved analytically.

The Schrodinger Equation in Spherical Coordinates

In chapter 5, we separated time and position to arrive at the time independent Schrodinger equation which is

$$\mathcal{H}\,\big|E_i\!> = E_i\big|E_i\!>, \tag{10 – 1}$$

where E_i are eigenvalues and $\big|E_i\!>$ are energy eigenstates. Also in chapter 5, we developed a one dimensional position space representation of the time independent Schrodinger equation, changing the notation such that $E_i \to E$, and $\big|E_i\!> \to \psi$. In three dimensions the Schrodinger equation generalizes to

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi,$$

where ∇^2 is the Laplacian operator. Using the Laplacian in spherical coordinates, the Schrodinger equation becomes **[Laplacian operator in spherical coordinates]**

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi + V(r)\psi = E\psi. \tag{10 – 2}$$

radial
angular
ansatz

In spherical coordinates, $\psi = \psi(r,\theta,\phi)$, and the plan is to look for a variables separable solution such that $\boxed{\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi).}$ We will in fact find such solutions where $Y(\theta,\phi)$ are the spherical harmonic functions and $R(r)$ is expressible in terms of associated Laguerre functions. Before we do that, interfacing with the previous chapter and arguments of linear algebra may partially explain why we are proceeding in this direction.

Complete Set of Commuting Observables for Hydrogen

Though we will return to equation (10–2), the Laplacian can be expressed

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \tag{10 – 3}$$

Compare the terms in parenthesis to equation 11–33. The terms in parenthesis are equal to $-\mathcal{L}^2/\hbar^2$, so assuming spherical symmetry, the Laplacian can be written

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\mathcal{L}^2}{r^2\hbar^2},$$

Laplacian operator in spherical coordinates

[2] Schwarzschild. "Optical Frequency Measurement is Getting a Lot More Precise," Physics Today 50(10) 19–21 (1997).

and the Schrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\mathcal{L}^2}{r^2\hbar^2} \right) + V(r) \right] \psi = E\psi. \qquad \textbf{TISE} \tag{10 – 4}$$

Assuming spherical symmetry, which we will have because a Coulomb potential will be used for $V(r)$, we have complicated the system of chapter 11 by adding a radial variable. Without the radial variable, we have a complete set of commuting observables for the angular momentum operators in $\mathcal{L}^2$ and $\mathcal{L}_z$. Including the radial variable, we need a minimum of one more operator, if that operator commutes with both $\mathcal{L}^2$ and $\mathcal{L}_z$. The total energy operator, the Hamiltonian, may be a reasonable candidate. What is the Hamiltonian here? It is the group of terms within the square brackets. Compare equations (10–1) and (10–4) if you have difficulty visualizing that. In fact,

$$\boxed{\left[\mathcal{H}, \, \mathcal{L}^2 \right] = 0, \qquad \text{and} \qquad \left[\mathcal{H}, \, \mathcal{L}_z \right] = 0,}$$

so the Hamiltonian is a suitable choice. The complete set of commuting observables for the hydrogen atom is $\mathcal{H}$, $\mathcal{L}^2$, and $\mathcal{L}_z$. We have all the eigenvalue/eigenvector equations, because the time independent Schrodinger equation is the eigenvalue/eigenvector equation for the Hamiltonian operator, *i.e.*, the the eigenvalue/eigenvector equations are

$$\boxed{\begin{aligned} \mathcal{H}\left|\psi\right> &= E_n\left|\psi\right>, \\ \mathcal{L}^2\left|\psi\right> &= l(l+1)\hbar^2\left|\psi\right>, \\ \mathcal{L}_z\left|\psi\right> &= m\hbar\left|\psi\right>, \end{aligned}}$$

simultaneous eigenvalue eigenvector problem

where we subscripted the energy eigenvalue with an n because that is the symbol conventionally used for the energy quantum number (per the particle in a box and SHO). Then the solution to the problem is the eigenstate which satisfies all three, denoted $\left|n, l, m\right>$ in abstract Hilbert space. The representation in position space in spherical coordinates is

$$\left<r, \theta, \phi\right|\left.n, l, m\right> = \psi_{nlm}(r, \theta, \phi).$$

Example 10–1: Starting with the Laplacian included in equation (10–2), show the Laplacian can be express as equation (10–3).

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\ &= \frac{1}{r^2}\left(2r\frac{\partial}{\partial r} + r^2\frac{\partial^2}{\partial r^2} \right) + \frac{1}{r^2\sin\theta}\left(\cos\theta\frac{\partial}{\partial\theta} + \sin\theta\frac{\partial^2}{\partial\theta^2} \right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\ &= \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\ &= \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right), \end{aligned}$$

which is the form of equation (10–3).

Example 10–2: Show $\left[\mathcal{H}, \, \mathcal{L}^2 \right] = 0$.

$$\left[\mathcal{H}, \, \mathcal{L}^2 \right] = \mathcal{H}\,\mathcal{L}^2 - \mathcal{L}^2\,\mathcal{H}$$

Separating Radial and Angular Dependence

In this and the following three sections, we illustrate how the angular momentum and magnetic moment quantum numbers enter the symbology from a calculus based argument. In writing equation (10–2), we have used a representation, so are no longer in abstract Hilbert space. One of the consequences of the process of representation is the topological arguments of linear algebra are obscured. They are still there, simply obscured because the special functions we use are orthogonal, so can be made orthonormal, and complete, just as bras and kets in a dual space are orthonormal and complete. The primary reason to proceed in terms of a position space representation is to attain a position space description. One of the by–products of this chapter may be to convince you that working in the generality of Hilbert space in Dirac notation can be considerably more efficient. Since we used topological arguments to develop angular momentum in the last chapter, and arrive at identical results to those of chapter 11, we rely on connections between the two to establish the meanings of of l and m. They have the same meanings within these calculus based discussions.

As noted, we assume a variables separable solution to equation (10–2) of the form

product ansatz

$$\boxed{\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi).} \qquad (10-5)$$

An often asked question is "How do you know you can assume that?" You do not know. You assume it, and if it works, you have found a solution. If it does not work, you need to attempt other methods or techniques. Here, it will work. Using equation (10–5), equation (10–2) can be written **put it into the TISE**

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r)\,Y(\theta,\phi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)R(r)\,Y(\theta,\phi)$$
$$+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}R(r)\,Y(\theta,\phi) - \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R(r)\,Y(\theta,\phi) = 0$$
$$\Rightarrow \quad Y(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) + R(r)\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi)$$
$$+R(r)\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) - \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R(r)\,Y(\theta,\phi) = 0.$$

mess around

Dividing the equation by $R(r)\,Y(\theta,\phi)$, multiplying by r^2, and rearranging terms, this becomes

$$\left\{\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) - \frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big]\right\}$$
$$+\left[\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)\right] = 0.$$

The two terms in the curly braces depend only on r, and the two terms in the square brackets depend only upon angles. With the exception of a trivial solution, the only way the sum of the groups can be zero is if each group is equal to the same constant. The constant chosen is known as the **separation constant**. Normally, an arbitrary separation constant, like K, is selected and then you solve for K later. In this example, we are instead going to stand on the shoulders of some of the physicists and mathematicians of the previous 300 years, and make the enlightened choice of $l(l+1)$ as the separation constant. It should become clear l is the angular momentum quantum number introduced in chapter 11. Then

Radial Equation
$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) - \frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big] = l(l+1) \qquad (10-6)$$

which we call the **radial equation**, and

Angular Eqn
$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) + \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi) = -l(l+1), \qquad (10-7)$$

which we call the **angular equation**. Notice the signs on the right side are opposite so they do, in fact, sum to zero.

solutions are the spherical harmonics

The Angular Equation

they also separate

The solutions to equation (10–7) are the spherical harmonic functions, and the l used in the separation constant is, in fact, the same used as the index l in the spherical harmonics $Y_{l,m}(\theta,\phi)$. In fact, it is the angular momentum quantum number. But where is the index m? How is the magnetic moment quantum number introduced? To answer these questions, remember the spherical harmonics are also separable, *i.e.*, $\boxed{Y_{l,m}(\theta,\phi) = f_{l,m}(\theta)\,g_m(\phi)}$. We will use such a solution in the angular equation, without the indices until we see where they originate. Using the solution $Y(\theta,\phi) = f(\theta)\,g(\phi)$ in equation (10–7),

product ansatz

put it in
$$\frac{1}{f(\theta)\,g(\phi)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)\,g(\phi) + \frac{1}{f(\theta)\,g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}f(\theta)\,g(\phi) = -l(l+1)$$

$$\Rightarrow\quad \frac{1}{f(\theta)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta) + \frac{1}{g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}g(\phi) = -l(l+1).$$

Multiplying the equation by $\sin^2\theta$ and rearranging,

mess around
$$\frac{\sin\theta}{f(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta) + l(l+1)\,\sin^2\theta + \frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi) = 0.$$

only theta — only phi

The first two terms depend only on θ, and the last term depends only on ϕ. Again, the only non–trivial solution such that the sum is zero is if the groups of terms each dependent on a single variable is equal to the same constant. Again using an enlightened choice, we pick m^2 as the separation constant, so

theta and phi separate

$$\frac{\sin\theta}{f(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)f(\theta) + l(l+1)\,\sin^2\theta = m^2, \qquad (10-8)$$

$$\frac{1}{g(\phi)}\frac{d^2}{d\phi^2}g(\phi) = -m^2, \qquad (10-9)$$

and that is how the magnetic moment quantum number is introduced. Again, (10–8) and (10–9) need to sum to zero so the separation constant has opposite signs on the right side in the two equations.

The Azimuthal Angle Equation

The solution to the azimuthal angle equation, equation (10–9), is

$$g(\phi) = e^{im\phi} \quad \Rightarrow \quad \boxed{g_m(\phi) = e^{im\phi},} \qquad \textbf{solutions} \qquad (10-10)$$

where the subscript m is added to $g(\phi)$ because it is now clear there are as many solutions as there are allowed values of m.

Example 10–4: Show $g_m(\phi) = e^{im\phi}$ is a solution to equation (10–9).

$$\frac{d^2}{d\phi^2} g_m(\phi) = \frac{d^2}{d\phi^2} e^{im\phi} = \frac{d}{d\phi}(im)e^{im\phi} = (im)^2 e^{im\phi} = -m^2 g_m(\phi).$$

Using this in equation (10–9),

$$\frac{1}{g(\phi)} \frac{d^2}{d\phi^2} g(\phi) = -m^2 \quad \Rightarrow \quad \frac{1}{g(\phi)} \Big(-m^2 g_m(\phi) \Big) = -m^2 \quad \Rightarrow \quad -m^2 = -m^2,$$

therefore $g_m(\phi) = e^{im\phi}$ is a solution to equation (10–9).

The Polar Angle Equation

This section is a little more substantial than the last. Equation (10–8) can be written

theta equation

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

Evaluating the first term,

do the derivatives

$$\begin{aligned}
\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d}{d\theta}\right) f(\theta) &= \sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\,f(\theta)}{d\theta}\right) \\
&= \sin\theta \left(\cos\theta \frac{d\,f(\theta)}{d\theta} + \sin\theta \frac{d^2 f(\theta)}{d\theta^2}\right) \\
&= \sin^2\theta \frac{d^2 f(\theta)}{d\theta^2} + \sin\theta\,\cos\theta \frac{d\,f(\theta)}{d\theta}.
\end{aligned}$$

Using this, equation (10–8) becomes

=>

$$\sin^2\theta \frac{d^2 f(\theta)}{d\theta^2} + \sin\theta\,\cos\theta \frac{d\,f(\theta)}{d\theta} + l(l+1) \sin^2\theta \, f(\theta) - m^2 f(\theta) = 0. \qquad (10-11)$$

We are going to change variables using $x = \cos\theta$, and will comment on this substitution later. We then need the derivatives with respect to x vice θ, so

change variables

$$\frac{d\,f(\theta)}{d\theta} = \frac{d\,f(x)}{dx}\frac{dx}{d\theta} = \frac{d\,f(x)}{dx}\big(-\sin\theta\big) = -\sin\theta \frac{d\,f(x)}{dx},$$

and

$$\frac{d^2 f(\theta)}{d\theta^2} = \frac{d}{d\theta}\left(-\sin\theta\,\frac{d\,f(x)}{dx}\right) = -\cos\theta\,\frac{d\,f(x)}{dx} - \sin\theta\,\frac{d}{d\theta}\,\frac{d\,f(x)}{dx}$$
$$= -\cos\theta\,\frac{d\,f(x)}{dx} - \sin\theta\,\frac{d}{dx}\,\frac{dx}{d\theta}\,\frac{d\,f(x)}{dx} = -\cos\theta\,\frac{d\,f(x)}{dx} - \sin\theta\,\frac{d}{dx}\Big(-\sin\theta\Big)\frac{d\,f(x)}{dx}$$
$$= -\cos\theta\,\frac{d\,f(x)}{dx} + \sin^2\theta\,\frac{d^2\,f(x)}{dx^2}.$$

Substituting just the derivatives in the equation (10–11),

$$\sin^2\theta\left(\sin^2\theta\frac{d^2\,f(x)}{dx^2} - \cos\theta\,\frac{d\,f(x)}{dx}\right) + \sin\theta\cos\theta\left(-\sin\theta\frac{d\,f(x)}{dx}\right) + l(l+1)\sin^2\theta f(x) - m^2\,f(x) = 0,$$

which gives us an equation in both θ and x, which is not formally appropriate. This is, however, an informal text, and it becomes difficult to keep track of the terms if all the substitutions and reductions are done at once. Dividing by $\sin^2\theta$, we get

$$\sin^2\theta\,\frac{d^2\,f(x)}{dx^2} - \cos\theta\,\frac{d\,f(x)}{dx} - \cos\theta\,\frac{d\,f(x)}{dx} + l(l+1)\,f(x) - \frac{m^2}{\sin^2\theta}f(x) = 0.$$

The change of variables is complete upon summing the two first derivatives, using $\cos\theta = x$, and $\sin^2\theta = 1 - \cos^2\theta = 1 - x^2$, which is

in the new variable x

$$\left(1-x^2\right)\frac{d^2\,f(x)}{dx^2} - 2x\,\frac{d\,f(x)}{dx} + l(l+1)\,f(x) - \frac{m^2}{1-x^2}f(x) = 0.$$

This is the **associated Legendre equation**, which reduces to **Legendre equation** when $m = 0$. The function has a single argument so there is no confusion if the derivatives are indicated with primes, and the associated Legendre equation is often written

$$\left(1-x^2\right)f''(x) - 2x\,f'(x) + l(l+1)\,f(x) - \frac{m^2}{1-x^2}f(x) = 0,$$

and becomes the Legendre equation, **when m=0, reduces to the Legendre equation**

$$\left(1-x^2\right)f''(x) - 2x\,f'(x) + l(l+1)\,f(x) = 0,$$

when $m = 0$. The solutions to the associated Legendre equation are the associated Legendre polynomials discussed briefly in the last section of chapter 11. To review that in the current context, associated Legendre polynomials can be generated from Legendre polynomials using

Legendre polynomials

$$P_{l,m}(x) = (-1)^m\sqrt{(1-x^2)^m}\,\frac{d^m}{dx^m}P_l(x),$$

where the $P_l(x)$ are Legendre polynomials. Legendre polynomials can be generated using

$$P_l(x) = \frac{(-1)^l}{2^l l!}\,\frac{d^l}{dx^l}(1-x^2)^l.$$

generating function

The use of these generating functions was illustrated in example 11–26 as intermediate results in calculating spherical harmonics.

The first few Legendre polynomials are listed in table 10–1. Our interest in those is to generate associated Legendre functions. The first few associated Legendre polynomials are listed in table 10–2.

no azimuthal dependence

$P_0(x) = 1$	$P_3(x) = \frac{1}{2}\big(5x^3 - 3x\big)$
$P_1(x) = x$	$P_4(x) = \frac{1}{8}\big(35x^4 - 30x^2 + 3\big)$
$P_2(x) = \frac{1}{2}\big(3x^2 - 1\big)$	$P_5(x) = \frac{1}{8}\big(63x^5 - 70x^3 + 15x\big)$

Table 10 – 1. The First Six Legendre Polynomials.

$P_{0,0}(x) = 1$	$P_{2,0}(x) = \frac{1}{2}\big(3x^2 - 1\big)$
$P_{1,1}(x) = -\sqrt{1-x^2}$	$P_{3,3}(x) = -15\big(\sqrt{1-x^2}\big)^3$
$P_{1,0}(x) = x$	$P_{3,2}(x) = 15x\,\big(1-x^2\big)$
$P_{2,2}(x) = 3\big(1-x^2\big)$	$P_{3,1}(x) = -\frac{3}{2}\big(5x^2 - 1\big)\sqrt{1-x^2}$
$P_{2,1}(x) = -3x\,\sqrt{1-x^2}$	$P_{3,0}(x) = \frac{1}{2}\big(5x^3 - 3x\big)$

Table 10 – 2. The First Few Associated Legendre Polynomials.

Two comment concerning the tables are appropriate. First, notice $P_l = P_{l,0}$. That makes sense. If the Legendre equation is the same as the associated Legendre equation with $m = 0$, the solutions to the two equations must be the same when $m = 0$. Also, many authors will use a positive sign for all associated Legendre polynomials. This is a different choice of phase. We addressed that following table 11–1 in comments on spherical harmonics. We choose to include a factor of $(-1)^m$ with the associated Legendre polynomials, and the sign of all spherical harmonics will be positive as a result.

Finally, remember the change of variables $x = \cos\theta$. That was done to put the differential equation in a more elementary form. In fact, a dominant use of associated Legendre polynomials is in applications where the argument is $\cos\theta$. One example is the generating function for spherical harmonic functions,

include azimuthal dependence

spherical harmonics

$$Y_{l,m}(\theta,\phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\, P_{l,m}(\cos\theta)\, e^{im\phi} \qquad m \geq 0, \qquad (10-10)$$

and

$$Y_{l,-m}(\theta,\phi) = Y^*_{l,m}(\theta,\phi), \qquad m < 0,$$

where the $P_{l,m}(\cos\theta)$ are associated Legendre polynomials. If we need a spherical harmonic with $m < 0$, we will calculate the spherical harmonic with $m = |m|$, and then calculate the adjoint.

To summarize the last three sections, we separated the angular equation into an azimuthal and a polar portion. The solutions to the azimuthal angle equation are exponentials including the magnetic moment quantum number in the argument. The solutions to the polar angle equation are the associated Legendre polynomials, which are different for each choice of orbital angular momentum and magnetic moment quantum number. Both quantum numbers are introduced into in 3d

THREE STANDARD COORDINATE SYSTEMS

CARTESIAN x, y, z

SPHERICAL r, θ, φ

CYLINDRICAL ρ, θ, z

∇^2 LOOKS DIFFERENT!

SOLUTIONS ARE DIFFERENT

OF COURSE, YOU CAN USE ANY COORDINATE SYSTEM

" IF THE BOUNDARY CONDITIONS ARE NOT SEPARABLE, MOST LIKELY WE ARE HOSED."

→ NEXT PAGE

http://quantumrelativity.calsci.com/Physics/EandM7.html

If the boundary conditions are not separable, most likely we're hosed

Generally speaking, if the boundary conditions are separable, there's a good chance the solution is separable. If the boundary conditions are not separable, most likely we're hosed.

This is Bessel's equation. The solutions are Bessel functions, Neumann functions, and Hankel functions, and we've officially entered Graduate Student Hell.

http://www.urbandictionary.com/define.php?term=hosed

$$\boxed{\begin{array}{l}\text{IN 3d} \quad \nabla^2 V = 0 \\ \text{SEPARATES IN } 11 + 2 = 13 \text{ COORD SYSTEMS}\end{array}}$$

$V(x,y,z) = X(x)\,Y(y)\,Z(z)$ CARTESIAN

$V(r,\theta,\varphi) = R(r)\,\Theta(\theta)\,\Phi(\varphi)$ SPHERICAL

$V(r,\theta,z) = R(r)\,\Theta(\theta)\,Z(z)$ CYLINDRICAL

Cartesian Coordinates

ONE EQN FOR EACH COORD

$$\frac{d^2 X}{dx^2} = c_1 X$$

$$\frac{d^2 Y}{dy^2} = c_2 Y$$

$$\frac{d^2 Z}{dz^2} = c_3 Z$$

$$c_1 + c_2 + c_3 = 0$$

Coordinate System	Variables	Solution Functions
=> Cartesian	$X(x)Y(y)Z(z)$	exponential functions, circular functions, hyperbolic functions
=> circular cylindrical	$R(r)\Theta(\theta)Z(z)$	Bessel functions, exponential functions, circular functions
conical		ellipsoidal harmonics, power
ellipsoidal	$\Lambda(\lambda)M(\mu)N(\nu)$	ellipsoidal harmonics
elliptic cylindrical	$U(u)V(v)Z(z)$	Mathieu function, circular functions
oblate spheroidal	$\Lambda(\lambda)M(\mu)N(\nu)$	Legendre polynomial, circular functions
=> parabolic		Bessel functions, circular functions
parabolic cylindrical		parabolic cylinder functions, Bessel functions, circular functions
paraboloidal	$U(u)V(v)\Theta(\theta)$	circular functions
prolate spheroidal	$\Lambda(\lambda)M(\mu)N(\nu)$	Legendre polynomial, circular functions
=> spherical	$R(r)\Theta(\theta)\Phi(\phi)$	Legendre polynomial, power, circular functions

Laplace's equation can be solved by separation of variables in all 11 coordinate systems that the Helmholtz differential equation can. The form these solutions take is summarized in the table above. In addition to these 11 coordinate systems, separation can be achieved in two additional coordinate systems by introducing a multiplicative factor. In these coordinate systems, the separated form is

http://mathworld.wolfram.com/LaplacesEquation.html

LECTURE 11 7-10-09

GENERAL SOLUTION

General Solutions

CARTESIAN

$$V(x,y,z) \sim e^{\pm i\alpha x}\ e^{\pm i\beta y}\ e^{\pm \gamma z}$$

SPHERICAL (AXIAL SYMMETRY)

$$V(r,\theta) = \sum_{\ell=0}^{\infty} \left[A_\ell r^\ell + B_\ell \frac{1}{r^{\ell+1}} \right] P_\ell(\cos\theta)$$

LEGENDRE POLYNOMIALS

SPHERICAL (WO AXIAL SYMMETRY)

$$V(r,\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \left[A_\ell r^\ell + B_\ell \frac{1}{r^{\ell+1}} \right] Y_{\ell m}(\theta,\varphi)$$

SPHERICAL HARMONICS

CYLINDRICAL (W CYLINDRICAL SYMMETRY)

$$V(r,\theta) = A_0 + B_0 \ln r + \sum_{m=1}^{\infty} \left[A_m r^m + B_m \frac{1}{r^m} \right] \left[C_m \cos(m\theta) + D_m \sin(m\theta) \right]$$

CYLINDRICAL HARMONICS

$$\boxed{\text{CYLINDRICAL} \quad (\text{WO CYLINDRICAL SYMMETRY})}$$

$$V(r,\theta,z) \sim \sum_{\substack{m\\n}} \left[A_{mn} J_n(k_m r) + B_{mn} N_n(k_m r) \right]$$

$$e^{\pm i n \theta} \qquad e^{\pm k_m (z)}$$

$J_n \; N_n$ CYLINDRICAL BESSEL FCNS

Spherical Coordinates

SPHERICAL COORDINATES

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2} = 0$$

$\Phi(r,\theta,\varphi) = R(r)P(\theta)Q(\varphi)$ **product ansatz**

$$\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{r^2 P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{1}{r^2 Q\sin^2\theta}\frac{d^2Q}{d\varphi^2} = 0$$

multiply with $r^2\sin^2\theta$:

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) = -\frac{1}{Q}\frac{d^2Q}{d\varphi^2}$$

The left-hand side depends only on r and θ, while the right-hand side depends only on ϕ. Thus the two sides must be a constant, m^2.

$$\frac{d^2Q}{d\varphi^2} + m^2Q = 0 \quad ; \quad Q(\varphi) \sim e^{\pm im\varphi} \quad ; \quad m = 0,1,2\ldots$$

azimuthal solutions

Note: If the physical problem limits ϕ to a restricted range m can be a non-integer.

Now we return to the left-hand side and rearrange the terms:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{1}{P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{m^2}{\sin^2\theta}$$

The new left-hand side depends only on r and the right-hand side on only θ. Thus, they must be a constant, $l(l+1)$.

We get

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-l(l+1)R=0$$ **radial equation**

and

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

To solve the first, we make the ansatz: $R=Ar^{\alpha}$ and obtain the two solutions r^{l} and $r^{-(l+1)}$. The general solution is then

$$R_l(r)=A_l r^l+B_l\frac{1}{r^{l+1}}$$ **solutions to the radial equation**

For the polar-angle function $P(\theta)$ it is customary to make the substitution

$$\cos\theta\rightarrow x \quad ; \quad -\frac{1}{\sin\theta}\frac{d}{d\theta}\rightarrow\frac{d}{dx}$$

This gives **associated Legendre equation**

$$\frac{d}{dx}\left[\left(1-x^2\right)\frac{dP}{dx}\right]+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P=0$$

We will first limit ourselves to axial or azimuthal symmetry.

Axial symmetry

if m=0

$$\boxed{\left(1-x^2\right)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+l(l+1)P=0}$$

Legendre's equation

Note that if $x=\pm 1$ are excluded from the problem l may be non-integer.

The solution is the *Legendre polynomial* of order l: $P_l(\cos\theta)$

Thus we have the general solution to Laplace's equation in spherical coordinates for the special case of axial symmetry as:

$$\boxed{\Phi(r,\theta)=\sum_{l=0}^{\infty}\left[A_l r^l+B_l\frac{1}{r^{l+1}}\right]P_l(\cos\theta)}$$

the general solution when the problem has axial symmetry

The Legendre polynomials can be obtained from

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

Rodrigues' formula

or from the *generating function*

$$F(x,\mu)=\frac{1}{\left(1-2x\mu+\mu^2\right)^{1/2}}=\sum_{l=0}^{\infty}\mu^l P_l(x)$$

or from *recursion relations* such as:

$$(l+1)P_{l+1}(x)=(2l+1)xP_l(x)-lP_{l-1}(x)$$

or

$$\left(1-x^2\right)\frac{dP_l}{dx}=-lxP_l(x)+lP_{l-1}(x)$$

The polynomials form a *complete, orthogonal set* of functions in the domain -1≤x≤1 (0≤θ≤π)

$$f(x) = \sum_{l=0}^{\infty} A_l P_l(x)$$

$$A_l = \frac{2l+1}{2} \int_{-1}^{1} f(x) P_l(x) dx$$

University of Nebraska
Department of Physics and Astronomy

Polarized Electron Physics

News

Pssst...Hey Mister...Wanna See a Picture of a Hexacontatetrapole?

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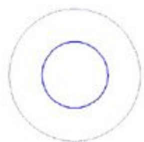
So what *is* a hexacontatetrapole moment, anyway?

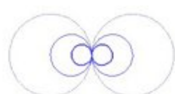
A sum of sines and cosines can be used to model period functions, given the correct coefficients (a Fourier series). Similarly, a special set of polynomials known as Legendres can model functions in a spherical coordinate system: specifically, spherical harmonics. In our lab, we care about spherical harmonics when we're talking about atomic orbitals--these charge clouds can be modeled using a series of Legendres. The collection of necessary parameters are known as the multipole moments.

Multipoles have many uses throughout the physical sciences. One common example comes from computational chemistry: predicting the electric potential (voltage) field due to a complex molecule. You could find the components of the field at each point due to every atom, but this becomes a tremendous task with a large molecule. Instead, the molecule can be decomposed into a handful of multipole moments which provide simple equations for predicting the field.

In essence, multipoles describe how much something behaves like another system that we can predict easily.



We start by asking, "How much does this act like a ball of charge?" In that case, the potential field is distributed evenly in all directions, and our multipole moment is an estimate of the total charge.



Next, we ask about how much the field behaves like a dipole: two opposite charges seperated by a small distance. In this case, the field has two bulbous ends, one with a positive potential and the other with negative potential. This multipole moment is something like the center of charge, giving us a clue to the distance between our origin and the center of charge. In some sense, the dipole is similar to the center of mass for a solid object.

As more charges are arranged together, they start creating strange looking fields. The beauty of the mathematics is that all the fields fit together to create a more complete picture of the field. We have information about the charge and center of mass from the first two poles, then keep adding finer and finer details until we have an adequate idea of the field's behavior. In the case of our hexacontatetrapole, that's seven poles deep, and we have an excellent measurement of how the system is behaving.

In an experiment, we start with data, extract multipoles, and try to reassemble the original field. Depending on the mathematics, this can give a single field solution or a set of solutions. While we can go backwards in some cases, the important information is not necessarily the original field, but how that field behaves. This is again where the multipoles come in handy: based on the multipole data, we can anticipate a reaction to the field without knowing what it true shape is, and we can gather hints about what the shape might be.

Let's take three examples, and look at what we can predict about the fields based on the multipoles. We'll use a football, a discus, and a bowling pin as familiar examples with differing poles. Each has a well defined axis of rotation, but differ in their symmetries around an equatorial axis. The football is longer in the axial direction, whereas the discus is wider in the equatorial direction than it is long. The bowling pin is not symmetric about its equator, since one end bulges out much more than the other.

To calculate the multipoles, we took a photograph of each object, then plotted points along its outline to simulate data. Next, we used integration to fit multipoles to the data sets, similar to the experiments in our lab. Those values are listed in the following table:

Order	Name	Football	Discus	Bowling Pin
0	Monopole	1	1	1
1	Dipole	0	0	-3.15×10^{-2}
2	Quadrupole	2.35×10^{-3}	-4.13×10^{-3}	5.22×10^{-3}

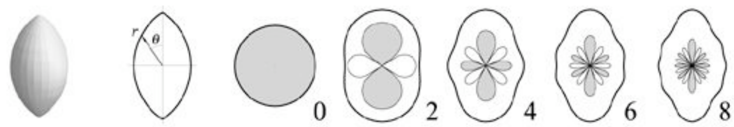
3	Octupole	0	0	-1.56×10^{-4}
		. . .		
6	Hexacontatetrapole	1.38×10^{-7}	-4.84×10^{-7}	6.61×10^{-7}

The first thing to notice is that if the object or field is symmetric, like the football and discus, all the odd-ordered multipoles are zero. These odd multipoles are all based on Legendre polynomials that are non-symmetric, so we wouldn't expect them in a symmetric object. Secondly, the sign of the multipole indicates whether there is an addition or subtraction from the field. The football has positive multipoles, and continues to grow slowly in the axial direction. The discus alternates sign, causing it to shrink a small amount more than it grows in the axial direction, making it wider in the equatorial direction.

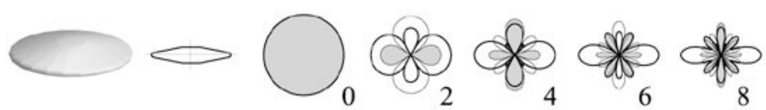
Great, we can calculate interactions. But what about the original field?

Multipoles can give us a good idea of how the field *behaves* without having to know the original field. In some cases, we can actually go backwards to create a field. For our sports balls, we can only generate one field of an infinite number of fields, but we'll see that given some guesses about the original size, our generalizations about what multipoles come from which shape will hold.

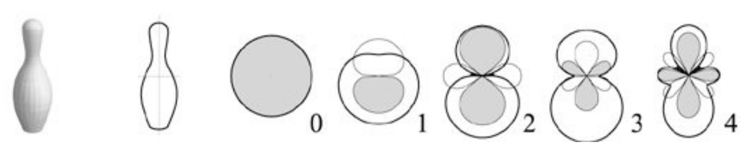
Again using multipoles, we can create spheres of varying density that yield pure multipole moments. A sphere with a density that varies in the same way as a dipole will end up with *only* a dipole momen, nothing else. By assembling these spheres together with the right weights, we create a new sphere that is composed of only pure multipole moments, and will thus yield the same multipoles.



Above is a reconstruction of the football, assuming a radius of 15 cm. The index is the highest order of multipoles used in that reconstruction, with zero being the monopole and six being the hexacontatetrapole. We've taken the mutipole spheres and graphed radius as a function of density; these are the thick black lines. Each additional multipole is shown in grey and white, where grey is an addition and white is a subtraction. These illustrate how the multipoles influence the overall shape. With the football, the "shape", or the thick black line, becomes longer in the axial direction, and has the general shape of a football.



The discus is quite a bit different from the football. It gets shorter in the axial direction and slowly grows in the equatorial direction. The shape line is complex, so it's hard to say that at this order we've got a discus, but many of the characteristics are the same. Note that this shape gives the same multipoles as the discus we are familiar with. In this reconstruction, the bulbous ends of the multipoles along the axis alternate positive and negative, just as the multipole moments did. However, there is always a grey positive addition along the equatorial plane.



The bowling pin is unique in that it has both odd and even multipoles. As the reconstruction progresses, the bottom end becomes larger and the top end becomes slightly smaller. The neck region shrinks, and the net shape resembles the beginnings of a bowling pin. The multipoles have signs such that the grey positive addition is towards the bulbous end.

These examples illustrate that you can get a general sense of the original field based on the multipoles, but (depending on the mathematics) the original field may not be reconstructable.

So, what is a hexacontatetrapole?

Despite the long name, it's just the 7th layer (6th order) of detail for a system represented by multipoles. It gives another level of information for understanding exactly what's going on in an interaction. In the end, we even have a better idea of what the charge cloud looks like in the system under study.

For our lab, and many other areas of physical science, multipoles are useful tools.

General case, no axial symmetry.

In this case we have in general a non-zero m value and the differential equation for P is more elaborate. The Legendre polynomials are replaced by the *associated Legendre polynomials*, $P_l^m(\cos\theta)$. For a given l-value there are $2l+1$ possible m-values: $m = 0, \pm 1, \pm 2,, \pm 3, ...$

There is a more general *Rodrigues' formula* for these functions:

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

For any given m the functions $P_l^m(\cos\theta)$ and $P_{l'}^m(\cos\theta)$ are orthogonal and the associated Legendre polynomials for a fixed m form a complete set of functions in the variable x.

The product of $P_l^m(x)$ and $e^{im\varphi}$ forms a complete set for the expansion of an arbitrary function on the surface of a sphere. These functions are called *spherical harmonics*.

$$\boxed{Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi}}$$

Spherical Harmonics

They are orthonormal

$$\int_{4\pi} Y_l^m(\theta,\varphi)Y_{l'}^{m'}{}^*(\theta,\varphi)d\Omega$$
$$= \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta Y_l^m(\theta,\varphi)Y_{l'}^{m'}{}^*(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$$

$$f(\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_l^m Y_l^m(\theta,\varphi)$$

and

$$C_l^m = \int_{4\pi} f(\theta,\varphi) Y_l^m{}^*(\theta,\varphi) d\Omega$$

The general solution to Laplace's equation in terms of spherical harmonics is

$$\boxed{\Phi(r,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[A_l^m r^l + B_l^m \frac{1}{r^{l+1}} \right] Y_l^m(\theta,\varphi)}$$

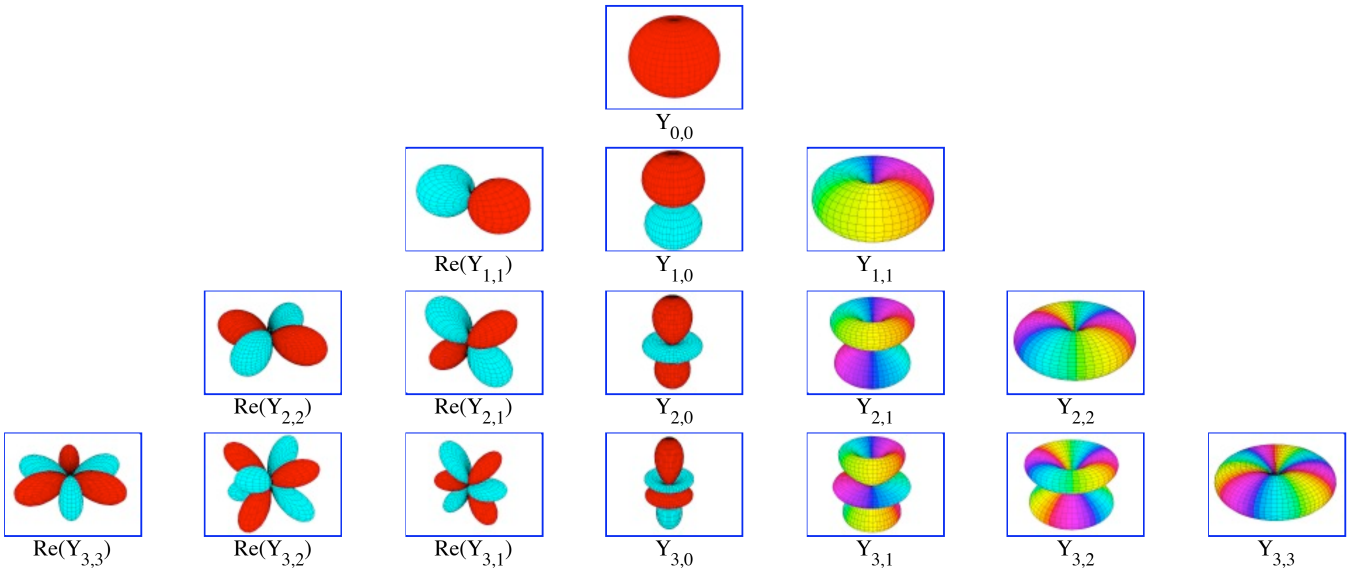
bound states **scattering states**

Spherical Harmonics

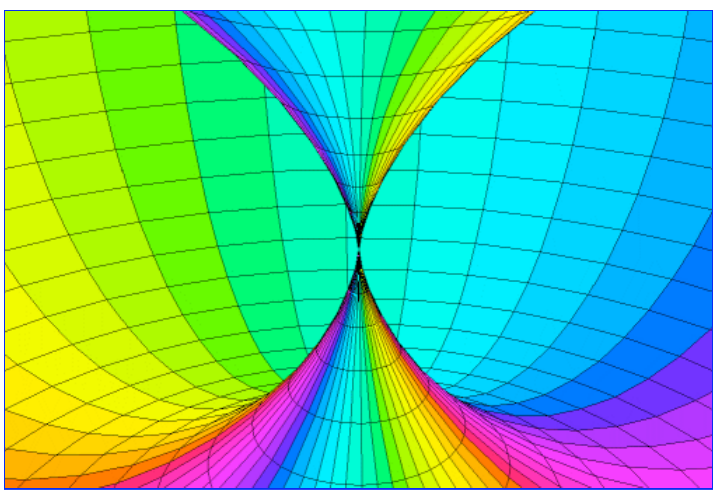
The Spherical Harmonics, $Y_{\ell,m}(\theta, \phi)$, are functions defined on the sphere. They are used to describe the wave function of the electron in a hydrogen atom, oscillations of a soap bubble, etc. The spherical harmonics describe non-symmetric solutions to problems with spherical symmetry.

The $Y_{\ell,m}$'s are complex valued. The radius of the figure is the magnitude, and the color shows the phase, of $Y_{\ell,m}(\theta, \phi)$. These are the numbers on the unit circle: 1 is red, i is purple, -1 is cyan (light blue), and -i is yellow-green.

For each value of ℓ, there are $2\ell + 1$ linearly independent functions $Y_{\ell,m}$, where $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$. I have chosen a different set of $2\ell + 1$ functions, as you see below.



The following figure is called "inside $Y_{2,2}$". My son, Michael, made this by holding down the "Page Up" key until the viewpoint gets *inside* the surface. (He suggests that you set the figure rotating continuously, and move the viewpoint a bit down before zooming in.)



Oscillations of a Soap Bubble

The volume of the bubble is constant, so $Y_{0,0}$ is not used. The center of mass of the bubble is constant, so $Y_{1,m}$ is not used. The lowest frequency oscillations of a soap bubble are $\ell = 2$. The radius of the soap film is $r = 1 + \varepsilon\, Y_{2,m}(\theta, \phi)$. The oscillations with different m all have the same frequency. The shape of the oscillations with m = 1 and m = 2 are the same up to a rotation, but the m = 0 oscillation is different.

Physics and Math notation

WARNING: Spherical coordinates are different in physics and mathematics. The symbols θ and ϕ are switched! The math notation makes r and θ the same in cylincrical and spherical coordinates. DPGraph uses math notation.

$$x^2 + y^2 + z^2 = r^2 \text{ (physics)} = r^2 \text{ (math)}$$
$$\arccos(z/r) = \theta \text{ (physics)} = \phi \text{ (math)}$$

Cylindrical Coordinates

CYLINDRICAL COORDINATES

$$\nabla^2\Phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial z^2} = 0$$

$$\boxed{\Phi(r,\theta,z) = R(r)Q(\theta)Z(z)}$$

Ansatz

$$\frac{1}{rR(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right) + \frac{1}{r^2Q(\theta)}\frac{d^2Q(\theta)}{d\theta^2} + \frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = 0$$

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right) + \frac{r^2}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\frac{1}{Q(\theta)}\frac{d^2Q(\theta)}{d\theta^2} = n^2$$

$$\frac{d^2Q}{d\theta^2} + n^2Q = 0$$

theta equation

theta solutions

$Q(\theta) \sim e^{\pm in\theta}$; $n = 0,1,2,\ldots$ (n may sometimes be non-integer)

$$\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right) - \frac{n^2}{r^2} = -\frac{1}{Z}\frac{d^2Z}{dz^2} = -k^2$$

$$\frac{d^2Z}{dz^2} - k^2Z = 0$$

z equation

$$Z(z) \sim e^{\pm kz}$$

z solutions

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \left(k^2r^2 - n^2\right)R = 0$$

r equation

Cylindrical symmetry and Cylindrical Harmonics

Then we may let k vanish and

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right)-n^2R=0$$

when no z dependence

The $n = 0$ term has to be treated separately

$$R_n(r)=\begin{cases} A_0+B_0\ln r, & (n=0) \\ A_n r^n+B_n\dfrac{1}{r^n}, & (n=1,2,3\ldots) \end{cases}$$

$$Q_n(\theta)=\begin{cases} C_0\left[+D_0\theta\right], & (n=0) \\ C_n\cos n\theta+D_n\sin n\theta, & (n=1,2,3\ldots) \end{cases}$$

General solution in cylindrical coordinates with no z-dependence.

$$\boxed{\Phi(r,\theta)=A_0+B_0\ln r+\sum_{n=1}^{\infty}\left[A_n r^n+B_n\frac{1}{r^n}\right]\left[C_n\cos n\theta+D_n\sin n\theta\right]}$$

The terms are called *cylindrical harmonics*.

cylindrical harmonics

No cylindrical symmetry and Bessel functions.

Now, we have to keep the constant k in the differential equation for R.

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left(k^2r^2-n^2\right)R=0$$

To solve this one usually makes the substitution

$$u=kr \quad ; \quad \frac{d}{dr}=k\frac{d}{du}$$

This leads to *Bessel's equation*:

$$\boxed{u^2\frac{d^2R}{du^2}+u\frac{dR}{du}+\left(u^2-n^2\right)R=0}$$

Bessel's equation

The solution to this equation is the so-called *Bessel function of order* n, $J_n(u)$. $J_{-n}(u)$ is also a solution. These are linearly dependent for integer orders but not for non-integer orders.

One usually introduces another function instead of $J_{-n}(u)$, the so-called *Neumann function* or *Bessel function of the second kind*, $N_n(u)$.

$$N_n(u)=\frac{J_n(u)\cos n\pi-J_{-n}(u)}{\sin n\pi}$$

General solution to Bessel's equation may be written as

$$\boxed{R_n(kr)=A_nJ_n(kr)+B_nN_n(kr)}$$

cylindrical Bessel functions

$J_n(u)$ is regular at origin and at infinity. **bound states**
$N_n(u)$ is <u>not</u> regular at origin but at infinity. **scattering states**

general solution is called Fourier-Bessel

The general solution to Laplace's equation in cylindrical coordinates can be written as the *Fourier-Bessel expansion*:

$$\boxed{\Phi(r,\theta,z) \sim \sum_{m,n}\left[A_{mn}J_n(k_m r) + B_{mn}N_n(k_m r)\right]e^{\pm in\theta}e^{\pm k_m z}}$$

decaying along the z direction

Other useful properties of the Bessel function

Let $k_m\rho$ be the mth root of $J_n(kr)$, i.e., $J_n(k_m\rho) = 0$.

Then $J_n(k_m r)$ form a complete orthogonal set for the expansion of a function of r in the interval $0 \le r \le \rho$.

$$f(r) = \sum_{m=1}^{\infty} D_{mn}J_n(k_m r) \qquad (\text{for any } n)$$

Fourier-Bessel series

$$D_{mn} = \frac{2}{\rho^2 J_{n+1}^2(k_m\rho)}\int_0^{\infty} f(r)J_n(k_m r)rdr$$

analogous to the Fourier transform.

Discussion: If we had chosen $+k^2$ instead of $-k^2$:

$$\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right)-\frac{n^2}{r^2}=-\frac{1}{Z}\frac{d^2Z}{dz^2}=+k^2$$

The z- dependence had been plane waves instead of exponentials and the r dependence had been found as solutions to the *modified Bessel equation:*

$$\boxed{u^2\frac{d^2R}{du^2}+u\frac{dR}{du}-\left(u^2+n^2\right)R=0}$$

with the modified Bessel functions $I_n(u)$ and $K_n(u)$ as solutions. The first is bounded for small arguments and the second for large.

Thus, an alternative expression for the general solution is

$$\boxed{\Phi(r,\theta,z)\sim\sum_{m.n}\left[A_{mn}I_n\left(k_m r\right)+B_{mn}K_n\left(k_m r\right)\right]e^{\pm in\theta}e^{\pm ik_m z}}$$

oscillating along the z direction

Cartesian Coordinates

RECTANGULAR COORDINATES

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}+\frac{\partial^2\Phi}{\partial z^2}=0$$

Assume we may write

$$\Phi(x,y,z)=X(x)Y(y)Z(z)$$ **product ansatz**

$$YZ\frac{d^2X}{dx^2}+XZ\frac{d^2Y}{dy^2}+XY\frac{d^2Z}{dz^2}=0$$

Note that the derivatives are no longer partial.

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}=0$$

The first term depends on x only, the second on y only and the third on z only. The equation can only be valid if each of the terms is a constant:

$$\boxed{\begin{aligned}&\frac{1}{X}\frac{d^2X}{dx^2}=\alpha'^2\\ &\frac{1}{Y}\frac{d^2Y}{dy^2}=\beta'^2\\ &\frac{1}{Z}\frac{d^2Z}{dz^2}=\gamma'^2\\ &\alpha'^2+\beta'^2+\gamma'^2=0\end{aligned}}$$

sign of the coefficient determines whether oscillating or decaying

condition on the components

Since we are considering the electrostatic potential it is real valued. This means that all these squares are real valued, but the last relation shows that the constants themselves cannot all be real valued, neither can they all be imaginary.

real coefficient => oscillating exp

imaginary coefficient => decaying exp

We can only have the following cases

a) two real, one imaginary
b) one real, two imaginary
c) one real, one imaginary, one zero
d) three zero

Four Cases

An imaginary separation constant leads to an oscillatory solution while a real valued leads to an exponential.

Let us arbitrarily let α' and β' be imaginary:

$$\alpha'^2 \equiv -\alpha^2$$
$$\beta'^2 \equiv -\beta^2$$
$$\gamma'^2 \equiv \gamma^2$$

α, β and γ are all real valued.

$$\frac{d^2X}{dx^2} + \alpha^2 X = 0$$
$$\frac{d^2Y}{dy^2} + \beta^2 Y = 0$$
$$\frac{d^2Z}{dz^2} - \gamma^2 Z = 0$$
$$\gamma^2 = \alpha^2 + \beta^2 \quad ; \quad \gamma = \sqrt{\alpha^2 + \beta^2}$$

$$\boxed{\begin{aligned} X(x) &= Ae^{i\alpha x} + Be^{-i\alpha x} \\ Y(y) &= Ce^{i\beta y} + De^{-i\beta y} \\ Z(z) &= Ee^{\gamma z} + Fe^{-\gamma z} \end{aligned}}$$

The complete solution is

$$\Phi(x,y,z) = X(x)Y(y)Z(z)$$

$$\sum_{r,s=1}^{\infty}\left(A_r e^{i\alpha_r x} + B_r e^{-i\alpha_r x}\right)\left(C_s e^{i\beta_s y} + D_s e^{-i\beta_s y}\right)$$

$$\cdot\left(E_{rs} e^{\gamma_{rs} z} + F_{rs} e^{-\gamma_{rs} z}\right)$$

Short hand notation:

$$\boxed{\Phi(x,y,z) \sim e^{\pm i\alpha x} e^{\pm i\beta y} e^{\pm \gamma z}}$$

All the constants will be determined from the boundary conditions of the problem.