Central Forces

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Abstract

The two body problem is treated classically. The reduced mass is used to reduce the two body problem to an equivalent one body problem. Conservation of angular momentum is derived and exploited to simplify the problem. Spherical coordinates are chosen to respect this symmetry. The equations of motion are obtained in two different ways: using Newton's second law, and using energy conservation. Kepler's laws are derived. The concept of an effective potential is introduced. The equations of motion are solved for the orbits in the case that the force obeys an inverse square law. The equations of motion are also solved, up to quadrature (i.e. in terms of definite integrals) and numerical integration is used to explore the solutions.

2 INTRODUCTION

In the Central Forces paradigm, we will examine a mathematically tractable and physically useful problem - that of two bodies interacting with each other through a force that has two characteristics: (a) it depends only on the separation between the two bodies, and (b) it points along the line connecting the two bodies. Such a force is called a central force. Perhaps the most common examples of this type of force are those that follow the $\frac{1}{r^2}$ behavior, specifically the Newtonian gravitational force between two point masses or spherically symmetric bodies and the Coulomb force between two point or spherically symmetric electric charges. Clearly both of these examples are idealizations - neither ideal point masses or charges nor perfectly spherically symmetric mass or charge distributions exist in nature, except perhaps for elementary particles such as electrons. However, deviations from ideal behavior are often small and can be neglected to within a reasonable approximation.

These notes discuss two solutions to the central force problem—classical behavior exemplified by the gravitational interaction and quantum behavior exemplified by the Coulomb interaction. In this way, we will be able to explore the strong similarities and the important differences between classical and quantum physics. Notice the difference in length scale: the archetypal gravitational example is planetary motion—at astronomical length scales, the archetypal Coulomb example is the hydrogen atom—at atomic length scales. We will also consider forces that depend on r in other ways and the kinds of motion they produce.

One of the unifying themes of this topic is the importance of *angular momentum*. You should have covered angular momentum in your introductory physics course. Before starting these notes, you might find it helpful to review the definition of angular momentum, how it enters into dynamical equations (Newton's laws and kinetic energy, for example), and the law of conservation of angular momentum.

You should read these notes in conjunction with the assigned readings in your textbooks. You should note that the development of the classical central force problem in other textbooks may use a formulation based on Lagrangians, which you will not cover until the Classical Mechanics Capstone. We will use a different approach in these notes. You are not responsible for learning the Lagrangian formalism for this course, but your reading in other books will be clearer if you know that the Lagrangian is defined simply as the

difference between kinetic energy and potential energy: $\mathcal{L} = T - U$. And be sure you don't confuse the various symbols. Some books use L to represent the Lagrangian instead of $\mathcal{L}$, $\boldsymbol{L}$ to represent the angular momentum vector, and l to represent the magnitude of the angular momentum. We will also use L_u $(u = x, y, z)$ to represent the components of the angular momentum vector. Some authors use K to represent kinetic energy or V to represent potential energy.

We will obtain the equations of motion in two equivalent ways, 1) using Newton's second law and 2) using energy conservation. The second approach is slightly more sophisticated in that it exploits more of the symmetries from the beginning.

3 Systems of Particles

Consider a system of n different masses m_i, interacting with each other and being acted on by external forces. We can write Newton's second law for the positions $\boldsymbol{r}_i$ of each of these masses with respect to a fixed origin $\boldsymbol{O}$, thereby obtaining a system of equations governing the motion of the masses.

$$\begin{aligned} m_1 \frac{d^2 \boldsymbol{r}_1}{dt^2} &= \boldsymbol{F}_1 + \ 0 \ + \boldsymbol{f}_{12} + \boldsymbol{f}_{13} + \ \dots \ + \boldsymbol{f}_{1n} \\ m_2 \frac{d^2 \boldsymbol{r}_2}{dt^2} &= \boldsymbol{F}_2 + \boldsymbol{f}_{21} + \ 0 \ + \boldsymbol{f}_{23} + \ \dots \ + \boldsymbol{f}_{2n} \\ &\vdots \\ m_n \frac{d^2 \boldsymbol{r}_n}{dt^2} &= \boldsymbol{F}_n + \boldsymbol{f}_{n1} + \boldsymbol{f}_{n2} + \ldots + \boldsymbol{f}_{n(n-1)} + 0 \end{aligned} \tag{1}$$

Here, we have chosen the notation $\boldsymbol{F}_i$ for the net external forces acting on mass m_i and $\boldsymbol{f}_{ij}$ for the internal force of mass m_j acting on m_i.

In general, each internal force $\boldsymbol{f}_{ij}$ will depend on the positions of the particles $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ in some complicated way, making (1) a set of **coupled** differential equations. To solve (1), we first need to **decouple** the differential equations, i.e. find an equivalent set of differential equations in which each equation contains only one variable.

The weak form of Newton's third law states that the force $\boldsymbol{f}_{12}$ of m_2 on m_1 is equal and opposite to the force $\boldsymbol{f}_{21}$ of m_1 on m_2. We see that each internal force appears twice in the system of equations (1), once with a

positive sign and once with a negative sign. Therefore, if we add all of the equations in (1) together, the internal forces will all cancel, leaving:

$$\sum_{i=1}^{n} m_i \frac{d^2 \boldsymbol{r}_i}{dt^2} = \sum_{i=1}^{n} \boldsymbol{F}_i \tag{2}$$

Notice what a surprising equation (2) is. The right-hand side directs us to add up all of the external forces, each of which acts on a different mass; something you were taught never to do in introductory physics.

The left-hand side of (2) directs us to add up (the second derivatives of) n "weighted" position vectors pointing from the origin to different masses. We can simplify the left-hand side of (2) if we multiply and divide by the total mass $M = m_1 + m_2 + \ldots + m_n$ and use the linearity of differentiation to "factor out" the derivative operator:

$$\begin{aligned} \sum_{i=1}^{n} m_i \frac{d^2 \boldsymbol{r}_i}{dt^2} &= M \sum_{i=1}^{n} \frac{m_i}{M} \frac{d^2 \boldsymbol{r}_i}{dt^2} && (3) \\ &= M \frac{d^2}{dt^2} \left(\sum_{i=1}^{n} \frac{m_i}{M} \boldsymbol{r}_i \right) && (4) \\ &= M \frac{d^2 \boldsymbol{R}}{dt^2} && (5) \end{aligned}$$

We recognize (or define) the quantity in the parentheses on the right-hand side of (4) as the position vector $\boldsymbol{R}$ from the origin to the "center of mass" of the system of particles.

$$\boldsymbol{R} = \sum_{i=1}^{n} \frac{m_i}{M} \boldsymbol{r}_i \tag{6}$$

With these simplifications, equation (2) becomes:

$$M \frac{d^2 \boldsymbol{R}}{dt^2} = \sum_{i=1}^{n} \boldsymbol{F}_i \tag{7}$$

which has the form of Newton's 2nd Law for a fictitious particle with mass M sitting at the center of mass of the system of particles and acted on by all of the external forces from the original system.

We can define the momentum of the center of mass as the total mass times the time derivative of the position of the center of mass:

$$\boldsymbol{P} = M\frac{d\boldsymbol{R}}{dt} \tag{8}$$

If there are no external forces acting, then the acceleration of the center of mass is zero and the momentum of the center of mass is constant in time (conserved).

$$M\frac{d^2\boldsymbol{R}}{dt^2} = \frac{d\boldsymbol{P}}{dt} = 0 \tag{9}$$

Notice that the entire discussion above applies even if all of the internal forces are zero $\boldsymbol{f}_{ij} = 0$, i.e. none of the particles have any way of knowing that the others are even present. Such particles are called non-interacting. The position of the center of mass of the system will still move according to equation (7).

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1 Problems

1. (TM 9.6) Consider two particles of equal mass m. The forces on the particles are $\boldsymbol{F}_1 = 0$ and $\boldsymbol{F}_2 = F_0\hat{\imath}$. If the particles are initially at rest at the origin, find the position, velocity, and acceleration of the center of mass as functions of time. Solve this problem in two ways, with or without theorems about the center of mass motion and write a short description comparing the two solutions.)

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4 REDUCED MASS

So far, we have found one decoupled equation to replace (2.1). What about the other $n-1$ equations? It turns out that, in general, there is no way to decouple and solve the other equations. Physicists often say, "The n-body problem can not be solved in general." Whenever you are stuck trying to solve a general problem, it often pays to start with simpler examples to build up your intuition. We will make several assumptions to simplify this problem and keep track of them in a list.

1. Assume that there are no external forces acting.

2. Assume that there are only two masses.

The system of equations (2.1) reduces to:

$$\begin{aligned} m_1 \frac{d^2 \boldsymbol{r}_1}{dt^2} &= -\boldsymbol{f}_{21} \\ m_2 \frac{d^2 \boldsymbol{r}_2}{dt^2} &= \boldsymbol{f}_{21} \end{aligned} \tag{10}$$

Because we added the two equations of motion to find the equation of motion for the center-of-mass, we are led now to consider subtracting the equations so as to get $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$. Figure 1 shows the basic geometry of our problem. $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the position vectors of the two masses measured with respect to an arbitrary coordinate origin **O**. We call the displacement

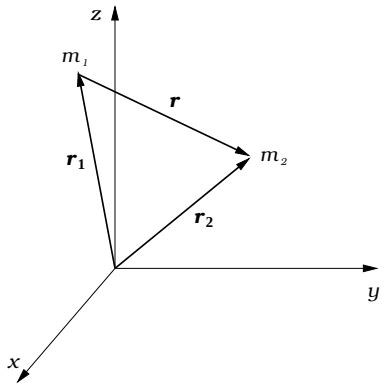

Figure 1: The position vectors for m_1 and m_2 and the displacement vector between them.

between the two masses $\boldsymbol{r}$. The magnitude of this displacement is r and the direction is $\hat{\boldsymbol{r}}$. These quantities can be found from $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ by:

$$\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1 \tag{11}$$

$$r = |\boldsymbol{r}| = |\boldsymbol{r}_2 - \boldsymbol{r}_1| \tag{12}$$

$$\hat{\boldsymbol{r}} = \frac{\boldsymbol{r}}{r} \tag{13}$$

We see that before we subtract, we should multiply the first equation in (11) by m_2 and the second equation by m_1 so that the factors in front of the second derivative are the same. Subtracting the first equation from the second and regrouping, we obtain:

$$m_1 m_2 \frac{d^2}{dt^2}\left(\boldsymbol{r}_2 - \boldsymbol{r}_1\right) = m_1 m_2 \frac{d^2}{dt^2}\left(\boldsymbol{r}\right) = \left(m_1 + m_2\right)\boldsymbol{f}_{21} \tag{14}$$

or rearranging:

$$\frac{m_1 m_2}{m_1 + m_2}\frac{d^2\boldsymbol{r}}{dt^2} = \mu \frac{d^2\boldsymbol{r}}{dt^2} = \boldsymbol{f}_{21} \tag{15}$$

The combination of masses

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{16}$$

is called the reduced mass. This equation is in the same form as Newton's law for a single fictitious mass μ, with position vector $\boldsymbol{r}$, moving subject to the force $\boldsymbol{f}_{21}$. For the rest of these notes, we will talk about "the mass", meaning this fictitious particle. Note that to solve the original two mass problem we started with, we will need to transform the solutions for $\boldsymbol{r}$ back to $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. See Problem 1.1.

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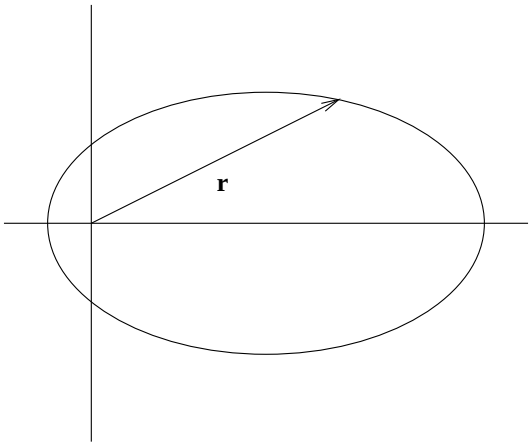
1 Problems

1. The figure below shows the orbit of a "fictitious" reduced mass, μ, traveling around the center-of-mass at the origin. The position vector $\mathbf{r}$ locates the particle at a particular instant t. Assume that $m_2 = m_1$ and draw on the figure the position vectors for m_1 and m_2 corresponding to $\mathbf{r}$. Also sketch the orbits for m_1 and m_2. Give an example of a physical situation that might produce this type of motion. (NOTE: Do this problem "by hand." Do not use MAPLE or a graphing calculator.)



Repeat this problem for $m_2 > m_1$ and $m_2 >> m_1$.

2. Find $\boldsymbol{r}_{\rm sun} - \boldsymbol{r}_{\rm cm}$ and μ for the Sun–Earth system. Compare $\boldsymbol{r}_{\rm sun} - \boldsymbol{r}_{\rm cm}$ to the radius of the Sun and to the distance from the Sun to the Earth. Repeat the calculation for the Sun–Jupiter system.

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5 CENTRAL FORCES

Our ultimate goal is to solve the equations of motion for two masses m_1 and m_2 subject to a central force acting between them. When you considered this problem in introductory physics, you assumed that one of the masses was so large that it effectively remained at rest while all of the motion belonged to the other object. This assumption works fairly well for the Earth orbiting around the Sun or for a satellite orbiting around the Earth, but in general we are going to have to solve for the motion of *both* objects.

In the introduction, we defined a central force to satisfy two characteristics. We can now write turn these descriptions of the characteristics into equations:

(a) a central force depends only on the separation between the two bodies

$$\boldsymbol{f}_{21} = -\boldsymbol{f}_{12} = \boldsymbol{f}(\boldsymbol{r}_2 - \boldsymbol{r}_1) \tag{17}$$

(b) it points along the line connecting the two bodies

$$\boldsymbol{f}_{21} = -\boldsymbol{f}_{12} = \boldsymbol{f}(\boldsymbol{r}_2 - \boldsymbol{r}_1) = f(\boldsymbol{r})\,\hat{\boldsymbol{r}} \tag{18}$$

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1 Problems

1. If a central force is the only force acting on a system of two masses (i.e. no external forces), what will the motion of the center of mass be?

2. Which of the forces which we found in the Static Fields Paradigm (*i.e.* $\vec{g}$, $q\vec{E}$, $q\vec{v} \times \vec{B}$) can be central forces? which cannot?

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6 ANGULAR MOMENTUM

Consider the angular momentum of the reduced mass system $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times \mu\boldsymbol{v}$. How does $\boldsymbol{L}$ change with time? We have:

$$\begin{aligned}
\frac{d\boldsymbol{L}}{dt} &= \frac{d}{dt}\left(\boldsymbol{r} \times \mu\boldsymbol{v}\right) && (19)\\
&= \boldsymbol{r} \times \mu\dot{\boldsymbol{v}} + \boldsymbol{v} \times \mu\boldsymbol{v} && (20)\\
&= \boldsymbol{r} \times \mu\boldsymbol{a} && (21)\\
&= \boldsymbol{r} \times \boldsymbol{F} && (22)\\
&= r\hat{\boldsymbol{r}} \times f(r)\hat{\boldsymbol{r}} && (23)\\
&= 0 && (24)
\end{aligned}$$

(To get from (19) to (20), use the product rule, which is valid for cross products as long as you don't change the order of the factors. The second term in (20) is zero since $\boldsymbol{v} \times \boldsymbol{v} = 0$.) Recall that $\boldsymbol{r} \times \boldsymbol{F}$ which occurs in (22) is called the torque τ. We have shown that in the case of central forces the time derivative of the angular momentum, and hence the torque, are zero. Therefore:

$$\tau = \frac{d\boldsymbol{L}}{dt} = 0 \qquad \Rightarrow \qquad \boldsymbol{L} = \text{constant} \tag{25}$$

i.e. the angular momentum is conserved.

The force $\boldsymbol{F}(r)$ depends only on the distance of the reduced mass from the center of mass and not on the orientation of the system in space. Therefore, this system is spherically symmetric; it is invariant (unchanged) under rotations. Noether's theorem states that whenever the laws of physics are invariant under a particular motion or other operation, there will be a corresponding conserved quantity. In this case, we see that the conservation of angular momentum is related to the invariance of the physical system under rotations. Noether's theorem, in general, is most easily discussed using Lagrangian techniques. You will see this again the Classical Mechanics Capstone.

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1 Problems

1. Which of the equations in the derivation of (19)–(24) are valid only for central forces, and which are true more generally?

2. (Challenging) What invariances of physics are related to conservation of linear momentum and conservation of energy?

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7 COORDINATES

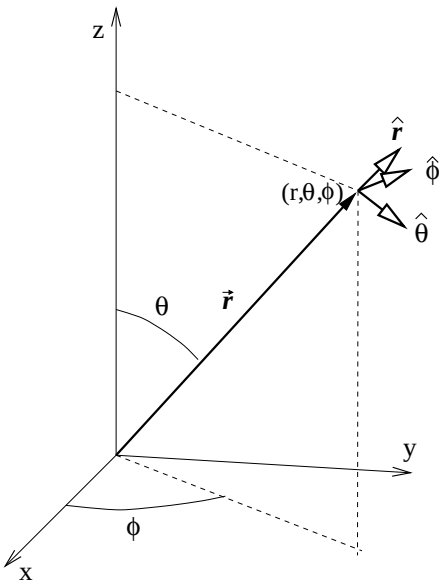
The time has come to choose a coordinate system. We have argued that the problem is spherically symmetric in nature. Therefore, it will be to our advantage to use spherical coordinates, defined by:

$$x = r\sin\theta\cos\phi \tag{26}$$
$$y = r\sin\theta\sin\phi \tag{27}$$
$$z = r\cos\theta \tag{28}$$

(see Figure 2), rather than the more comfortable Cartesian coordinates x, y, and z.

In fact, in the present classical mechanics context, we can do even better. For a central force:

$$\boldsymbol{F} = f(r)\,\hat{\boldsymbol{r}} \tag{29}$$



Spherical Coordinates

x=r sin θ cos φ
y=r sin θ sin φ
z=r cos θ

Figure 2: Spherical Coordinates.

the force, and hence the acceleration, are in the radial direction. Therefore, the path of the motion (orbit) will be in the plane determined by the position vector $\boldsymbol{r}$ and velocity vector $\boldsymbol{v}$ of the reduced mass at any one moment of time. Since there is never a component of force out of this plane, the subsequent motion must remain in the plane. In this plane, choose plane polar coordinates:

$$x = r\cos\phi \tag{30}$$
$$y = r\sin\phi \tag{31}$$

Notice that many textbooks choose to call the angle of plane polar coordinates θ. See Practice Problem 1.3 for the reason that we choose to call the angle ϕ.

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1 Problems

1. Convince yourself that the plane of the orbit is perpendicular to the angular momentum vector $\boldsymbol{L}$.

2. Show that a central force is **always** conservative. Find the scalar potential U corresponding to the central force $\boldsymbol{F} = f(r)\,\hat{r}$ and show that it depends only on the distance from the center of mass $U = U(r)$.

3. Show that the plane polar coordinates we have chosen are equivalent to spherical coordinates if we make the choices:

   (a) The direction of z in spherical coordinates is the same as the direction of $\boldsymbol{L}$.

   (b) The θ of spherical coordinates is chosen to be $\pi/2$, so that the orbit is in the equatorial plane of spherical coordinates.

   Some textbooks argue that you can obtain plane polar coordinates in terms of r and the polar angle θ by taking spherical coordinates (26)–(28) and making the choice $d\phi = 0$. Why is this choice actually misleading? Hint: In spherical coordinates, what is the range of θ? These textbooks label the angle θ because this is the most common convention for polar coordinates alone. However, if you do this, polar coordinates do **not** correspond in any nice way to spherical coordinates. Because I want you to see the relationship between classical and quantum mechanics and because the quantum version of central forces will require the use of spherical coordinates, we will call the polar coordinate angle ϕ.)

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8 VELOCITY & ACCELERATION

Newton's Laws require a knowledge of velocity and acceleration. With our choice of polar coordinates:

$$x = r\cos\phi \tag{32}$$
$$y = r\sin\phi \tag{33}$$

we must deal with the problem of how to compute velocity and acceleration as time derivatives of the position vector $\boldsymbol{r}$ in terms of the coordinates r and ϕ. A difficulty arises because $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ are not independent of position and therefore are not independent of time. This problem does not present itself in Cartesian coordinates because $\hat{\boldsymbol{\imath}}$, $\hat{\boldsymbol{\jmath}}$, and $\hat{\boldsymbol{k}}$ are independent of position. We can exploit this Cartesian independence to help us in polar coordinates. $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ are given, in terms of $\hat{\boldsymbol{\imath}}$ and $\hat{\boldsymbol{\jmath}}$, by

$$\hat{\boldsymbol{r}} = \cos\phi\,\hat{\boldsymbol{\imath}} + \sin\phi\,\hat{\boldsymbol{\jmath}} \tag{34}$$

$$\hat{\boldsymbol{\phi}} = -\sin\phi\,\hat{\boldsymbol{\imath}} + \cos\phi\,\hat{\boldsymbol{\jmath}} \tag{35}$$

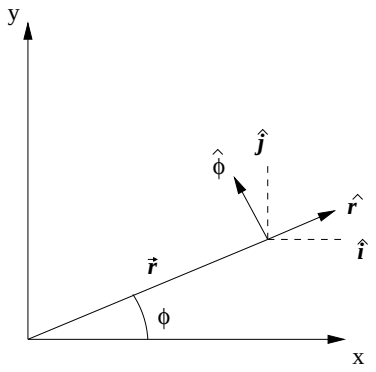

Figure 3: The relationship between unit vectors in polar coordinates ($\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{\phi}}$) and unit vectors in Cartesian coordinates ($\hat{\boldsymbol{\imath}}$, $\hat{\boldsymbol{\jmath}}$).

You should recognize this basis change as a rotation performed on the $\hat{\boldsymbol{\imath}}$, $\hat{\boldsymbol{\jmath}}$ basis. As Figure 3 shows:

$$\begin{pmatrix} \hat{\boldsymbol{r}} \\ \hat{\boldsymbol{\phi}} \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{\imath}} \\ \hat{\boldsymbol{\jmath}} \end{pmatrix} = R(\phi) \begin{pmatrix} \hat{\boldsymbol{\imath}} \\ \hat{\boldsymbol{\jmath}} \end{pmatrix} \tag{36}$$

Using the chain rule, the general velocity vector is given by:

$$\boldsymbol{v} = \frac{d\boldsymbol{r}}{dt} = \frac{d}{dt}(r\hat{r}) = \frac{dr}{dt}\hat{\boldsymbol{r}} + r\frac{d\hat{\boldsymbol{r}}}{dt} \tag{37}$$

To evaluate (37), we need the derivatives of $\hat{\boldsymbol{r}}$ (and $\hat{\boldsymbol{\phi}}$) with respect to time. Using the definitions in (36) above, we obtain:

$$\frac{d\hat{\boldsymbol{r}}}{dt} = \frac{d}{dt}(\cos\phi\hat{\boldsymbol{\imath}} + \sin\phi\hat{\boldsymbol{\jmath}}) = -\sin\phi\frac{d\phi}{dt}\hat{\boldsymbol{\imath}} + \cos\phi\frac{d\phi}{dt}\hat{\boldsymbol{\jmath}} = \frac{d\phi}{dt}\hat{\boldsymbol{\phi}} \tag{38}$$

$$\frac{d\hat{\boldsymbol{\phi}}}{dt} = \frac{d}{dt}\left(-\sin\phi\hat{\boldsymbol{\imath}} + \cos\phi\hat{\boldsymbol{\jmath}}\right) = -\cos\phi\frac{d\phi}{dt}\hat{\boldsymbol{\imath}} - \sin\phi\frac{d\phi}{dt}\hat{\boldsymbol{\jmath}} = -\frac{d\phi}{dt}\hat{\boldsymbol{r}} \quad (39)$$

Combining this with equation (37) gives:

$$\boldsymbol{v} = \dot{r}\hat{\boldsymbol{r}} + r\dot{\phi}\,\hat{\boldsymbol{\phi}} \quad (40)$$

Notice that we have used the convenient notation of putting a dot over a symbol to denote time derivative.

Taking another derivative of (40) with respect to time shows that the acceleration is given by:

$$\boldsymbol{a} = \dot{\boldsymbol{v}} = \ddot{\boldsymbol{r}} = \left(\ddot{r} - r\dot{\phi}^2\right)\hat{\boldsymbol{r}} + \left(r\ddot{\phi} + 2\dot{r}\dot{\phi}\right)\hat{\boldsymbol{\phi}} \quad (41)$$

(40) can be used to show that the kinetic energy T of the reduced mass in polar coordinates is given by:

$$T = \frac{1}{2}\mu\, v^2 = \frac{1}{2}\mu\, \boldsymbol{v}\cdot\boldsymbol{v} = \frac{1}{2}\mu\left(\dot{r}^2 + r^2\dot{\phi}^2\right) \quad (42)$$

Similarly, the magnitude of the angular momentum $\boldsymbol{L}$ of the reduced mass μ is given in polar coordinates by:

$$|\boldsymbol{L}| = |\boldsymbol{r}\times\mu\boldsymbol{v}| = l = \mu r^2\dot{\phi} \quad (43)$$

Since the angular momentum is a constant in central force problems, it's magnitude l is also constant. Therefore (43) can be used to rewrite differential equations, getting rid of $\dot{\phi}$'s in favor of the variable r and the constant l.

Kepler's second law says that the areal velocity of a planet in orbit is constant in time. This is equivalent to equation (43). To see why, read in section 8.3 of Marion and Thornton, page 294, from equation 8.10 to the bottom of the page.

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1 Practice Problems

1. Work through the steps deriving equations (41), (42), and (43) from (40).

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9 EQUATIONS OF MOTION: $\boldsymbol{F} = \mu \boldsymbol{a}$

The problem is now to the point where we can write the equations of motion in a form we can solve. However, the importance of the preceding sections cannot be stressed enough. The strategies that we used are important to the success of problem solving in many complicated physics situations. Drawing a picture, exploiting symmetries, choosing a convenient origin, and using the most appropriate coordinate system all combine to make the analysis as easy as possible. These and other tricks should always be regarded as a good beginning to any problem.

Newton's second law, reduced and modified for our specific problem is:

$$f(r)\hat{\boldsymbol{r}} = \mu\, \ddot{\boldsymbol{r}} = \mu \left((\ddot{r} - r\dot{\phi}^2)\hat{\boldsymbol{r}} + (r\ddot{\phi} + 2\dot{r}\dot{\phi})\hat{\boldsymbol{\phi}} \right) \tag{44}$$

The vector equation breaks up, in polar coordinates, into two coupled differential equations for $r(t)$ and $\phi(t)$:

$$f(r) = \mu\,(\ddot{r} - r\dot{\phi}^2) \tag{45}$$

$$0 = \mu\,(r\ddot{\phi} + 2\dot{r}\dot{\phi}) \tag{46}$$

Equation (46) is just the polar coordinate statement of angular momentum conservation, which we have already discussed, i.e.:

$$0 = r\,\mu\,(r\ddot{\phi} + 2\dot{r}\dot{\phi}) = \frac{d}{dt}\left(\mu\, r^2\dot{\phi}\right) = \frac{dl}{dt} \tag{47}$$

(To derive verify the equalities in (47) it is easiest to work from right to left!) Therefore

$$\mu r^2\dot{\phi} = l = \text{constant} \tag{48}$$

(48) can be solved for $\dot{\phi}$ and used in (45) to obtain a messy, second order ODE for $r(t)$:

$$\ddot{r} = \frac{l^2}{\mu^2 r^3} + \frac{1}{\mu} f(r) \tag{49}$$

In principle, we could now insert the particular form of $f(r)$ we are concerned with, solve equation (49) for r as a function of t, and insert this value in (48) and solve for $\phi(t)$. We would then have solved the equations of motion for r, and ϕ, parameterized by the time t. In practice, for any but the simplest forms of $f(r)$, it is impossible to solve the differential equations analytically. Computers to the rescue! On Day 4, you will use a Maple worksheet which will allow you to explore numerical solutions for some important physical examples.

10 SHAPE OF THE ORBIT

If we are only interested in the shape of the orbit, we can do something simpler than solving the equations of motion for r and ϕ as functions of t; we can solve for the shape of the orbit, i.e. instead of using the variable t as a parameter in (49), we will use the variable ϕ and solve for $r(\phi)$. To do this, we need to change the time derivatives into ϕ derivatives.

$$\frac{d}{dt} = \frac{d\phi}{dt}\frac{d}{d\phi} = \dot{\phi}\frac{d}{d\phi} = \frac{\ell}{\mu r^2}\frac{d}{d\phi} \tag{50}$$

It turns out that the differential equation which we obtain will be much easier to solve if we also change independent variables from r to

$$u = r^{-1} \tag{51}$$

(There is no way that you could guess this, yourself.) Therefore,

$$\frac{dr}{dt} = \frac{\ell}{\mu r^2}\frac{dr}{d\phi} = -\frac{\ell}{\mu}\frac{d\,r^{-1}}{d\phi} = -\frac{\ell}{\mu}\frac{du}{d\phi} \tag{52}$$

(To verify the second equality, work from right to left.) Then the second derivative is given by

$$\frac{d^2r}{dt^2} = \frac{d}{dt}\frac{dr}{dt} = \frac{\ell}{\mu}\,u^2\,\frac{d}{d\phi}\left(-\frac{\ell}{\mu}\frac{du}{d\phi}\right) = -\frac{\ell^2}{\mu^2}\,u^2\,\frac{d^2u}{d\phi^2} \tag{53}$$

Plugging (51) and (53) into (49), dividing through by u^2, and rearranging, we obtain the orbit equation

$$\frac{d^2u}{d\phi^2} + u = -\frac{\mu}{\ell^2}\,\frac{1}{u^2}\,f\left(\frac{1}{u}\right) \tag{54}$$

For the special case of inverse square forces $f(r) = -k/r^2$ (spherical gravitational and electric sources), it turns out that the right-hand side of (54) is constant so that the equation is particularly easy to solve. First solve the homogeneous equation (with $f(r) = 0$), which is just the harmonic oscillator equation with general solution

$$u_{\rm h} = A\cos(\phi + \delta) \tag{55}$$

Add to this any particular solution of the inhomogeneous equation (with $f(r) = -k/r^2$). By inspection, such a solution is just

$$u_{\rm p} = \frac{\mu\, k}{\ell^2} \tag{56}$$

so that the general solution of (54) for an inverse square force is

$$r^{-1} = u = u_{\rm h} + u_{\rm p} = A\cos(\phi + \delta) + \frac{\mu\, k}{\ell^2} \tag{57}$$

Then solving for r in (57) we obtain

$$r = \frac{1}{\frac{\mu k}{\ell^2} + A\cos(\phi + \delta)} = \frac{\frac{\ell^2}{\mu k}}{1 + A'\cos(\phi + \delta)} \tag{58}$$

You can explore how the graph of this equation depends on the various parameters using the Maple worksheet *conics.mws*

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1 Practice Problems

1. Go through all the steps in the derivation of (54) from (49). (49) is the same as equation 8.18 in section 8.4 on page 296 of Marion and Thornton; an alternative derivation of (54) can be found following equation 8.18. Use whichever technique is easiest for you to follow, but make sure you understand at least one. This kind of change of variables is very common in physics.

2. How do the physical constants in (58) correspond to the mathematical constants: amplitude α, phase δ, and the eccentricity ϵ, from the Maple worksheet *conics.mws*?

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11 EQUATIONS OF MOTION: $E = T + U$

Another theoretical tool we can use to arrive at an equation for the orbit is conservation of energy. The central force $\boldsymbol{F}$ is conservative and can be

derived from a potential $U(r)$ which depends only on the distance from the center of mass (see practice problem 1.2):

$$\boldsymbol{F} = -\nabla U = -\frac{\partial U(r)}{\partial r} \tag{59}$$

The statement of energy conservation:

$$E = T + U \tag{60}$$

becomes, using (42), (43), and (59):

$$E = \frac{1}{2}\mu\,\dot{r}^2 + \frac{1}{2}\frac{l^2}{\mu r^2} + U(r) \tag{61}$$

(61) can be solved for $\dot{r}$ to give:

$$\dot{r} = \pm\sqrt{\frac{2}{\mu}(E - U(r)) - \frac{l^2}{\mu^2 r^2}} \tag{62}$$

(62) is an equivalent alternative to (49) as an equation of motion for $r(t)$. You might be surprised that (62) is a first order differential equation, whereas (49) is second order. This means that only one initial condition is required for the solution of (62) whereas two are needed for the solution of (49). There is nothing surprising going on here. We have already provided the extra information (the extra initial condition) by specifying the constant total energy E.

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1 Practice Problems

1. (Challenging) Show that the equation of motion derived from Newton's Law (49) is equivalent to the equation of motion derived from energy conservation (62). Hint: Multiply (49) by $2\dot{r}\,dt$ and integrate both sides.

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12 EVERYTHING ELSE

You should now work through sections 8.4-8.7 of Taylor. Pay particular attention to the concept of the effective potential.

There are many areas left to explore if you are interested: questions of the stability of orbits under perturbations, the precession of the orbit, and whether it is open or closed. There are many interesting examples, even within our solar system, that show the varied and unique outcomes of central force interactions: Lagrange points, resonant orbits, horseshoe orbits, to name a few. There are also other types of central forces. The repulsive inverse square force was very important to early atomic experiments. Rutherford bombarded a lattice of gold with alpha particles (helium nuclei). The repulsive electrostatic interaction can be handled easily by our preceding analysis. The theory fit experiment well until the alpha particle energies became high enough to overcome the effective potential and hit the nucleus head-on.

Many of the ideas in our analysis are handled nicely by the Lagrangian formalism which you will study in the Classical Mechanics Capstone. Lagrangian mechanics provides yet another starting point for obtaining the equations of motion. The ideas of symmetry and conservation are more easily recognized and handled within that context, which proves to be very powerful in more complicated situations. When you reach that point, remember some of the techniques we used here and then appreciate the simplicity and beauty provided by the new viewpoint.

QUANTUM CENTRAL FORCES

Abstract

The Schrödinger equation in a central potential is examined. The separation of variables procedure is used to turn this partial differential equation into a set of ordinary differential equations. The angular equations are solved, first for a particle confined to a ring and then for a particle confined to a sphere, thereby building up, one dimension at a time, toward the eigenstates of the hydrogen atom. Special attention is paid to linear combinations of states and time-dependent states.

The properties of the spherical harmonics are explored, including a brief introduction to angular-momentum raising and lowering operators. The relationship of spherical harmonics to spin 1 systems is discussed. The eigenstates on the surface of a sphere are shown to be the same as the rigid rotor problem and the properties of rotational spectra are discussed.

The radial equation is solved and the properties of the eigenstates of the (unperturbed) hydrogen atom are explored.

13 INTRODUCTION

We now begin our analysis of the central force problem in quantum mechanics. We will find that there are some similarities and some differences between the handling of this problem in classical mechanics and quantum mechanics. Concepts such as acceleration or Newton's third law have no counterpart in quantum physics. However, we shall find that reduction of the two-body problem to a fictitious one-body problem is also a characteristic of the quantum analysis. And we will again find that angular momentum is a critical aspect of our description of the motion of the system, related to spherical symmetry.

As we did in analyzing our classical central force problem, we again assume a two-particle system in which the only interaction is the mutual interaction of the two particles. We assume that this interaction depends only on the separation distance between the particles and not on any angle or orientation in space. In this case, as in the classical problem, we will find that the angular momentum is a constant of the motion, but in quantum mechanics angular momentum (like energy) is quantized.

As always in quantum mechanics, we begin with Schrödinger's equation

$$H_{\rm op}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

14 Reduced Mass

It is helpful to consider briefly how the quantum two-body problem separates into an equation governing the center of mass and an equation describing the system around the center of mass, comparing this process to the classical problem. The quantum two-body problem in three dimensions is very messy, but all the essential features of the calculation show up in a simple one-dimensional model. So, for simplicity, let's consider a system of two particles, m_1 and m_2, lying on a line at positions x_1 and x_2, and let the interaction between the particles be represented by a potential energy U that depends only on $x = x_1 - x_2$, the separation distance between the particles. Don't worry about how the particles can get past each other on the line—this is a simple toy model; just imagine that they can pass right through each other.

Our first job, as always, is to identify the Hamiltonian $H_{\rm op}$ for the system. Because energies are additive, the kinetic part of the Hamiltonian is just the sum of the kinetic parts for two individual particles and the potential $U(x)$ describes the interaction between them. Therefore the Hamiltonian is

$$H_{\rm op} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + U(x) \tag{63}$$

and the wave function Ψ is a function of the positions of both particles (and of course time) $\Psi = \Psi(x_1, x_2, t)$.

Inspired by our experience with classical two-body systems, we will try rewriting the Hamiltonian (63) in terms of the center-of-mass coordinate X, given by

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \tag{64}$$

and the relative coordinate x. We will use the chain rule of calculus to transform the partial derivatives in equation (63) to derivatives with respect to x and X. (Please see Appendix A , especially the worked example on plane polar coordinates.) The transformations for first derivatives are:

$$\frac{\partial}{\partial x_1} = \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} = \frac{\partial}{\partial x} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial X} \tag{65}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_2}\frac{\partial}{\partial X} = -\frac{\partial}{\partial x} + \frac{m_2}{m_1+m_2}\frac{\partial}{\partial X} \tag{66}$$

It is important to note that we cannot simply write equations (65–66) for the second derivative, which is what we need for the Hamiltonian (63). To find the second derivative, we must apply the first derivative rules (65–66) twice:

$$\begin{aligned}
\frac{\partial^2}{\partial x_1^2}\Psi &= \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_1}\Psi & (67)\\
&= \left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\Psi & (68)\\
&= \frac{\partial^2}{\partial x^2}\Psi + \frac{2m_1}{m_1+m_2}\frac{\partial^2}{\partial x \partial X}\Psi + \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}\Psi & (69)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial^2}{\partial x_2^2}\Psi &= \frac{\partial}{\partial x_2}\frac{\partial}{\partial x_2}\Psi & (70)\\
&= \left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\Psi & (71)\\
&= \frac{\partial^2}{\partial x^2}\Psi - \frac{2m_1}{m_1+m_2}\frac{\partial^2}{\partial x \partial X}\Psi + \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}\Psi & (72)
\end{aligned}$$

Substituting into the Hamiltonian (63), we obtain for Schrödinger's equation

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2(m_1+m_2)}\frac{\partial^2}{\partial X^2} + U(x)\right\}\Psi(X,x,t) = i\hbar\frac{\partial}{\partial t}\Psi(X,x,t) \tag{73}$$

By transforming to these coordinates, the middle terms in equations (69) and (72) have canceled, enabling us to separate the dependence on x from the dependence on X. We can now write

$$\Psi(x,X,t) = \psi_M(X)\psi_\mu(x)T(t) \tag{74}$$

After a separation of variables procedure (see Appendix B) on equation (74), we find that the ordinary differential equation governing the variable X has a simple, recognizable form (see Problem 14.3b). The solution has the same form as the free-particle solution to the Schrödinger equation (also called the plane-wave solution to the equation)

$$\psi_M(X) = e^{iP_X X/\hbar} \tag{75}$$

where P_X represents the momentum associated with the motion of the center of mass. All observables in quantum mechanics involve the probability density, i.e. terms of the form $\Psi^*\Psi$, so if we are evaluating observables associated with the relative motion, the pure phase contribution from the center-of mass has no effect. We can therefore ignore the center-of-mass motion and concentrate only on the relative motion.

We have arrived at a conclusion in the quantum analysis of the two-body problem that is similar to our analysis of the classical problem (but for different reasons). We have again replaced the more complicated two-body system with a fictitious one-body system, involving the relative coordinate and the reduced mass. Once we have solved the problem and found $\psi_\mu(x)$ and $T(t)$, we can then reverse the procedure in this section to find the wave function $\Psi(x_1, x_2, t)$ describing the original two-body system. The analysis in three dimensions is the same, except that we must do the calculation three times, once for each of the rectangular coordinates.

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1 Problems

1. Work through the steps of the chain rule to show that equation (73) follows from equation (63)

2. Where does the mass of a particle appear in Schrödinger's equation? In equation (73), what is the mass associated with the center-of-mass coordinate X? what is the mass associated with the relative position coordinate x? Does this make sense?

3. Use the separation of variables procedure in Appendix B to break equation (73) up into three ordinary differential equations.

   (a) How many separation constants do you have? Is this the number you expect? Explain.

   (b) Solve the equations for $\psi_M(X)$. What are the possible eigenvalues?

   (c) Give an appropriate name to the eigenvalues of the (unsolved) equation for $\psi_\mu(x)$.

   (d) Solve the equation for $T(t)$. Discuss how the energy E of the system depends on the separation constants.

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15 SCHRÖDINGER'S EQUATION IN SPHERICAL COORDINATES

Schrödinger's equation is

$$H_{\text{op}}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{76}$$

For one-dimensional waves, the Hamiltonian is

$$H_{\text{op}} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + U(x) \tag{77}$$

In a central potential the role of the second derivative with respect to x is played by the Laplacian operator ∇^2 and the potential energy is a function only on the separation variable $U = U(r)$, making the Hamiltonian:

$$H_{\text{op}} = -\frac{\hbar^2}{2\mu}\nabla^2 + U(r) \tag{78}$$

Because of the parameter r, this problem is clearly asking for the use of spherical coordinates, centered at the origin of the central force.

In rectangular coordinates, we know that the Laplacian ∇^2 is given by:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{79}$$

What is the Laplacian in spherical coordinates? Since $\nabla^2 \stackrel{\text{def}}{=} \vec{\nabla}\cdot\vec{\nabla}$, we can combine the spherical coordinate definitions of gradient and divergence

$$\vec{\nabla}V = \frac{\partial V}{\partial r}\,\hat{r} + \frac{1}{r}\frac{\partial V}{\partial\theta}\,\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial V}{\partial\phi}\,\hat{\phi} \tag{80}$$

$$\vec{\nabla}\cdot\vec{v} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 v_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta v_\theta) + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial\phi} \tag{81}$$

to obtain:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{82}$$

For convenience, we will give the combination of angular derivatives which appears in (82) a new name:

$$L^2_{\rm op} \stackrel{\rm def}{=} -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \tag{83}$$

Notice the conventional factor of $-\hbar^2$. $\hbar$ is a constant, 1.05459×10^{-27} erg-sec $= 6.58217 \times 10^{-16}$ eV-sec. Notice that the dimensions of $\hbar$ are those of angular momentum. With this definition, (82) becomes:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} L^2_{\rm op} \tag{84}$$

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1 Practice Problems

1. Review the definition of spherical coordinates. Remember that in our conventions θ is always the angle measured from the z axis and ranges from 0 to π. ϕ is the angle in the x-y plane measured from the x axis towards the y axis and ranges from 0 to 2π.

2. Review the definition of gradient and divergence in spherical coordinates. See Griffiths E&M, Appendix A, for a nice derivation. What is the fastest place to look-up expressions for gradient, etc. in spherical and cylindrical coordinates?

3. Using the definition of gradient (80) and divergence (81) in spherical coordinates, derive equation (82).

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16 SEPARATION OF VARIABLES

We will use the "separation of variables" procedure (see Appendix B) on the Schrödinger equation in a central potential. Most of the calculation will involve using this procedure on the Laplacian operator. Since the Laplacian comes up in almost all physics problems with spherical symmetry, you will find yourself using the results of this section many times in your career.

Because there are several spatial dimensions, the procedure requires a number of rounds, each consisting of the same set of six steps. In the first round, we will separate out an ordinary differential equation in the time variable.

Step 1: Write the partial differential equation in appropriate coordinate system. For Schrödinger's equation in any potential we have:

$$H_{\rm op}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{85}$$

Step 2: Assume that the solution Ψ can be written as the product of functions, at least one of which depends on only one variable, in this case t. The other function(s) must not depend at all on this variable, i.e. assume

$$\Psi(r,\theta,\phi,t) = \psi(r,\theta,\phi)T(t) \tag{86}$$

Plug this assumed solution (255) into the partial differential equation (85). Because of the special form for Ψ, the partial derivatives each act on only one of the factors in Ψ.

$$\left(H_{\rm op}\psi\right)T = i\hbar\psi\,\frac{dT}{dt} \tag{87}$$

Any partial derivatives that act only on a function of a single variable may be rewritten as total derivatives.

Step 3: Divide by Ψ in the form of (255).

$$\frac{1}{\psi}\left(H_{\rm op}\psi\right) = i\hbar\frac{dT}{dt}\frac{1}{T} \tag{88}$$

Step 4: Isolate **all** of the dependence on one coordinate on one side of the equation. Do as much algebra as you need to do to achieve this. In our example, notice that in (257), all of the t dependence is on the right-hand side of the equation while all of the dependence on the spatial variable is on the other side. In this case, the t dependence is already isolated, without any algebra on our part.

Step 5: Now imagine changing the isolated variable t by a small amount. In principle, the right-hand side of (257) could change, but nothing on the left-hand side would. Therefore, if the equation is to be true for all values of t, the particular combination of t dependence on the right-hand side must be constant. By convention, we call this constant E.

$$\frac{1}{\psi}\left(H_{\rm op}\psi\right) = i\hbar\frac{dT}{dt}\frac{1}{T} \stackrel{\rm def}{=} E \tag{89}$$

In this way we have broken our original partial differential equation up into a pair of equations, one of which is an ordinary differential equation involving only t, the other is a partial differential equation involving only the three spatial variables.

$$\frac{1}{\psi} H_{\text{op}} \psi = E \tag{90}$$

$$i\hbar \frac{dT}{dt} \frac{1}{T} = E \tag{91}$$

The separation constant E appears in both equations.

Step 6: Write each equation in standard form by multiplying each equation by its unknown function to clear it from the denominator.

$$H_{\text{op}} \psi = E\psi \tag{92}$$

$$\frac{dT}{dt} = -\tfrac{i}{\hbar} ET \tag{93}$$

Notice that (261) is an eigenvalue equation for the operator H_{op}. You may never have thought of the derivation of this "time independent version of the Schrödinger equation" from the Schrödinger equation as just a simple example of the separation of variables procedure. At the moment, the eigenvalue E could be anything. Much of the rest of the Paradigm will be directed toward finding the possible values of E!

Now we must repeat the steps until each of the variables has been separated out into its own ordinary differential equation. In the next round, we will isolate the r dependence.

Step 1: Since we want to isolate the r dependence, we must rewrite H_{op} to show the r dependence explicitly using (84)

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} L^2_{\text{op}} \right] \psi + U(r)\psi = E\psi \tag{94}$$

Step 2: Assume $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$.

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) Y - \frac{1}{\hbar^2 r^2} R(L^2_{\text{op}} Y) \right] + U(r)RY = ERY \tag{95}$$

Step 3:

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{d}{dr} \frac{1}{R} \left(r^2 \frac{dR}{dr} \right) - \frac{1}{\hbar^2 r^2} \frac{1}{Y} (L^2_{\text{op}} Y) \right] + U(r) = E \tag{96}$$

Step 4: To isolate the r dependence we must first clear the r dependence from the angular term (involving angular derivatives in $L_{\rm op}$ and angular functions in Y). To do this, we need to multiply (96) by r^2 to clear this factor out of the denominators of the angular pieces. Further rearranging (96) to get all of the r dependence on the right-hand side, we obtain:

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L^2_{\rm op}Y) = -\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R} - \frac{2\mu}{\hbar^2}(E-U(r))r^2 \tag{97}$$

Step 5: In this case, I have called the separation constant A.

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L^2_{\rm op}Y) = -\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R} - \frac{2\mu}{\hbar^2}(E-U(r))r^2 \stackrel{\rm def}{=} A \tag{98}$$

In principle, A can be any complex number.

Step 6: Rearranging (98) slightly, we obtain the radial and angular equations in the more standard form:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}(E-U(r))r^2\,R + AR = 0 \tag{99}$$

$$L^2_{\rm op}Y + \hbar^2 AY = 0 \tag{100}$$

Notice that the only place that the central potential enters the set of differential equations is in the radial equation (99). (99) is not yet in the form of an eigenvalue equation since it contains two unknown constants E and A. (100) is an eigenvalue equation for the operator $L^2_{\rm op}$ with eigenvalue $\hbar^2 A$; it is independent of the form of the central potential.

In the last round, we must separate the θ dependence from the ϕ dependence. I will leave this as an important Practice Problem. The answer is:

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) - A\sin^2\theta P - BP = 0 \tag{101}$$

$$\frac{d^2\Phi}{d\phi^2} + B\Phi = 0 \tag{102}$$

(102) is an eigenvalue equation for the operator $d^2/d\phi^2$ with eigenvalue B. (101) is not yet in the form of an eigenvalue equation since it contains two unknown constants A and B.

We started with a partial differential equation in four variables and we ended up with four ordinary differential equations (262), (99), (101), (102) by introducing **three** separation constants (E, A, and B). You should always get one fewer separation constant than the number of variables you started with; each separation constant should appear in two of the final set of equations.

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1 Practice Problems

1. Work carefully through all of the derivations in this section.

2. Use the separation of variables procedure on (100) to obtain (101) and (102).

3. Consider the problem of the motion of a quantum particle of mass μ confined to move on a ring of radius r_0. Redo the separation of variables procedure in this section, assuming that $r = r_0$ is a constant and $\theta = \frac{\pi}{2}$ is a constant so that $\Psi = T(t)\Phi(\phi)$ only. How do the equations you get differ from the equations of this section? The solutions of these equations will be the subject of the next section.

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17 Motion on a Ring

To begin our study of the angular properties of the solutions of Schrödinger's equation, we consider the motion of a quantum particle of mass μ confined to move on a ring of constant radius r_0. As with classical orbits, let's assume that the ring lies in the x, y plane, so that in spherical coordinates $\theta = \frac{\pi}{2}$ =const. Then, since Ψ is independent of r and θ, derivatives with respect to those variables give zero and Schrödinger's equation reduces to

$$H_{\text{op}}\Psi = -\frac{\hbar^2}{2\mu}\frac{1}{r_0^2}\frac{\partial^2}{\partial\phi^2}\Psi + U(r_0)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{103}$$

Redoing the separation of variables procedure of the last section (see Practice Problem 1.3), and assuming that $\Psi = T(t)\Phi(\phi)$ only, we obtain the following separated ordinary differential equations

$$\frac{d^2\Phi}{d\phi^2} = -\frac{2I}{\hbar^2}\left(E - U(r_0)\right)\Phi \tag{104}$$

$$\frac{dT}{dt} = -\frac{i}{\hbar}ET \tag{105}$$

where we have used the substitution $\mu r_0^2 = I$, in which I would be the moment of inertia of a classical particle of mass μ traveling in a ring about the center-of-mass.

Alternatively, we could have obtained equations (104) and (105) from the results of our original separation of variables procedure (262), (99), (101), (102), by restricting the variables r and θ to the equator, noticing that the functions R and P are therefore constant, and that equation (99) reduces to:

$$A = \frac{2\mu}{\hbar^2}\left(E - U(r_0)\right)r_0^2$$

and equation (101) then reduces to:

$$B = -\frac{2\mu}{\hbar^2}\left(E - U(r_0)\right)r_0^2$$

Since the coefficient of Φ on the right-hand-side of (104) is a constant

$$\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} = \text{constant} \tag{106}$$

the solutions of the Φ equation (104), are

$$\Phi_m(\phi) \stackrel{\text{def}}{=} N\, e^{im\phi} \tag{107}$$

where

$$m = \pm\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} \tag{108}$$

and N is a normalization constant.

There is no "boundary" on the ring, on which we can impose boundary conditions. However, there is one very important property of the wave function that we can invoke: it must be single-valued. The variable ϕ is geometrically an angle, so that $\phi + 2\pi$ is physically the same point as ϕ. If we go once around the ring and return to our starting point, the value of the wave function must remain the same. Therefore the solutions must satisfy the periodicity condition $\Phi_m(\phi + 2\pi) = \Phi_m(\phi)$. This is impossible unless m is real so that the solutions are oscillatory, i.e. $E - U(r_0) > 0$. Furthermore, the solutions must have the correct period, i.e.

$$m \in \{0, \pm 1, \pm 2, \ldots\} \tag{109}$$

The quantum number m is called the *azimuthal* or *magnetic quantum number*. Note that the solution permits both positive and negative values of m as well as zero.

Solving (108) for the possible eigenvalues of energy, we obtain

$$E_m = \frac{\hbar^2}{2I}\, m^2 + U(r_0) \tag{110}$$

For this simplified ring problem, we can choose the potential energy $U(r_0)$ to be zero, but we will have to remember that we should not make this choice when we are working on the full hydrogen atom problem. There is a degeneracy that arises in this calculation. Note that the wave functions corresponding to $+|m|$ and $-|m|$ have the same energy but represent (as we will see) different states of the motion.

As usual, we choose the normalization N in (107) so that, if the particle is in an eigenstate, the probability of finding it somewhere on the ring is unity.

$$1 = \int_0^{2\pi} \Phi_m^*(\phi)\, \Phi_m(\phi)\, r_0 d\phi = \int_0^{2\pi} N^* e^{-im\phi}\, N e^{im\phi}\, r_0 d\phi = 2\pi r_0 |N|^2 \tag{111}$$

$$\Rightarrow \quad N = \frac{1}{\sqrt{2\pi r_0}} \tag{112}$$

This is a one-dimensional problem, just like the problem of a particle-in-a-box which you solved in the Waves Paradigm (now in ϕ instead of x) and the solutions have the same oscillatory form. Everything that you learned in that Paradigm is immediately applicable here. As in that problem, the energy eigenvalues are discrete because of a boundary condition. The only difference is that the boundary condition appropriate to this problem is periodicity, since ϕ is a physical angle, rather than $\Psi(x) = 0$ at the boundaries, appropriate to an infinite potential.

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1 Practice Problems

1. Show that (107) and (108) are solutions of (104).

2. Why is there a factor of r_0 in the integral in (111)?

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18 ANGULAR MOMENTUM OF THE PARTICLE ON A RING

Classically, a particle moving in a circle has an angular momentum perpendicular to the plane of the circle, which for a ring in the x, y–plane would be in the z direction. Since angular momentum is defined by $\vec{L} = \vec{r} \times \vec{p}$, we have $L_z = xp_y - yp_x$. To make the transition to quantum mechanics, we replace p_x and p_y by their operator equivalents:

$$L_z = xp_y - yp_x \Rightarrow x\frac{\hbar}{i}\frac{\partial}{\partial y} - y\frac{\hbar}{i}\frac{\partial}{\partial x} \tag{113}$$

Using a straightforward application of the chain rule (see Practice Problems, below) to replace the Cartesian partial derivatives with their polar representations, we obtain

$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi} \tag{114}$$

The effect of operating on the ring eigenfunctions with this operator is:

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(\frac{1}{\sqrt{2\pi}}\,e^{im\phi}\right) = m\hbar\left(\frac{1}{\sqrt{2\pi}}\,e^{im\phi}\right) \tag{115}$$

The energy eigenfunctions $\Phi_m(\phi)$ are thus also eigenfunctions of $\hat{L}_z$ with eigenvalues $m\hbar$. Because the $\Phi_m(\phi)$ are eigenfunctions of both energy and angular momentum, we can make simultaneous determinations of the eigenvalues of energy and angular momentum.

Considering the angular momentum helps us understand the degeneracy of the eigenfunctions with respect to energy. The $\pm m$ degeneracy of the energy eigenstates corresponds to $L_z = +m\hbar$ and $L_z = -m\hbar$. That is, the two degenerate states represent particles rotating in opposite directions around the ring.

For a classical particle rotating in a circular path in the x, y-plane, the kinetic energy is $T = \frac{1}{2}I\omega^2 = L_z^2/2I$, where I is the rotational inertia (moment of inertia). The rotational inertia of a single particle of mass μ moving in a circle of radius r_0 is $I = \mu r_0^2$. The Hamiltonian for the system is thus

$$H = T + U = \frac{L_z^2}{2I} + U = -\frac{\hbar^2}{2\mu r_0^2}\frac{\partial^2}{\partial\phi^2} + U_0 \tag{116}$$

It is apparent from this approach that the energy and the angular momentum have simultaneous eigenvalues because they are commuting operators. Clearly $[L_z^2, L_z] = 0$, so that E and L_z have the same eigenfunctions. Therefore, we see that (104) and (115) are the position-space representations of the eigenvalue equations

$$\hat{H}\,|m\rangle = E_m|m\rangle \tag{117}$$

$$\hat{L}_z\,|m\rangle = \hbar m\,|m\rangle \tag{118}$$

Because the Φ_m are simultaneous eigenstates of both $\hat{H}$ and $\hat{L}_z$, it is possible to make simultaneous measurements of both the energy and the z-component of angular momentum.

In setting up the problem of the particle on the ring, we constrained the motion to the x, y-plane, so that the angular momentum vector is in the z direction. However, according to quantum mechanics (yet another form of the Heisenberg uncertainty relationships) it is not possible to know the direction of the angular momentum vector. Our knowledge of the angular momentum vector is limited to its length and any one component. If the

vector lies along the z-axis, then we would know all three of its components (the x and y components being zero). We'll see how the three-dimensional problem solves this contradiction.

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1 Practice Problems

1. Using a the chain rule for partial derivatives, show that (113) is indeed the same as (114), thereby showing that this operator is the quantum analogue of the z-component of angular momentum.

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19 TIME DEPENDENCE OF RING STATES

We know, from the theory of Fourier series, that we can write any initial probability distribution, which is necessarily periodic, as a sum of the energy eigenstates.

$$\Phi(\phi) = \sum_{m=-\infty}^{\infty} c_m \, \Phi_m(\phi) = \sum_{m=-\infty}^{\infty} c_m \left(\frac{1}{\sqrt{2\pi \, r_0}} \, e^{im\phi} \right) \tag{119}$$

where, for the probability distribution to be normalized, we must have:

$$\sum_{m=-\infty}^{\infty} |c_m|^2 = 1 \tag{120}$$

To find the time evolution of the eigenstates $\Phi_m(\phi)$, we must solve the t equation (105). Since, for each Φ_m, we have now found the value of the constant $E = E_m$, given by (110), we can solve (105) trivially.

$$T(t) = e^{-\frac{i}{\hbar} E_m t} \tag{121}$$

A deep theorem in the theory of partial differential equations states that if you have found an expansion of the initial probability density in terms of the eigenstates of the Hamiltonian, then the time evolution of that probability

density is simply obtained by multiplying each eigenstate individually by the appropriate time evolution.

$$\Phi(\phi, t) = \sum_{m=-\infty}^{\infty} c_m \, \Phi_m(\phi) \, e^{-\frac{i}{\hbar} E_m t} \tag{122}$$

BE CAREFUL! There are an infinite number of different values for the energy, depending on the eigenstate of the Hamiltonian. It is incorrect to multiply the initial state (119) by a single over-all exponential time factor. Each term in the series gets its own time evolution.

20 Motion on a Sphere

We will now relax the restriction that the mass be confined to the ring, and instead, let it range over the surface of a sphere of radius r_0. The results of this analysis yield predictions that can be successfully compared with experiment for molecules and nuclei that rotate more than they vibrate. For this reason, the problem of a mass confined to a sphere is often called the rigid rotor problem. Furthermore, the solutions that we will find for equations (101) and (102), called spherical harmonics, will occur whenever one solves a partial differential equation that involves spherical symmetry.

For homework, you will write down the Schrödinger equation for a particle restricted to a sphere and use the separation of variables procedure to obtain an equivalent set of ordinary differential equations. One of the equations you obtain will be (102), with solutions exactly as we found them for the ring. The other equation will be (101) with slightly different labels for the unknown constants. So, to solve either Schrödinger's equation for the hydrogen atom or for a particle restricted to a sphere, we need to solve (101). This will be the job of the next five sections.

21 Change of Variables

Since we have solved the ϕ equation (102) and found the possible values of the separation constant $\sqrt{B} = m \in \{0, \pm 1, \pm 2, \ldots\}$, the θ equation becomes an eigenvalue/eigenfunction equation for the unknown separation constant A and the unknown function $P(\theta)$.

$$\left(\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-A\sin^2\theta-m^2\right)P(\theta)=0 \tag{123}$$

We start with a change of independent variable $z=\cos\theta$ where z is the usual rectangular coordinate in three-space. As θ ranges from 0 to π, z ranges from 1 to -1. We see from Figure 4 that:

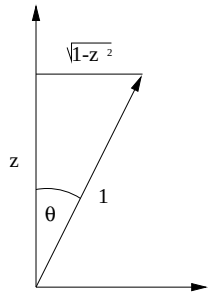

Figure 4: Relationship between z and θ.

$$\sqrt{1-z^2}=\sin\theta \tag{124}$$

Using the chain rule for partial derivatives, we have:

$$\frac{\partial}{\partial\theta}=\frac{\partial z}{\partial\theta}\frac{\partial}{\partial z}=-\sin\theta\frac{\partial}{\partial z}=-\sqrt{1-z^2}\frac{\partial}{\partial z} \tag{125}$$

Notice, particularly, the last equality: we are trying to change variables from θ to z, so it is important to make sure we change **all** the θ's to z's. Multiplying by $\sin\theta$ we obtain:

$$\sin\theta\frac{\partial}{\partial\theta}=-\left(1-z^2\right)\frac{\partial}{\partial z} \tag{126}$$

Be careful finding the second derivative; it involves a product rule:

$$\begin{aligned}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)&=\left(1-z^2\right)\frac{\partial}{\partial z}\left(\left(1-z^2\right)\frac{\partial}{\partial z}\right)\\&=\left(1-z^2\right)^2\frac{\partial^2}{\partial z^2}-2z\left(1-z^2\right)\frac{\partial}{\partial z}\end{aligned} \tag{127}$$

Inserting (124) and (127) into (123), we obtain a standard form of the Associated Legendre's equation:

$$\left(\left(1-z^2\right)\frac{\partial^2}{\partial z^2}-2z\frac{\partial}{\partial z}-A-\frac{m^2}{(1-z^2)}\right)P(z)=0 \tag{128}$$

In §22 and §25, we will solve this equation. After we have found the eigenfunctions $P(z)$, we will substitute $z = \cos\theta$ everywhere to find the eigenfunctions of the original equation (123).

22 SERIES SOLUTIONS OF ODE'S

The simplest possible ϕ–dependence on the ring is, of course, $\Phi(\phi) = \text{constant}$, which corresponds in equation (123) to $m = 0$. We will first find solutions for this special case, which is known as *Legendre's equation*.

$$\left(\left(1 - z^2\right) \frac{\partial^2}{\partial z^2} - 2z \frac{\partial}{\partial z} - A \right) P(z) = 0 \tag{129}$$

Let's use series methods to find a solution of (129), i.e. let's assume that the solution can be written as a Taylor series

$$P(z) = \sum_{n=0}^{\infty} a_n \, z^n \tag{130}$$

and solve for the coefficients a_n. Then we have

$$\frac{dP}{dz} = \sum_{n=0}^{\infty} a_n \, n \, z^{n-1} \tag{131}$$

$$\frac{d^2P}{dz^2} = \sum_{n=0}^{\infty} a_n \, n(n-1) \, z^{n-2} \tag{132}$$

and then plug (130)–(132) into (129) to obtain

$$0 = \sum_{n=0}^{\infty} a_n \, n(n-1) \, z^{n-2} - z^2 \sum_{n=0}^{\infty} a_n \, n(n-1) \, z^{n-2} - 2z \sum_{n=0}^{\infty} a_n \, n \, z^{n-1} - A \sum_{n=0}^{\infty} a_n \, z^n \tag{133}$$

In (133), the summation variable n is a dummy variable (just like a dummy variable of integration). Therefore, in the first sum, we can shift $n \to n + 2$.

$$\sum_{n=0}^{\infty} a_n \, n(n-1) \, z^{n-2}$$

$$\rightarrow \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1)z^n$$

$$= a_{-2}(-2+2)(-2+1)z^{-2} + a_{-1}(-1+2)(-1+1)z^{-1} + \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)z^n$$

$$= \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)z^n$$

Pay special attention to what happened to the lower limit of the sum. The new sum would start at $n = -2$, but since the factor of $(n+2)$ in the first term and the factor of $(n+1)$ in the second term means that these terms are zero and we can eliminate them from the sum. At the same time, bring any overall factors of z into the corresponding sums. Finally, since each sum now has a factor of z^n and runs over the same range, group the sums together.

$$\sum_{n=-2}^{\infty} a_{n+2}\,(n+2)(n+1)\,z^n - \sum_{n=0}^{\infty} a_n\,n(n-1)\,z^n - 2\sum_{n=0}^{\infty} a_n\,n\,z^n - A\sum_{n=0}^{\infty} a_n\,z^n \tag{134}$$

$$= \sum_{n=0}^{\infty} \left[a_{n+2}\,(n+2)(n+1) - a_n\,n(n-1) - 2\,a_n\,n - A\,a_n\right] z^n = 0 \tag{135}$$

Now comes the MAGIC part. Since (135) is true *for all values of* z, the coefficient of z^n for each term in the sum must separately be zero, i.e.

$$a_{n+2}\,(n+2)(n+1) - a_n\,n(n-1) - 2\,a_n\,n - A\,a_n = 0 \tag{136}$$

and therefore we can solve for a_{n+2} in terms of a_n

$$a_{n+2} = \frac{n(n+1)+A}{(n+2)(n+1)}\,a_n \tag{137}$$

By plugging successive even values of n into the recurrence relation (137) allows us to find a_2, a_4, etc. in terms of the arbitrary constant a_0 and successive odd values of n allow us to find a_3, a_5, etc. in terms of the arbitrary constant a_1. Thus, for the second order differential equation (129) we obtain two solutions as expected. a_0 becomes the normalization constant for a solution with only even powers of z and a_1 becomes the normalization constant for a solution with only odd powers of z. For example:

$$a_2 = \frac{A}{2}\,a_0 \tag{138}$$

$$a_4 = \frac{6+A}{12}\,a_2 = \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right)\,a_0 \qquad \text{etc.} \tag{139}$$

$$a_3 = \frac{2+A}{6}\,a_1 \tag{140}$$

$$a_5 = \frac{12+A}{20}\,a_2 = \left(\frac{12+A}{20}\right)\left(\frac{6+A}{12}\right)\,a_0 \qquad \text{etc.} \tag{141}$$

so that

$$P(z) = a_0\left[\frac{A}{2}\,z^0 + \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right)\,z^2 + \ldots\right] \tag{142}$$

$$+ \quad a_1\left[\frac{2+A}{6}\,z^1 + \left(\frac{12+A}{20}\right)\left(\frac{2+A}{6}\right)\,z^3 + \ldots\right] \tag{143}$$

In general, the solutions of an ordinary linear differential equation can blow-up only where the coefficients of the equation itself are singular, in this case at $z = \pm 1$, which correspond to the north and south poles $\theta = 0, \pi$. But there is nothing special about physics at these points, only the choice of coordinates is special there. Therefore, we want to choose solutions of (129) which are regular (non-infinite) at $z = \pm 1$. This is an important example of a problem where the choice of coordinates for a partial differential equation end up imposing boundary conditions on the ordinary differential equation which comes from it. Therefore, the infinite series (130) could possibly blow up at the endpoints $z = \pm 1$, but a polynomial could not. So if we choose the special values for the separation constant A to be $A = -\ell(\ell+1)$ where ℓ is a non-negative integer, we see from (137) that for $n \geq \ell$ the coefficients become zero and the series terminates in a polynomial. The solutions for these special values of A are polynomials of degree ℓ, denoted P_ℓ, and called Legendre polynomials.

23 LEGENDRE POLYNOMIALS

It turns out that the Legendre polynomials can also be found from Rodrigues' formula

$$P_\ell(z) = \frac{1}{2^\ell \ell!}\,\frac{d^\ell}{dz^\ell}\left(z^2-1\right)^\ell \tag{144}$$

(The proof is lengthy, but beautiful. Ask!) Rodrigues' Formula can be used to generate solutions quickly. To do this, write

$$\left(z^2-1\right)^\ell = (z-1)^\ell (z+1)^\ell = a^\ell b^\ell \tag{145}$$

and use the product rule

$$\frac{d^\ell}{dz^\ell}\left(z^2-1\right)^\ell = \left(\frac{d^\ell a^\ell}{dz^\ell}\right) b^\ell + \ell\left(\frac{d^{\ell-1}a^\ell}{dz^{\ell-1}}\right)\left(\frac{db^\ell}{dz}\right) + \frac{\ell(\ell-1)}{2!}\left(\frac{d^{\ell-2}a^\ell}{dz^{\ell-2}}\right)\left(\frac{d^2b^\ell}{dz^2}\right) + ... + a^\ell\left(\frac{d^\ell b^\ell}{dz^\ell}\right) \tag{146}$$

where the coefficient of the i^{th} term in the product rule is the binomial coefficient

$$\binom{\ell}{i} = \binom{\ell}{\ell-i} = \frac{\ell!}{(\ell-i)!\,i!} \tag{147}$$

The first few Legendre polynomials are:

$$P_0(z) = 1 \tag{148}$$
$$P_1(z) = z \tag{149}$$
$$P_2(z) = \frac{1}{2}\left(3z^2-1\right) \tag{150}$$
$$P_3(z) = \frac{1}{2}\left(5z^3-3z\right) \tag{151}$$
$$P_4(z) = \frac{1}{8}\left(35z^4-30z^2+3\right) \tag{152}$$
$$P_5(z) = \frac{1}{8}\left(63z^5-70z^3+15z\right) \tag{153}$$

There are several useful patterns to the Legendre polynomials:

- The overall coefficient for each solution is conventionally chosen so that $P_\ell(1) = 1$. *As discussed in the next section, this is an inconvenient convention that we are stuck with!*
- $P_\ell(z)$ is a polynomial of degree ℓ.
- Each $P_\ell(z)$ contains only odd or only even powers of z, depending on whether ℓ is even or odd. Therefore, each $P_\ell(z)$ is either an even or an odd function.
- Since the differential operator in (129) is Hermitian (unproven), we are guaranteed by a deep theorem of mathematics that the Legendre

polynomials are orthogonal for different values of ℓ (just as with Fourier series) [1] , i.e.

$$\int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz = \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} \tag{154}$$

The "squared norm" of P_ℓ is just $1/(\ell + \frac{1}{2})$. To normalize each $P_\ell(z)$ it should be multiplied by $\sqrt{\ell + \frac{1}{2}}$.

Notice that the differential equation

$$\frac{\partial^2 P}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial P}{\partial z} + \frac{\ell(\ell+1)}{1-z^2} P = 0 \tag{155}$$

is a **different** equation for different values of ℓ. For a given value of ℓ, you should expect two solutions of (155). Why? We have only given one. It turns out that the "other" solution for each value of ℓ is not regular (i.e. it blows up) at $z = \pm 1$. In cases where the separation constant A does not have the special value $l(l+1)$ for non-negative integer values of ℓ, it turns out that *both* solutions blow up. We discard these irregular solutions as unphysical for the problem we are solving.

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1 Practice Problems

1. Use Rodrigues' formula, by hand, to find the first 5 Legendre polynomials.

2. Go through the worksheet `legendre.mws`. You do not need to turn anything in. However, there are two things you should get out of this worksheet:

   (a) Get a feel for what the Legendre polynomials look like. There are some questions in the worksheet to help guide your exploration.

   (b) Learn the syntax for writing a "loop" in Maple. There is a discussion of this in the worksheet. Loops are one of the most useful of all computer programming techniques.

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[1] One shows this using Rodrigues' Formula and repeated integration by parts, noting that the "surface terms" always vanish.

24 LEGENDRE POLYNOMIAL SERIES

There is a very powerful mathematical theorem which says that *any* sufficiently smooth function $f(z)$, defined on the interval $-1 < z < 1$, can be expanded as a linear combination of Legendre polynomials

$$f(z) = \sum_{\ell=0}^{\infty} c_\ell \, P_\ell(z) \tag{156}$$

(This theorem is the analogue of the theorem which says that any sufficiently smooth periodic function can be expanded in a Fourier series.) You will have several occasions in physics to expand functions in Legendre polynomial series, so we will explore the technique in this section.

We can find the coefficients c_ℓ by taking the inner product of both sides of (156) in turn with each "basis vector" P_k and using (154). This yields

$$\begin{aligned}
\int_{-1}^{1} P_k^*(z)\, f(z)\, dz &= \int_{-1}^{1} P_k^*(z) \sum_{\ell=0}^{\infty} c_\ell \, P_\ell(z)\, dz && (157)\\
&= \sum_{\ell=0}^{\infty} c_\ell \int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz && (158)\\
&= \sum_{\ell=0}^{\infty} c_\ell \, \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} && (159)\\
&= \frac{c_k}{k + \frac{1}{2}} && (160)
\end{aligned}$$

or equivalently

$$c_k = \left(k + \frac{1}{2}\right) \int_{-1}^{1} P_k^*(z)\, f(z)\, dz \tag{161}$$

This expression should be compared with the exponential version of a Fourier series for $f(z)$ on the same interval $-1 \le z \le 1$, namely

$$f(z) = \sum_{n=-\infty}^{\infty} C_n \, e^{in\pi z} \tag{162}$$

where

$$C_n = \frac{1}{2}\int_{-1}^{1} e^{-in\pi z} f(z)\, dz \tag{163}$$

Note the analogous role played by the *normalization constants* $k+\frac{1}{2}$ and $\frac{1}{2}$. If we had made an unconventional, but more convenient, choice for the normalization for the Legendre polynomials such that the value of the integrals in (154) were simply $\delta_{k\ell}$, then we would not need to carry around the extra factor of $k+\frac{1}{2}$ in (161).

1 Example: Legendre Expansion of $\varepsilon(z)$

Consider the step function

$$\varepsilon(z) = 2\,\Theta(z) - 1 = \begin{cases} +1 & (z>0) \\ -1 & (z<0) \end{cases} \tag{164}$$

where Θ is the Heaviside step function; note that $\varepsilon(z)$ is an *odd* function of z. Using (161) leads to

$$c_\ell = \left(\ell+\frac{1}{2}\right)\int_{-1}^{1} P_\ell^*(z)\,\varepsilon(z)\,dz \tag{165}$$

$$= -\left(\ell+\frac{1}{2}\right)\int_{-1}^{0} P_\ell^*(z)\,dz + \left(\ell+\frac{1}{2}\right)\int_{0}^{1} P_\ell^*(z)\,dz \tag{166}$$

and each integral in the final expression is an elementary integral of a polynomial. Furthermore, it is easily seen that these two integrals cancel if ℓ is even, and add if ℓ is odd, so that

$$c_\ell = \begin{cases} 0 & (\ell \text{ even}) \\ 2\left(\ell+\frac{1}{2}\right)\displaystyle\int_{0}^{1} P_\ell^*(z)\,dz & (\ell \text{ odd}) \end{cases} \tag{167}$$

These coefficients are easily evaluated on Maple for as many values of ℓ as desired.

25 ASSOCIATED LEGENDRE FUNCTIONS

We now return to equation (128) to consider the cases with $m \neq 0$. We can solve these equations with (a slightly more sophisticated version of) the series techniques from the $m = 0$ case. We would again find solutions that are regular at $z = \pm 1$ whenever we choose $A = -\ell(\ell+1)$ for $\ell \in \{0, 1, 2, 3, \ldots\}$. With this value for A, we obtain the standard form of Legendre's associated equation, namely

$$\left(\frac{\partial^2}{\partial z^2} - \frac{2z}{1-z^2} \frac{\partial}{\partial z} + \frac{\ell(\ell+1)}{1-z^2} - \frac{m^2}{(1-z^2)^2} \right) P(z) = 0 \tag{168}$$

Recall that this equation was obtained by separating variables in spherical coordinates. Solutions of this equation which are regular at $z = \pm 1$ are called *associated Legendre functions*, and turn out to be given by

$$P_\ell^m(z) = P_\ell^{-m}(z) = (1-z^2)^{m/2} \frac{d^m}{dz^m} \left(P_\ell(z) \right) \tag{169}$$

$$= (1-z^2)^{m/2} \frac{d^{m+\ell}}{dz^{m+\ell}} \left((z^2-1)^\ell \right) \tag{170}$$

where $m \geq 0$. [2] Note that if $z = \cos\theta$, then $P_\ell(z)$ is a polynomial in $\cos\theta$, while

$$(1-z^2)^{m/2} = (\sin^2\theta)^{m/2} = \sin^m\theta \tag{171}$$

so that $P_\ell^m(z)$ is a polynomial in $\cos\theta$ times a factor of $\sin^m\theta$. Some other properties of the associated Legendre functions are

- $P_\ell^m(z) = 0$ if $|m| > \ell$
- $P_\ell^{-m}(z) = P_\ell^m(z)$
- $P_\ell^m(\pm 1) = 0$ for $m \neq 0$ (cf. factor of $(1-z^2)^{m/2}$)
- $P_\ell^m(-z) = (-1)^{\ell-m} P_\ell^m(z)$ (behavior under parity)
- $\displaystyle\int_{-1}^{1} P_\ell^m(z) P_q^m(z)\, dz = \frac{2}{(2\ell+1)} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell q}$

The last property shows that for each given value of m, the Associated Legendre functions form an orthonormal basis on the interval $-1 \leq z \leq 1$. Any function on this interval can be expanded in terms of anyone of these bases.

[2] Some authors define $P_\ell^{-m}(z)$ with a different phase.

26 SPHERICAL HARMONICS

We have found that normalized solutions of the ϕ equation (102) satisfying periodic boundary conditions are

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi} \qquad\qquad (m = 0, \pm 1, \pm 2, ...) \tag{172}$$

and normalized solutions of the θ equation (101 which are regular at the poles are given by

$$P(\cos\theta) = \sqrt{\frac{(2\ell+1)}{2}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta) \tag{173}$$

Combining these yields via multiplication (we assumed solutions of this type when we first did the separation of variables procedure), we obtain the *spherical harmonics*

$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta)\, e^{im\phi} \tag{174}$$

where the somewhat peculiar choice of phase is conventional.

The spherical harmonics are orthonormal on the unit sphere:

$$\int_0^{2\pi}\int_0^{\pi} \left(Y_{\ell_1}^{m_1}\right)^* Y_{\ell_2}^{m_2} \sin\theta\, d\theta\, d\phi = \delta_{\ell_1\ell_2}\delta_{m_1m_2} \tag{175}$$

since $dz = \sin\theta\, d\theta$. They are complete in the sense that any sufficiently smooth function f on the unit sphere can be expanded in a *Laplace series* as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m}\, Y_\ell^m(\theta,\phi) \tag{176}$$

where

$$a_{\ell m} = \int_0^{2\pi}\int_0^{\pi} (Y_\ell^m)^*\, f(\theta,\phi)\, \sin\theta\, d\theta\, d\phi \tag{177}$$

1 Example

Suppose you want a function of (θ, ϕ) which satisfies

$$f(\theta,\phi) = \begin{cases} \sin\theta & 0 < \theta < \frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases} \tag{178}$$

Then f takes the form (176), and the constants $a_{\ell m}$ can be determined from (177), yielding

$$a_{\ell m} = \int_0^{2\pi} \int_0^{\pi/2} (Y_\ell^m)^* \sin^2\theta \, d\theta \, d\phi \tag{179}$$

$$= N_{\ell m} \int_0^{2\pi} e^{-im\phi} \, d\phi \int_0^{\pi/2} P_\ell^m(\cos\theta) \, \sin^2\theta \, d\theta \tag{180}$$

where

$$N_{\ell m} = (-1)^{(m+|m|)/2} \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} \tag{181}$$

Thus,

$$a_{\ell m} = \begin{cases} 0 & (m \neq 0) \\ \sqrt{(2\ell+1)\,\pi} \displaystyle\int_0^{\pi/2} P_\ell(\cos\theta) \, \sin^2\theta \, d\theta & (m = 0) \end{cases} \tag{182}$$

For $m = 0$, the integral is most easily computed with the substitution $z = \cos\theta$; the first few coefficients are:

$$\begin{aligned} a_{00} &= \frac{\pi}{8} \qquad a_{10} = \frac{1}{2} \qquad a_{20} = -\frac{5\pi}{64} \\ a_{30} &= -\frac{7}{12} \qquad a_{40} = -\frac{9\pi}{512} \qquad a_{50} = \frac{77}{240} \end{aligned} \tag{183}$$

(each of which should be multiplied by $\sqrt{4\pi/(2\ell+1)}$). As you can check by graphing, however, it requires at least twice this many terms to obtain a good approximation.

27 ANGULAR MOMENTUM

1 Classical Angular Momentum

Consider the angular momentum of the reduced mass system $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times \mu \boldsymbol{v}$. We have:

$$\begin{aligned} \frac{d\boldsymbol{L}}{dt} &= \frac{d}{dt}(\boldsymbol{r} \times \mu \boldsymbol{v}) && (184) \\ &= \boldsymbol{r} \times \mu \dot{\boldsymbol{v}} + \boldsymbol{v} \times \mu \boldsymbol{v} && (185) \\ &= \boldsymbol{r} \times \mu \boldsymbol{a} && (186) \\ &= \boldsymbol{r} \times \boldsymbol{F} && (187) \\ &= r\hat{\boldsymbol{r}} \times f(r)\hat{\boldsymbol{r}} && (188) \\ &= 0 && (189) \end{aligned}$$

(The second term in (185) is zero since $\boldsymbol{v} \times \boldsymbol{v} = 0$.) $\boldsymbol{r} \times \boldsymbol{F}$ which occurs in (187) is called the torque. We have shown that in the case of central forces the time derivative of the angular momentum, and hence the torque, are zero. Therefore:

$$\tau = \frac{d\boldsymbol{L}}{dt} = 0 \qquad \Rightarrow \qquad \boldsymbol{L} = \text{constant} \tag{190}$$

i.e. the angular momentum is conserved.

The force $\boldsymbol{F}(r)$ depends only on the distance of the reduced mass from the center of mass and not on the orientation. Therefore, this system is spherically symmetric; it is invariant (unchanged) under rotations. Noether's theorem states that whenever the laws of physics are invariant under a particular motion or other operation, there will be a corresponding conserved quantity. In this case, we see that the conservation of angular momentum is related to the invariance of the physical situation under rotations. Noether's theorem, in general, is most easily discussed using Lagrangian techniques. You will see this again the Classical Mechanics Capstone.

. . . . . .

Practice Problem

1. (Challenging) Can you guess what invariances of physics are related to conservation of linear momentum and conservation of energy?

2 Quantum Angular Momentum

In quantum mechanics, momentum $\boldsymbol{p}$ becomes the differential operator $\frac{\hbar}{i}\boldsymbol{\nabla}$. Under this correspondence, the components of $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$ become the operators

$$L_x = yp_z - zp_y \quad \longmapsto \quad \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \tag{191}$$

$$L_y = zp_x - xp_z \quad \longmapsto \quad \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \tag{192}$$

$$L_z = xp_y - yp_x \quad \longmapsto \quad \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial \phi} \tag{193}$$

which we also call L_x, etc. Direct computation, which you will verify for homework, shows that

$$[L_x, L_y]f = i\hbar L_z f \tag{194}$$

and cyclic permutations. But the operator

$$\begin{aligned} L^2 &= \boldsymbol{L}\cdot\boldsymbol{L} = L_x^2 + L_y^2 + L_z^2 \\ &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \end{aligned} \tag{195}$$

does commute with $\boldsymbol{L}$, that is

$$[L^2, L_z] = 0 \tag{196}$$

and so forth.

This (Lie) algebra is the same as the algebra of the spin matrices

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{197}$$

that is

$$[S_x, S_y] = i\hbar S_z \tag{198}$$

and cyclic permuations.

3 Eigenvalues

What are the eigenvalues and eigenfunctions of the angular momentum operators? As you will show for homework,

$$L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m} \tag{199}$$
$$L_z Y_{\ell m} = \hbar m Y_{\ell m} \tag{200}$$
$$\tag{201}$$

28 The Radial Equation

So far we have obtained solutions to the angular (θ and ϕ) parts of the Schrödinger equation. The $Y_{lm}(\theta, \phi)$'s describe the spatial variation of the wave function on the surface of a sphere. Now we turn to the radial equation (99), plugging in the value of the separation constant $A = -\ell(\ell+1)$ that we obtained when solving the θ equation.

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}(E - U(r))r^2 R - \ell(\ell+1)R = 0 \tag{202}$$

The solution to equation (99) will depend on the potential energy $U(\vec{r})$; for central forces, the potential energy U depends only on r and is independent of θ and ϕ. As a result, the $Y_{lm}(\theta, \phi)$'s are solutions to the angular part for *any* central force.

We can rewrite equation(202) as:

$$\frac{d^2 R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left[E - U(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2}\right] R = 0 \tag{203}$$

which resembles the one-dimensional Schrödinger equation corresponding to an effective potential energy U_{eff}:

$$U_{\text{eff}}(r) = U(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \tag{204}$$

The term $\hbar^2 \ell(\ell+1)/2\mu\, r^2$ is the centrifugal contribution to the effective potential energy. It behaves like a repulsive force, and it increases with ℓ in exact analogy with classical mechanics.

We will solve the radial equation for a potential energy characteristic of an atom consisting of a single electron interacting with a nucleus of charge +Ze (H, He+, Li++, etc.):

$$U(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r} \tag{205}$$

Insert Graph

Practice Question:

As l increases, do you think the expectation value of r will increase or decrease? Later we will use the radial wave functions to calculate the expectation value of r, and we will see if the calculated value is consistent with your expectation.

With this choice of $U(r)$, we can write the radial equation as:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left[E + \frac{k}{r} - \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]R = 0 \tag{206}$$

where $k = Ze^2/4\pi\varepsilon_0$.

29 ASYMPTOTIC SOLUTIONS TO THE RADIAL EQUATION

At first glance there seems to be no obvious direct approach to solving equation (206), so let's see if we can get some clues to the form of the solution by looking at the limiting behavior of the solutions for large r and for small r.

For large r, the terms in equation (206) involving r^{-1} and r^{-2} can be neglected, so equation (206) becomes approximately

$$\frac{d^2R}{dr^2} + \frac{2\mu E}{\hbar^2}R = 0 \tag{207}$$

It is helpful to remind ourselves that $E < 0$ by writing equation (207) as

$$\frac{d^2R}{dr^2} = \frac{2\mu\,|E|}{\hbar^2}R \tag{208}$$

which has the familiar exponential solutions $R(r) = e^{\pm br}$ with $b = \sqrt{2\mu|E|/\hbar^2}$.

Note the $\pm$ symbol in the exponential, which is there because equation (208) involves the second derivative of R. Can we eliminate one of these

signs? As r goes to infinity, e^{+br} blows up. We will eventually want our solutions for the wave functions to give us reasonably behaved probability densities (that is, they must be finite everywhere), and we must therefore discard any solution that leads to an infinite probability. Our solution for the radial wave function in this limit then becomes:

$$R(r) \sim e^{-br} \qquad (\text{larger}) \tag{209}$$

Now let's look at the behavior of the solutions when r is small. In this limit, the r^{-2} term will dominate and we can neglect the other terms in the square brackets in equation (206). In this case, we obtain

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R = 0 \tag{210}$$

Practice Question: The solution to this equation apparently doesn't depend on $\hbar$. Don't all quantum-mechanical results depend in some way on Planck's constant?

By inspection, you can see that a solution of the form $R(r) = r^q$ can be made to satisfy equation (210) - note that for this choice of $R(r)$ each term in equation (210) will then depend on r^{q-2} and the three terms can sum to zero. With this substitution, we obtain

$$q(q-1)r^{q-2} + \frac{2}{r}qr^{q-1} - \frac{l(l+1)}{r^2}r^q = 0 \tag{211}$$

or

$$q(q+1) - l(l+1) = 0 \tag{212}$$

This quadratic equation for q yields two solutions: $q = l$ and $q = l - 1$. For small r, $r - l - 1$ blows up, so we discard this solution. We then have

$$R(r) \sim r^l \qquad (\text{small}r) \tag{213}$$

Combining equations (209) and (213), we expect the radial solution to look something like $R(r) \sim r^l e^{-br}$. Note that we have not violated the proper behavior at the limits by combining these two solutions; $R(r)$ remains well-behaved for $r = 0$ and $r \to \infty$. What else do we need to complete the solution? Perhaps an additional function $H(r)$, which gives the remaining radial dependence and is well-behaved by not blowing up at $r = 0$ (or blowing

up more slowly than r^{-l}) nor as $r \to \infty$ (or blowing up more slowly than e^{br}). Let us therefore seek solutions of the radial equation of the form

$$R(r) = r^l e^{-br} H(r) \tag{214}$$

Our next goal is to determine $H(r)$.

Practice Question:

Other than its asymptotic behavior, what other properties do you expect for $R(r)$? If we expect $R(r)$ to be a radial WAVE function, what type of behavior is missing from the other parts of $R(r)$ that $H(r)$ must provide?

30 SOLVING THE RADIAL EQUATION

Before we begin substituting into equation (206), we'll need the first two derivatives of $R(r)$.

$$\frac{dR}{dr} = lr^{l-1}e^{-br}H(r) - br^l e^{-br}H(r) + r^l e^{-br}H'(r) \tag{215}$$

where $H'(r) = dH/dr$, and

$$\begin{aligned} \frac{d^2R}{dr^2} &= l(l-1)r^{l-2}e^{-br}H(r) - 2blr^{l-1}e^{-br}H(r) + 2lr^{l-1}e^{br}H'(r) && (216) \\ &+ b^2r^l e^{-br}H(r) - 2br^l e^{-br}H'(r) + r^l e^{-br}H''(r) && (217) \end{aligned}$$

Substituting equations (215) and (217) into equation (206) and clearing terms, the result is

$$rH'' + [2(l+1) - 2br]\,H' + \left[-2b(l+1) + \frac{2\mu}{\hbar^2}k\right] H = 0 \tag{218}$$

It is convenient at this point to re-write this equation in terms of the dimensionless variables $\rho = 2br$ and $\lambda = \mu k/\hbar^2 b$:

$$\rho\frac{d^2H}{d\rho^2} + (2l + 2 - \rho)\frac{dH}{d\rho} + (\lambda - l - 1)H(\rho) = 0 \tag{219}$$

In analogy with our solution to the θ equation, equation (101), we'll use a power series expansion to find the solution to equation (219):

$$H(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \tag{220}$$

Taking derivatives, we obtain

$$H'(\rho) = \sum_{j=1}^{\infty} j c_j \rho^{j-1} \quad \text{and} \quad H''(\rho) = \sum_{j=2}^{\infty} j(j-1) c_j \rho^{j-2} \tag{221}$$

and substituting into equation (219 we find

$$\sum_{j=2}^{\infty} j(j-1) c_j \rho^{j-1} + (2l+2) \sum_{j=1}^{\infty} j c_j \rho^{j-1} - \sum_{j=1}^{\infty} j c_j \rho^{j} + (\lambda - l - 1) \sum_{j=0}^{\infty} c_j \rho^{j} = 0 \tag{222}$$

Expanding each of the sums gives a power series in ρ. For all terms of the series to add to zero for any and all values of ρ, the coefficient of each power of ρ must be zero. Before we develop the solution, let's write out the first few terms of equation (222):

$$[(2l+2)c_1 + (\lambda - l - 1)c_0]\rho^0 + [(4l+6)c_2 \tag{223}$$

$$+ \quad (\lambda - l - 2)c_1]\rho^1 + [(6l+12)c_3 + (\lambda - l - 3)c_2]\rho^2 + \ldots = 0 \tag{224}$$

Each term in square brackets must be zero for this equation to be valid for any value of ρ. From the first term in square brackets, we obtain a relationship between c_1 and c_0, from the second term in square brackets, we obtain a relationship between c_2 and c_1, from the third term in square brackets, we obtain a relationship between c_3 and c_2, and so forth. The value of c_0 thus determines the values of all of the remaining c_j.

Now let's find the complete solution to equation (222). It is convenient to begin by rewriting equation (222) so that all sums are given in terms of powers of ρ^j. We can accomplish this by replacing j with $j+1$ in the first two sums:

$$\sum_{j=1}^{\infty} (j+1)(j) c_{j+1} \rho^{j} \quad + \quad (2l+2) \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^{j} \tag{225}$$

$$- \quad \sum_{j=1}^{\infty} j c_j \rho^{j} + (\lambda - l - 1) \sum_{j=0}^{\infty} c_j \rho^{j} = 0 \tag{226}$$

Once again, the coefficient of each term in the sum must vanish. The coefficient of the general term ρ^j is

$$(j+1)(j) c_{j+1} + (2l+2)(j+1) c_{j+1} - j c_j + (\lambda - l - 1) c_j = 0 \tag{227}$$

This leads to the recursion relation

$$c_{j+1} = \frac{j - \lambda + l + 1}{(j+1)(j+2l+2)} c_j \tag{228}$$

which agrees with the results we obtained from the first few terms in the expansion of equation (222). As we deduced from that analysis, choosing c_0 determines all of the remaining expansion coefficients.

In our study of the polar wave functions, we found we had to force the series to terminate to prevent the wave function from becoming infinite. So far we have assumed that the upper limit of the series expansion of $H(\rho)$ is infinity. However, our analysis for the expansion coefficients does not depend on whether the series is finite or infinite. Let's see how we can use the properties of $R(r)$ to make this determination.

How does the recursion relationship, equation (228), behave in the limit of large j? As $j \to \infty$, equation (228) becomes approximately $c_{j+1} \sim c_j/j + 1$. That is, $c_1 = c_0$, $c_2 = c_1/2 = c_0/2$, $c_3 = c_2/3 = c_0/3!$, and so forth. In general, then, for large j, $c_j \sim c_0/j!$ and because $\sum_{j=0}^{\infty} \rho^j/j! = e^\rho$ we have $H(\rho) = c_0 e^\rho$. Recalling that $\rho = 2br$, equation (214) gives the behavior of $R(r)$ for large r as $R(r) \sim r^l e^{-br} e^{2br}$, which clearly blows up for large r. We cannot allow this to happen, and we can prevent it by arranging for the series expansion of $H(\rho)$ to terminate at some value $j_{\max}$ such that the numerator of the recursion relationship, equation (228), goes to zero:

$$j_{\max} - \lambda + l + 1 = 0 \tag{229}$$

Because j and l are integers, equation (229) can be satisfied only if λ is also an integer. Let's call this integer n:

$$j_{\max} = n - l - 1) \tag{230}$$

Using our previous definition of $\lambda = \mu k/\hbar^2 b$ with $\lambda = n$, we have

$$n = \frac{\mu k}{\hbar^2 b} = \frac{\mu (Ze^2/4\pi\varepsilon_0)}{\hbar^2 \sqrt{2\mu \left|E\right| /\hbar^2}} \tag{231}$$

or

$$E_n = -\frac{Z^2 e^4 \mu}{32\pi^2 \varepsilon_0^2 \hbar^2} \frac{1}{n^2} \tag{232}$$

This is the quantization condition on the energy levels of the hydrogenic atom, which agrees with the semi-classical condition of the Bohr model. Note that E depends only on n and not on l (even though $R(r)$ depends on both n and l). For $Z = 1$ and $\mu = m_e$ (the electron mass), the numerical factors in equation (232) evaluate to 13.6 eV.

Practice Question: What property did we impose on the radial wave functions that ultimately resulted in energy quantization?

It is also convenient at this point to define the quantity

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} \tag{233}$$

a_0 has the dimension of length and provides a convenient length scale for atomic systems. When $\mu = m_e$, a_0 is known as the *Bohr radius* and has the value 0.0529 nm = 52.9 pm. In terms of a_0, the parameter b can be written

$$b = \sqrt{\frac{2m\,|E|}{\hbar^2}} = \frac{\mu Z e^2}{4\pi\varepsilon_0\hbar^2 n} = \frac{Z}{a_0 n} \tag{234}$$

Before we discuss the general results for $H(\rho)$, let's look at the form of some of the solutions for particular values of n.

n=1:

In this case, equation (230) gives $j_{\max} = -l$, and since neither j nor l can be negative, the only possible solution is $j = l = 0$. In this case, $H(\rho) = c_0$ and $R(r)$ becomes

$$R_{10}(r) = c_0 e^{-Zr/a_0} \tag{235}$$

We have labeled the radial wave functions as $R_n l$ using the indices n and l. The constant c_0 can be determined from the normalization condition.

n=2:

In this case, $j_{\max} = 1 - l$. The possible l values are $l = 0$ (in which case $j_{\max} = 1$) and $l = 1$ (in which case $j_{\max} = 0$). For $l = 1$, only $j = 0$ contributes and $H(\rho) = c_0$. We then have

$$R_{21}(r) = c_0 r e^{-Zr/2a_0} \tag{236}$$

For $l = 0$, $j_{\max} = 1$ and thus $H(\rho) = c_0 + c_1$. We can use the recursion formula, equation (228), to determine c_1 in terms of c_0:

$$c_1 = \frac{0 - 2 + 0 + 1}{(1)(0 + 0 + 2)} c_0 = -\tfrac{1}{2} c_0 \tag{237}$$

so that $H(\rho) = c_0 \frac{1}{2} c_0 \rho = c_0(1 - \frac{1}{2}\rho)$ or $H(r) = c_0(1 - Zr/2a_0)$. We thus have

$$R_{20}(r) = c_0 e^{-Zr/2a_0}(1 - Zr/2a_0) \tag{238}$$

Practice problems:

Continue this process for $n = 3$ and show

$$R_{30}(r) = c_0 \left[1 - \frac{2Zr}{3a_0} + \frac{2}{27}\left(\frac{Zr}{a_0}\right)^2\right] e^{-Zr/3a_0} \tag{239}$$

$$R_{31}(r) = c_0 r \left(1 - \frac{Zr}{6a_0}\right) e^{-Zr/3a_0} \tag{240}$$

$$R_{32}(r) = c_0 r^2 e^{-Zr/3a_0} \tag{241}$$

31 THE COMPLETE RADIAL SOLUTION

The general solution of equation (219) is the *associated Laguerre polynomial*. First let's look at the *ordinary* Laguerre polynomials of degree q, which are obtained from the generating function

$$L_q(\rho) = e^{\rho} \frac{d^q}{d\rho^q}\left(\rho^q e^{-\rho}\right) \tag{242}$$

The *associated* Laguerre polynomials are then defined as

$$L_q^p(\rho) = \frac{d^p}{d\rho^p} L_q(\rho) \tag{243}$$

which is a polynomial of degree $q - p$. The general solution of equation (219) is the associated Laguerre polynomial:

$$H(\rho) = L_{n+l}^{2l+1}(\rho) \tag{244}$$

a polynomial of degree $(n+l)-(2l+1) = n-l-1$, as expected corresponding to the value of $j_{\max}$ given by equation (230).

The complete solution for $R(r)$ is then

$$R_{nl}(r) = N_{nl} r^l e^{-Zr/na_0} L_{n+l}^{2l+1}(2Zr/na_0) \tag{245}$$

where $N_{\rm nl}$ is a normalization constant. Because the $Y_l^m(\theta,\phi)$ are separately normalized, the normalization of $\psi(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$ then requires that the $R_{\rm nl}(r)$ be normalized:

$$\int_0^\infty r^2\,dr\,[R_{nl}(r)]^2 = 1 \tag{246}$$

Following a tedious but straightforward calculation,

$$N_{nl} = \left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2} \left(\frac{2Z}{na_0}\right)^l \tag{247}$$

so that the complete solution for $R(r)$ is then

$$R_{nl}(r) = \left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2} e^{-Zr/na_0} \left(\frac{2Zr}{na_0}\right)^l L_{n+l}^{2l+1}(2Zr/na_0) \tag{248}$$

The solution to the Schrödinger equation for the hydrogenic atom is

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi) \tag{249}$$

The solution to the time-dependent equation is

$$\Psi_{nlm}(r,\theta,\phi,t) = R_{nl}(r)Y_l^m(\theta,\phi)e^{-iE_nt/\hbar} \tag{250}$$

where E_n are the energy eigenvalues given in equation (232).

As is always the case for quantum systems, it is possible for the atom to exist in mixed states that are not pure eigenstates. These states can be described by appropriate linear combinations of the eigenfunctions given in equation (250):

$$\Psi(r,\theta,\phi,t) = \sum_{n,l,m} c_{nlm}R_{nl}(r)Y_l^m(\theta,\phi)e^{-iE_nt/\hbar} \tag{251}$$

Given any arbitrary (but mathematically well-behaved) function $f(r,\theta,\phi)$ that represents the state of the atom at $t = 0$, we can expand $f(r,\theta,\phi)$ in terms of the eigenfunctions:

$$f(r,\theta,\phi) = \sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} c_{nlm}R_{nl}(r)Y_l^m(\theta,\phi) \tag{252}$$

where

$$c_{nlm} = \int_0^\infty r^2\,dr \int_0^\pi \sin\theta\,d\theta \int_0^{2\pi} d\phi\, R_{nl}^*(r)Y_l^{m*}(\theta,\phi) \tag{253}$$

32 Appendix A: CHAIN RULE

Please see Riley, Hobsen, & Bence, 2nd edition, section 5.5-5.6 (The Chain Rule and Change of Variables), especially the worked example on plane polar coordinates.

33 Appendix B: SEPARATION OF VARIABLES

"Separation of variables" is a procedure that can turn a partial differential equation (i.e. a differential equation in several variables) into a system of ordinary differential equations (i.e. a set of differential equations, each in only a single variable). The procedure only works in very special cases involving a high degree of symmetry. Remarkably, the procedure works for many important physics examples. Here, we will use the procedure on the wave equation, as a simple example that illustrates the basic steps.

Step 1: Write the partial differential equation in an appropriate coordinate system. For the wave equation in one-dimension, we have:

$$\frac{\partial^2}{\partial x^2}\Psi(x,t) = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\Psi(x,t) \tag{254}$$

Step 2: Assume that the solution $\Psi(x,t)$ can be written as the product of functions, at least one of which depends on only one variable, in this case t; the other function(s) must not depend at all on this variable, i.e. assume

$$\Psi(x,t) = X(x)T(t) \tag{255}$$

This is a very strong assumption. Not all solutions will be of this form. However, it turns out that all of the solutions can be written as linear combinations of solutions of this form. The study of when and why this works is called Sturm-Liouville theory.

Plug this assumed solution (255) into the partial differential equation (254). Because of the special form for Ψ, the partial derivatives each act on only one of the factors in $\Psi = X(x)T(t)$.

$$\frac{d^2X(x)}{dx^2}\,T(t) = \frac{1}{v^2}X(x)\,\frac{d^2T(t)}{dt^2} \tag{256}$$

Notice that the partial derivatives $\frac{\partial^2}{\partial x^2}$ and $\frac{\partial^2}{\partial t^2}$ have turned into total derivatives $\frac{d^2}{dx^2}$ and $\frac{d^2}{dt^2}$. Any partial derivatives that act only on a function of a single variable may be rewritten as total derivatives.

Step 3: Divide by Ψ in the form of (255). The rest of the procedure doesn't work if you omit this step. Many, many students forget. Don't be one of them!

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \frac{1}{v^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} \tag{257}$$

Step 4: Isolate **all** of the dependence of one coordinate on one side of the equation. Do as much algebra as you need to do to achieve this. In our example, notice that in (257), all of the t dependence is on the right-hand side of the equation while all of the dependence on the spatial variable x is on the other side. In this case, the t dependence is already isolated, without any algebra on our part.

Step 5: Now imagine changing the isolated variable t by a small amount. In principle, the right-hand side of (257) could change, but nothing on the left-hand side would. (This argument is the magic of the separation of variables procedure–make sure that the logic is clear to you.) Therefore, if the equation is to be true for all values of t, the particular combination of t dependence on the right-hand side must be constant.

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \frac{1}{v^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} \stackrel{\text{def}}{=} A \tag{258}$$

In this way we have broken our original partial differential equation up into a pair of equations, one of which is an ordinary differential equation involving only x, the other is an ordinary differential equation involving only t.

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} \stackrel{\text{def}}{=} F \tag{259}$$

$$\frac{1}{v^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} \stackrel{\text{def}}{=} F \tag{260}$$

The separation constant F appears in both equations.

Step 6: Write each equation in standard form by multiplying each equation by its unknown function to clear it from the denominator.

$$\frac{d^2X(x)}{dx^2} \stackrel{\text{def}}{=} F\,X(x) \tag{261}$$

$$\frac{d^2T(t)}{dt^2} \stackrel{\text{def}}{=} F\,T(t) \tag{262}$$

Notice that (261) is an eigenvalue equation for the operator $\frac{d^2}{dx^2}$. At the moment, all we have done is mathematics and the eigenvalue F could be anything. Next we need to solve the system of ordinary differential equations and use physical information to find the possible values of F. In general the solution to the X equation will be

$$X(x) = A\cos(-\sqrt{F}x) + B\sin(-\sqrt{F}x) = A\cos kx + B\sin kx$$

where k is a conventional name for the constant $-\sqrt{F}$ and the allowed values of k are determined by the boundary conditions. We can then plug this value of F into the equation for T. Since we now know the value of F, the equation for T is **not** an eigenvalue equation. The solutions for T are, of course

$$T(t) = C\cos(-\sqrt{F}vt) + D\sin(-\sqrt{F}vt) = C\cos kvt + D\sin kvt$$

If the original partial differential equation had had more than two variables, we could have repeated the steps until each of the variables had been separated out into its own ordinary differential equation.