22.101 Applied Nuclear Physics (Fall 2006)
Lecture 4 (9/18/06)

Bound States in Three Dimensions – Orbital Angular Momentum

References --
R. L. Liboff, *Introductory Quantum Mechanics* (Holden Day, New York, 1980).
L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1955).
P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).

We will now extend the bound-state calculation to three-dimensional systems. The problem we want to solve is essentially the same as before, except that we wish to determine the bound-state energy levels and corresponding wave functions for a particle in a three-dimensional *spherical* well potential. Although this is a three-dimensional potential, we can take advantage of its symmetry in angular space and reduce the calculation to an equation still involving only one variable, the radial distance between the particle position and the origin. In other words, the spherical potential is still a function of one variable,

$$\begin{aligned} V(r) &= -V_o \qquad r < r_o \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{4.1}$$

Here r is the radial position of the particle relative to the origin. Any potential that is a function only of r, the magnitude of the position $\underline{r}$ and not the position vector itself, is called a central-force potential. As we will see, this form of the potential makes the solution of the Schrödinger wave equation particularly simple. For a system where the potential or interaction energy has no angular dependence, one can reformulate the problem by factorizing the wave function into a component that involves only the radial coordinate and another component that involves only the angular coordinates. The wave equation is then reduced to a system of uncoupled one-dimensional equations, each describing a radial component of the wave function. As to the justification for using a

central-force potential for our discussion, this will depend on which properties of the nucleus we wish to study.

We again begin with the time-independent wave equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\underline{r}) = E\psi(\underline{r}) \tag{4.2}$$

Since the potential function has spherical symmetry, it is natural for us to carry out the analysis in the spherical coordinate system rather than the Cartesian system. A position vector $\underline{r}$ then is specified by the radial coordinate r and two angular coordinates, θ and φ, the polar and azimuthal angles respectively, see Fig. 1. In this coordinate system

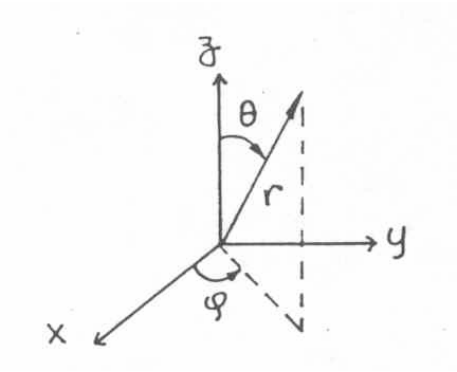

Fig. 1. The spherical coordinate system. A point in space is located by the radial coordinate r, and polar and azimuthal angles θ and φ.

the Laplacian operator ∇^2 is of the form

$$\nabla^2 = D_r^2 + \frac{1}{r^2}\left[\frac{-L^2}{\hbar^2}\right] \tag{4.3}$$

where D_r^2 is an operator involving only the radial coordinate,

$$D_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\right] \tag{4.4}$$

and the operator L^2 involves only the angular coordinates,

$$-\frac{L^2}{\hbar^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{4.5}$$

In terms of these operators the wave equation (4.2) becomes

$$\left[-\frac{\hbar^2}{2m}D_r^2 + \frac{L^2}{2mr^2} + V(r)\right]\psi(r\theta\varphi) = E\psi(r\theta\varphi) \tag{4.6}$$

For any potential V(r) the angular variation of ψ is always determined by the operator $L^2/2mr^2$. Therefore one can study the operator L^2 separately and then use its properties to simplify the solution of (4.6). This needs to be done only once, since the angular variation is independent of whatever form one takes for V(r). It turns out that L^2 is very well known (it is the square of L which is the angular momentum operator); it is the operator that describes the angular motion of a free particle in three-dimensional space.

We first summarize the basic properties of L^2 before discussing any physical interpretation. It can be shown that the eigenfunction of L^2 are the spherical harmonics functions, $Y_\ell^m(\theta,\varphi)$,

$$L^2Y_\ell^m(\theta,\varphi) = \hbar^2\ell(\ell+1)Y_\ell^m(\theta,\varphi) \tag{4.7}$$

where

$$Y_\ell^m(\theta,\varphi) = \left[\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}\right]^{1/2} P_\ell^m(\cos\theta)e^{im\varphi} \tag{4.8}$$

and

$$P_\ell^m(\mu) = \frac{(1-\mu^2)^{m/2}}{2^\ell\ell!}\frac{d^{\ell+m}}{d\mu^{\ell+m}}(\mu^2-1)^\ell \tag{4.9}$$

with $\mu = \cos\theta$. The function $P_\ell^m(\mu)$ is called the associated Legendre polynomials, which are in turn expressible in terms of Legendre polynomials $P_\ell(\mu)$,

$$P_\ell^m(\mu) = (1-\mu)^{|m|/2} \frac{d^{|m|}}{d\mu^{|m|}} P_\ell(\mu) \tag{4.10}$$

with $P_o(x) = 1$, $P_1(x) = x$, $P_2(x) = (3x^2 - 1)/2$, $P_3(x) = (5x^3-3x)/2$, etc. Special functions like Y_ℓ^m and P_ℓ^m are quite extensively discussed in standard texts [see, for example, Schiff, p.70] and reference books on mathematical functions [More and Feshbach, p. 1264]. For our purposes it is sufficient to regard them as well known and tabulated quantities like sines and cosines, and whenever the need arises we will invoke their special properties as given in the mathematical handbooks.

It is clear from (4.7) that $Y_\ell^m(\theta,\varphi)$ is an eigenfunction of L^2 with corresponding eigenvalue $\ell(\ell+1)\hbar^2$. Since the angular momentum of the particle, like its energy, is quantized, the index ℓ can take on only positive integral values or zero,

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

Similarly, the index m can have integral values from $-\ell$ to ℓ,

$$m = -\ell, -\ell+1, \ldots, -1, 0, 1, \ldots, \ell-1, \ell$$

For a given ℓ, there can be $2\ell+1$ values of m. The significance of m can be seen from the property of L_z, the projection of the orbital angular momentum vector $\underline{L}$ along a certain direction in space (in the absence of any external field, this choice is up to the observer). Following convention we will choose this direction to be along the z-axis of our coordinate system, in which case the operator L_z has the representation, $L_z = -i\hbar\partial/\partial\varphi$, and its eignefunctions are also $Y_\ell^m(\theta,\varphi)$, with eigenvalues $m\hbar$. The indices ℓ and m are called quantum numbers. Since the angular space is two-dimensional

(corresponding to two degrees of freedom), it is to be expected that two quantum numbers will emerge from our analysis. By the same token we should expect three quantum numbers in our description of three-dimensional systems. We should regard the particle as existing in various states which are specified by a unique set of quantum numbers, each one is associated with a certain orbital angular momentum which has a definite magnitude and orientation with respect to our chosen direction along the z-axis. The particular angular momentum state is described by the function $Y_\ell^m(\theta,\varphi)$ with ℓ known as the *orbital angular momentum quantum number*, and m the *magnetic quantum number*. It is useful to keep in mind that $Y_\ell^m(\theta,\varphi)$ is actually a rather simple function for low order indices. For example, the first four spherical harmonics are:

$$Y_0^0 = 1/\sqrt{4\pi}\,, \quad Y_1^{-1} = \sqrt{3/8\pi}e^{-i\varphi}\sin\theta\,, \quad Y_1^0 = \sqrt{3/4\pi}\cos\theta\,, \quad Y_1^1 = \sqrt{3/8\pi}e^{i\varphi}\sin\theta$$

Two other properties of the spherical harmonics are worth mentioning. First is that $\{Y_\ell^m(\theta,\varphi)\}$, with ℓ = 0, 1, 2, … and $-\ell \le m \le \ell$, is a *complete set* of functions in the space of $0 \le \theta \le \pi$ and $0 \le \varphi \le 2\pi$ in the sense that any arbitrary function of θ and φ can be represented by an expansion in these functions. Another property is orthonormality,

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi Y_\ell^{m*}(\theta,\varphi) Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'} \tag{4.11}$$

where $\delta_{\ell\ell'}$ denotes the Kronecker delta function; it is unity when the two subscripts are equal, otherwise the function is zero.

Returning to the wave equation (4.6) we look for a solution as an expansion of the wave function in spherical harmonics series,

$$\psi(r\theta\varphi) = \sum_{\ell,m} R_\ell(r) Y_\ell^m(\theta,\varphi) \tag{4.12}$$

Because of (4.7) the L^2 operator in (4.6) can be replaced by the factor $\ell(\ell+1)\hbar^2$. In view of (4.11) we can eliminate the angular part of the problem by multiplying the wave equation by the complex conjugate of a spherical harmonic and integrating over all solid angles (recall an element of solid angle is $\sin\theta d\theta d\varphi$), obtaining

$$\left[-\frac{\hbar^2}{2m}D_r^2+\frac{\ell(\ell+1)\hbar^2}{2mr^2}+V(r)\right]R_\ell(r)=ER_\ell(r) \tag{4.13}$$

This is an equation in one variable, the radial coordinate r, although we are treating a three-dimensional problem. We can make this equation look like a one-dimensional problem by transforming the dependent variable R_ℓ. Define the radial function

$$u_\ell(r)=rR_\ell(r) \tag{4.14}$$

Inserting this into (4.13) we get

$$-\frac{\hbar^2}{2m}\frac{d^2u_\ell(r)}{dr^2}+\left[\frac{\ell(\ell+1)\hbar^2}{2mr^2}+V(r)\right]u_\ell(r)=Eu_\ell(r) \tag{4.15}$$

We will call (4.15) *the radial wave equation*. It is the basic starting point of three-dimensional problems involving a particle interacting with a central potential field.

We observe that (4.15) is actually a system of uncoupled equations, one for each fixed value of the orbital angular momentum quantum number ℓ. With reference to the wave equation in one dimension, the extra term involving $\ell(\ell+1)$ in (4.15) represents the contribution to the potential field due to the centrifugal motion of the particle. The $1/r^2$ dependence makes the effect particularly important near the origin; in other words, centrigfugal motion gives rise to a barrier which tends to keep the particle away from the origin. This effect is of course absent in the case of ℓ = 0, a state of zero orbital angular momentum, as one would expect. The first few ℓ states usually are the only ones of interest in our discussion (because they tend to have the lowest energies); they are given special spectroscopic designations,

notation: **s, p, d, f, g, h**, …

ℓ = **0, 1, 2, 3, 4, 5**, …

where the first four letters stand for ‘sharp’, ‘principal’, ‘diffuse’, and ‘fundamental’ respectively. After f the letters are assigned in alphabetical order, as in h, i, j, … The wave function describing the state of orbital angular momentum ℓ is often called the ℓ th partial wave,

$$\psi_\ell(r\theta\varphi) = R_\ell(r)Y_\ell^m(\theta\varphi) \tag{4.16}$$

Notice that in the case of s-wave the wave function is spherically symmetric since Y_0^0 is independent of θ and φ.

Interpretation of Orbital Angular Momentum

In classical mechanics, the angular momentum of a particle in motion is defined as the vector product, $\underline{L} = \underline{r} \times \underline{p}$, where r is the particle position and p its linear momentum. L is directed along the axis of rotation (right-hand rule), as shown in Fig. 2.

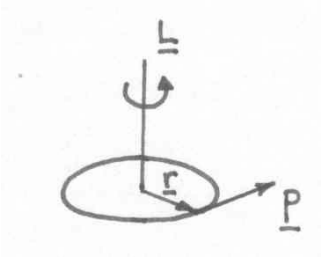

Fig. 2. Angular momentum of a particle at position r moving with linear momentum p (classical definition).

L is called an axial or pseudovector in contrast to r and p, which are polar vectors. Under inversion, $\underline{r} \to -\underline{r}$, and $\underline{p} \to -\underline{p}$, but $\underline{L} \to \underline{L}$. Quantum mechanically, L^2 is an operator with eigenvalues and eigenfunctions given in (4.7). Thus the magnitude of L is $\hbar\sqrt{\ell(\ell+1)}$, with ℓ = 0, 1, 2, …being the orbital angular momentum quantum number. We can specify the magnitude and one Cartesian component (usually called the z-

component) of L by specifying ℓ and m, an example is shown in Fig. 3. What about the x- and y-components? They are undetermined, in that they cannot be observed

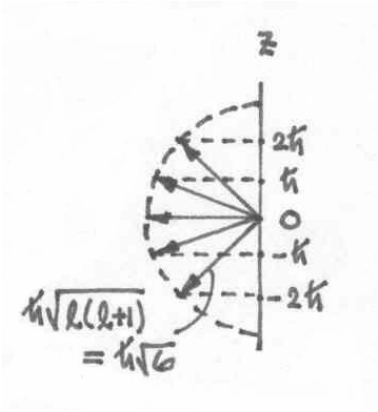

Fig. 3. The $\ell(\ell+1) = 5$ projections along the z-axis of an orbital angular momentum with $\ell = 2$. Magnitude of L is $\sqrt{6}\hbar$.

simultaneously with the observation of L^2 and L_z. Another useful interpretation is to look at the energy conservation equation in terms of radial and tangential motions. By this we mean that the total energy can be written as

$$E = \frac{1}{2}m(v_r^2 + v_t^2) + V = \frac{1}{2}mv_r^2 + \frac{L^2}{2mr^2} + V \qquad (4.17)$$

where the decomposition into radial and tangential velocities is depicted in Fig. 4. Eq.(4.17) can be compared with the radial wave equation (4.15).

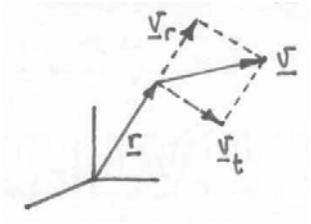

Fig. 4. Decomposing the velocity vector of a particle at position r into radial and tangential components.

Thus far we have confined our discussions of the wave equation to its solution in spherical coordinates. There are situations where it will be more appropriate to work in another coordinate system. As a simple example of a bound-state problem, we can consider the system of a free particle contained in a cubical box of dimension L along each side. In this case it is clearly more convenient to write the wave equation in Cartesian coordinates,

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi(xyz)=E\psi(xyz) \tag{4.17}$$

$0 < x, y, z < L$. The boundary conditions are $\psi = 0$ whenever x, y, or z is 0 or L. Since both the equation and the boundary conditions are separable in the three coordinates, the solution is of the product form,

$$\psi(xyz)=\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

$$=(2/L)^{3/2}\sin(n_x\pi x/L)\sin(n_y\pi y/L)\sin(n_z\pi z/L) \tag{4.18}$$

where n_x, n_y, n_z are positive integers (excluding zero), and the energy becomes a sum of three contributions,

$$E_{n_xn_yn_z}=E_{n_x}+E_{n_y}+E_{n_z}$$

$$=\frac{(\hbar\pi)^2}{2mL^2}\left[n_x^2+n_y^2+n_z^2\right] \tag{4.19}$$

We see that the wave functions and corresponding energy levels are specified by the set of three quantum numbers (n_x, n_x, n_z). While each state of the system is described by a unique set of quantum numbers, there can be more than one state at a particular energy level. Whenever this happens, the level is said to be *degenerate*. For example, (112),

(121), and (211) are three different states, but they are all at the same energy, so the level at $6(\hbar\pi)^2/2mL^2$ is triply degenerate. The concept of degeneracy is useful in our later discussion of the nuclear shell model where one has to determine how many nucleons can be put into a certain energy level. In Fig. 6 we show the energy level diagram for a particle in a cubical box. Another way to display the information is through a table, such as Table I.

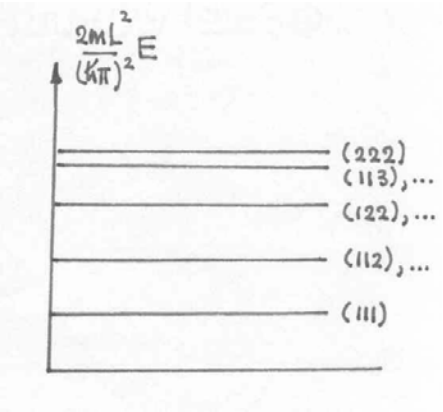

Fig. 6. Bound states of a particle in a cubical box of width L.

Table I. The first few energy levels of a particle in a cubical box which correspond to Fig. 6.

n_x n_y n_z	$\frac{2mL^2}{(\hbar\pi)^2}E$	degeneracy
1 1 1	3	1
1 1 2	6	3
1 2 1		
2 1 1		
1 2 2, …	9	3
1 1 3, …	11	3
2 2 2	12	1

The energy unit is seen to be $\Delta E = (\hbar\pi)^2 / 2mL^2$. We can use this expression to estimate the magnitude of the energy levels for electrons in an atom, for which m = 9.1 x10^{-28} gm and L ~ 3 x 10^{-8}cm, and for nucleons in a nucleus, for which m = 1.6x10^{-24} gm and L ~ 5F. The energies come out to be ~30 ev and 6 Mev respectively, values which are typical in atomic and nuclear physics. Notice that if an electron were in a nucleus, then it would have energies of the order 10^{10} ev !

In closing this section we note that Bohr had put forth the "correspondence principle" which states that quantum mechanical results will approach the classical results when the quantum numbers are large. Thus we have

$$\left|\psi_n\right|^2 = \frac{2}{L}\sin^2(n\pi x / L) \to \frac{1}{L} \qquad (4.20)$$

$$n \to \infty$$

What this means is that the probability of finding a particle anywhere in the box is 1/L, i.e., one has a uniform distribution, see Fig. 7.

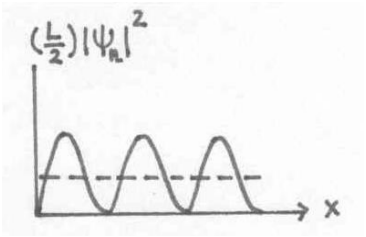

Fig. 7. The behavior of $\sin^2 nx$ in the limit of large n.

Parity

Parity is a symmetry property of the wave function associated with the inversion operation. This operation is one where the position vector $\underline{r}$ is reflected through the origin (see Fig. 1), so $\underline{r} \to -\underline{r}$. For physical systems which are not subjected to an external vector field, we expect these systems will remain the same under an inversion

operation, or the Hamiltonian is invariant under inversion. If $\psi(\underline{r})$ is a solution to the wave equation, then applying the inversion operation we get

$$H\psi(-\underline{r}) = E\psi(-\underline{r}) \tag{4.21}$$

which shows that $\psi(-\underline{r})$ is also a solution. A general solution is therefore obtained by adding or subtracting the two solutions,

$$H\left[\psi(\underline{r}) \pm \psi(-\underline{r})\right] = E\left[\psi(\underline{r}) \pm \psi(-\underline{r})\right] \tag{4.22}$$

Since the function $\psi_+(\underline{r}) = \psi(\underline{r}) + \psi(-\underline{r})$ is manifestly invariant under inversion, it is said to have positive parity, or its parity, denoted by the symbol π, is +1. Similarly, $\psi_-(\underline{r}) = \psi(\underline{r}) - \psi(-\underline{r})$ changes sign under inversion, so it has negative parity, or π = -1. The significance of (4.22) is that a physical solution of our quantum mechanical description should have definite parity; this is the condition we have previously imposed on our solutions in solving the wave equation (see Lec3). Notice that there are functions which do not have definite parity, for example, Asinkx + Bcoskx. This is the reason that we take either the sine function or the cosine function for the interior solution in Lec3. In general, one can accept a solution as a linear combination of individual solutions all having the same parity. A linear combination of solutions with different parities has no definite parity, and is therefore unacceptable.

In spherical coordinates, the inversion operation of changing $\underline{r}$ to $-\underline{r}$ is equivalent to changing the polar angle θ to $\pi - \theta$, and the azimuthal angle φ to $\varphi + \pi$. The effect of the transformation on the spherical harmonic function $Y_\ell^m(\theta,\varphi) \sim e^{im\varphi}P_\ell^m(\theta)$ is

$$e^{im\varphi} \rightarrow e^{im\varphi}e^{im\pi} = (-1)^m e^{im\varphi}$$

$$P_\ell^m(\theta) \rightarrow (-1)^{\ell-m} P_\ell^m(\theta)$$

so the parity of $Y_\ell^m(\theta,\varphi)$ is $(-1)^\ell$. In other words, the parity of a state with a definite orbital angular momentum is even if ℓ is even, and odd if ℓ is odd. All eigenfunctions of the Hamiltonian with a spherically symmetric potential are therefore either even or odd in parity.