CHAPTER SIX: Generalization to Three Dimensions

First step: generalize some obvious results to 3-D. Starting point: "grab bag" of results.

$$\vec{x}|\vec{x}'> = \vec{x}'|\vec{x}'>, \qquad \vec{p}|\vec{p}'> = \vec{p}'|\vec{p}'>. \tag{1}$$

The <u>Cartesian</u> bases (we will also encounter a <u>spherical</u> basis) $|\vec{x}'>$ and $|\vec{p}'>$ are <u>direct products</u> of the basis states in the three orthogonal directions: (One sometimes writes $|\vec{x}'> = |x_1'> \otimes |x_2'> \otimes |x_3'>$.)

$$\left.\begin{aligned} |\vec{x}'> &= |x_1'>|x_2'>|x_3'>, & |\vec{p}'> &= |p_1'>|p_2'>|p_3'> \\ &\equiv |x_1', x_2', x_3'> & &\equiv |p_1', p_2', p_3'> \end{aligned}\right\} \tag{2}$$

(I will try to consistently label the three orthogonal space directions as 1, 2 and 3 rather than as x, y and z from now on.) We also have (see (158) of Ch. 2)

$$<\vec{x}'|\vec{p}'> = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\vec{x}'\cdot\vec{p}'/\hbar}, \tag{3}$$

$$<\vec{x}'|\vec{x}''> = \delta^3(\vec{x}' - \vec{x}''), \quad <\vec{p}'|\vec{p}''> = \delta^3(\vec{p}' - \vec{p}''), \tag{4}$$

where

$$\left.\begin{aligned} \delta^3(\vec{x}' - \vec{x}'') &= \delta(x_1' - x_1'')\delta(x_2' - x_2'')\delta(x_3' - x_3''), \\ \delta^3(\vec{p}' - \vec{p}'') &= \delta(p_1' - p_1'')\delta(p_2' - p_2'')\delta(p_3' - p_3''). \end{aligned}\right\} \tag{5}$$

Also

$$1 = \int d^3x'|\vec{x}'><\vec{x}'|, \quad 1 = \int d^3p'|\vec{p}'><\vec{p}'|, \tag{6}$$

with

$$d^3x' = dx_1'dx_2'dx_3', \quad d^3p' = dp_1'dp_2'dp_3'. \qquad (7)$$

The formal energy eignevalue problem is still stated as

$$H|a'\rangle = E_{a'}|a'\rangle, \qquad (8)$$

where the $|a'\rangle$ are a complete, orthogonal set of states:

$$\sum_{a'} |a'\rangle\langle a'| = 1, \quad \langle a'|a''\rangle = \delta_{a'a''} . \qquad (9)$$

(Eq$^{\underline{n}}$ (9) assumes the energy eigenvalues are discrete and nondegenerate. What would the analogous equations in the more general situation look like?) Wavefunctions are given by the projections (see (174) of Ch. 2)

$$u_{a'}(\vec{x}') = \langle\vec{x}'|a'\rangle, \qquad (10)$$

which satisfy (using (6))

$$\int d^3x\; u^*_{a'}(\vec{x})u_{a'}(\vec{x}) = 1. \qquad (11)$$

Eq$^{\underline{n}}$ (11) tells us the engineering dimensions of the $u_{a'}(\vec{x})$ are

$$[u_{a'}(\vec{x})] \sim [\text{length}]^{-3/2} . \qquad (12)$$

For continuous spectra, we usually use a momentum rather than an energy basis to completely specify the state of the particle. Then defining*

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* Many books use $u_{\vec{k}}(\vec{x}) \equiv \hbar^{3/2}\, u_{\vec{p}}(\vec{x})$ as the momentum eigenfunction, in which case it is dimensionless.

$$u_{\vec{p}}(\vec{x}) = \langle \vec{x}' | \vec{p} \rangle , \tag{13}$$

we have (again from (6))

$$\int d^3x \; u^*_{\vec{p}}(\vec{x}) u_{\vec{p}'}(\vec{x}) = \delta^3(\vec{p} - \vec{p}') . \tag{14}$$

We will limit ourselves to consideration of Hamiltonians of the form

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}) . \tag{15}$$

The form of the potential, $V(\vec{x})$, will determine the nature of the spatial basis to be used. For example, for $V(\vec{x}) = F(x_1) + F(x_2) + F(x_3)$ (as for the 3-D harmonic oscillator) we would use a Cartesian basis; for $V(\vec{x}) = V(r)$, where $r = |\vec{x}|$, one would use a spherical basis. We must use a basis in which the time independent Schrödinger equation separates; for example $u_{a'}(\vec{x}) = u_1(x_1)u_2(x_2)u_3(x_3)$ in Cartesian coordinates or $u_{a'}(\vec{x}) = u_1(r)u_2(\theta)u_3(\phi)$ in spherical coordinates. The time independent Schrödinger equation is, of course, just Eq$\underline{^{n}}$ (8) projected into an explicit basis.

We will continue to assume that

$$[x_i, p_i] = i\hbar \tag{16}$$

for <u>each</u> i = 1,2,3, where x_i and p_i are <u>operators</u>. However, what about $[x_i, x_j]$ for $i \neq j$? In the Cartesian basis

$$[x_1, x_2] | \vec{x}' \rangle = (x_1 x_2 - x_2 x_1) | x_1', x_2', x_3' \rangle = 0 \tag{17}$$

Since (17) is true for any $|\vec{x}'>$,

$$\Rightarrow [x_1,x_2] = 0 \ . \qquad (18)$$

Similarly $[x_2,x_3] = [x_1,x_3] = 0$. Therefore

$$[x_i,x_j] = 0 \ . \qquad (19)$$

for all i,j. We learned before in Ch.4 that [A,B] is a measure of the "compatibility" of the operators A and B. Eq$^{\underline{n}}$ (19) above tells us that measurements of x_i do not limit the precision of measurements of x_j $(i \neq j)$ for a particle. Thus the x_i are simultaneously measurable for all states.

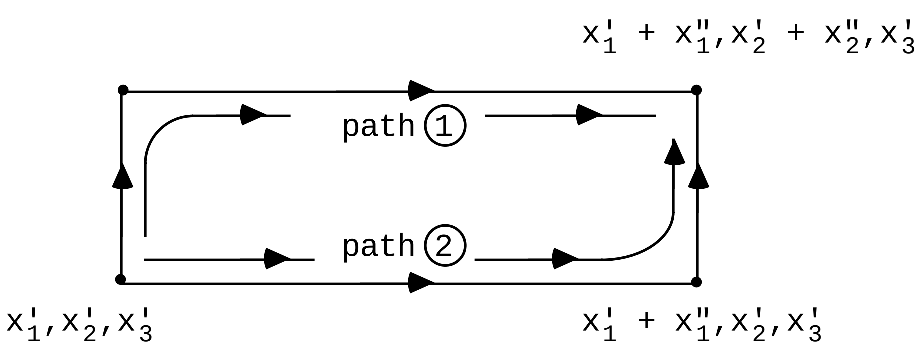
Let us generalize the unitary displacement operator we had before, also in Ch.4:

$$< x_1'|e^{ix_1''p_1/\hbar} = < x_1' + x_1''| \ . \qquad (20)$$

Now we have

$$< x_1',x_2',x_3'|e^{ix_1''p_1/\hbar} = < x_1' + x_1'',x_2',x_3'|, \qquad (21)$$

and similarly for displacements in the 2 and 3 directions. Now consider the following displacements:



We may get from (x_1', x_2', x_3') to $(x_1' + x_1'', x_2' + x_2'', x_3')$ along paths 1 or 2. Along path 1

$$< x_1', x_2', x_3' | e^{ix_2'' p_2/\hbar} \, e^{ix_1'' p_1/\hbar} = < x_1' + x_1'', x_2' + x_2'', x_3' | \; . \quad (22)$$

Along path 2:

$$< x_1', x_2', x_3' | e^{ix_1'' p_1/\hbar} \, e^{ix_2'' p_2/\hbar} = < x_1' + x_1'', x_2' + x_2'', x_3' | \; . \quad (23)$$

The equivalence of these two operators tells us that

$$[p_1, p_2] = 0. \quad (24)$$

This can obviously be done for the sets (p_2, p_3) and (p_1, p_3) also. The conclusion is

$$[p_i, p_j] = 0. \quad (25)$$

for all i,j. Thus the p_i are simultaneously measurable in all states. Notice that since (25) is true, we have

$$e^{ix_1' p_1/\hbar} \, e^{ix_2' p_2/\hbar} \, e^{ix_3' p_3/\hbar} = e^{i\vec{x}' \cdot \vec{p}/\hbar} \; , \quad (26)$$

so that a general displacement can be written as

$$< \vec{x}' | e^{i\vec{x}'' \cdot \vec{p}/\hbar} = < \vec{x}' + \vec{x}'' |. \quad (27)$$

What about mixed objects like $[x_1, p_2]$? Consider the infinitesimal change

$$< \vec{x}' | (1 + id\vec{x}'' \cdot \vec{p}/\hbar) = < \vec{x}' + d\vec{x}'' | \; . \quad (28)$$

Multiplying both sides by the operator $\vec{x}$, we have

$$\langle \vec{x}'|(1 + i d\vec{x}'' \cdot \vec{p}/\hbar)\vec{x} = \langle \vec{x}' + d\vec{x}''|(\vec{x}' + d\vec{x}''). \tag{29}$$

Now do these two operations in the opposite order:

$$\langle \vec{x}'|\vec{x}(1 + i d\vec{x}'' \cdot \vec{p}/\hbar) = \langle \vec{x}'|(1 + i d\vec{x}'' \cdot \vec{p}/\hbar)\vec{x}'$$
$$= \langle \vec{x}' + d\vec{x}''|\vec{x}'. \tag{30}$$

Therefore, we have that

$$\langle \vec{x}'|[(1 + i d\vec{x}'' \cdot \vec{p}/\hbar),\vec{x}] = \langle \vec{x}' + d\vec{x}''|d\vec{x}'', \tag{31}$$

$$\Rightarrow \langle \vec{x}'|\frac{i}{\hbar}[d\vec{x}'' \cdot \vec{p},\vec{x}] = \langle \vec{x}'|d\vec{x}'', \tag{32}$$

$$\Rightarrow \frac{i}{\hbar}[d\vec{x}'' \cdot \vec{p},\vec{x}] = d\vec{x}''. \tag{33}$$

This statement becomes more transparent in component language:

$$\frac{i}{\hbar}\sum_k dx''_k[p_k,x_j] = dx''_j, \tag{34}$$

$$\Rightarrow [p_k,x_j] = \frac{\hbar}{i}\delta_{kj}. \tag{35}$$

From the 1-D statement,

$$\langle x'|e^{ix''p_x/\hbar} = \langle x' + x''|, \tag{36}$$

I derived the result (Ch. 4, Eq$^{\underline{n}}$ (153))

$$\langle x'|p_x = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|. \tag{37}$$

Likewise in our 3-D Cartesian basis given Eq$^{\underline{n}}$ (27) above, it is easy to show that

$$<\vec{x}'|\vec{p} = \frac{\hbar}{i}\vec{\nabla}'<\vec{x}'|, \qquad (38)$$

where $\vec{\nabla}'$ is the usual gradient (differential) operator:

$$\vec{\nabla}' = \sum_i \hat{e}_i \frac{\partial}{\partial x_i'} . \qquad (39)$$

Likewise one can show that

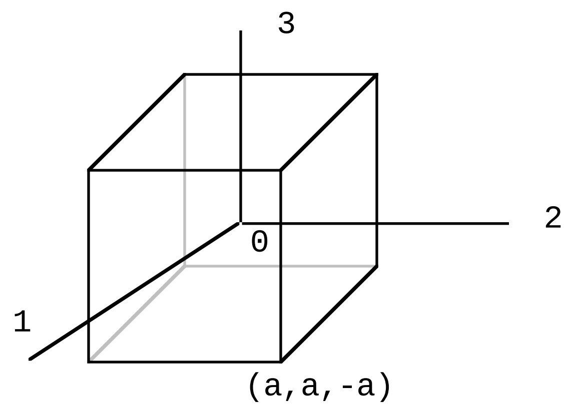
$$<\vec{p}'|\vec{x} = -\frac{\hbar}{i}\vec{\nabla}_p' <\vec{p}'|, \qquad (40)$$

where

$$\vec{\nabla}_p' = \sum_i \hat{e}_i \frac{\partial}{\partial p_i'} . \qquad (41)$$

Let us apply our Cartesian basis to a simple problem in 3-D. Consider the infinite 3-D square well:

(Origin at center)



$V = 0$ inside $\qquad -a \le x_1 \le a$

$V = +\infty$ outside $\qquad -a \le x_2 \le a$

$\qquad -a \le x_3 \le a$

The B.C. are

$$\left.\begin{aligned} u(\pm a, x_2, x_3) &= 0, \\ u(x_1, \pm a, x_3) &= 0, \\ u(x_1, x_2, \pm a) &= 0. \end{aligned}\right\} \qquad (42)$$

(In other words $u|_{surface} = 0$). Projected into the Cartesian basis, the energy eigenvalue condition $H|a'\rangle = E_{a'}|a'\rangle$ becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)u_{a'}(\vec{x}) = E_{a'}u_{a'}(\vec{x}). \tag{43}$$

This is obviously separable in x_1, x_2 and x_3. Let

$$u_{a'}(\vec{x}) = u_1(x_1)u_2(x_2)u_3(x_3). \tag{44}$$

Then (43) may be put into the form $\left(u_1'' \equiv \frac{\partial^2 u}{\partial x_1^2}\text{ , etc.}\right)$

$$\frac{u_1''}{u_1}+\frac{u_2''}{u_2}+\frac{u_3''}{u_3} = -\frac{2mE_{a'}}{\hbar^2}\text{ ,} \tag{45}$$

which means we may set

$$\left.\begin{aligned} -\frac{\hbar^2}{2m}u_1'' &= E_1u_1(x_1),\\ -\frac{\hbar^2}{2m}u_2'' &= E_2u_2(x_2),\\ -\frac{\hbar^2}{2m}u_3'' &= E_3u_3(x_3),\end{aligned}\right\} \tag{46}$$

where

$$E_1+E_2+E_3 = E_{a'}. \tag{47}$$

Eq$\underline{\text{n}}$s (46) and the B.C. (42) insure that the solution in each direction is identical to the one-dimensional case solved in Ch. 3. Let me remind you of these solutions:

$$u_{n-}(x) = \langle x|n-\rangle = \frac{1}{\sqrt{a}}\sin(k_{n-}x), \tag{48}$$

$$u_{n+}(x) = \langle x|n+\rangle = \frac{1}{\sqrt{a}}\cos(k_{n+}x), \tag{49}$$

where

$$n = 1,2,3,\ldots \begin{cases} k_{n-} = \dfrac{n\pi}{a} & (50) \\ k_{n+} = \dfrac{(n - 1/2)\pi}{a} & (51) \end{cases}$$

and $E = \dfrac{\hbar^2 k^2}{2m}$. Thus in 3-D, the solutions are

$$u_{a'}(\vec{x}) \equiv <\vec{x}'|a'> = <x_1|E_1><x_2|E_2><x_3|E_3> = u_{n_1P_1}(x_1)u_{n_2P_2}(x_2)u_{n_3P_3}(x_3), \qquad (52)$$

where each of the $u_{n_iP_i}$ are given in (48) and (49) with $P_{1,2,3} = \pm$ giving the parities of the state. Eq$\underline{^n}$ (47) says that the total energy is given by the sum of the E_1, E_2 and E_3 eigenenergies. This means that there are energy degeneracies. For example, consider energy levels for which $P_1 = P_2 = P_3 = -$,

$$E_- = \frac{\pi^2\hbar^2}{2ma^2}(n_1^2 + n_2^2 + n_3^2). \qquad (53)$$

Although the lowest energy above is specified by $n_1 = n_2 = n_3 = 1$, the first excited state can be given as ($n_1 = 2$, $n_2 = 1$, $n_3 = 1$), ($n_1 = 1$, $n_2 = 2$, $n_3 = 1$) or ($n_1 = 1$, $n_2 = 1$, $n_3 = 2$).

Can you find a complete set of commuting operators that uniquely specify the independent states?

A much more useful coordinate basis in physics is a spherical basis in which the position of a particle is specified by the three numbers r, θ, φ:

$$<x_1',x_2',x_3'| \rightarrow <r,\theta,\phi|. \qquad (54)$$

Based on what we have seen before, we expect that

$$1 = \int d^3r\,|r,\theta,\phi\rangle\langle r,\theta,\phi|, \tag{55}$$

where

$$d^3r = r^2 \sin\theta \; dr d\theta d\phi. \tag{56}$$

The range of these variables is as usual

$$\left.\begin{array}{l} r:\ 0 \to \infty, \\ \theta:\ 0 \to \pi, \\ \phi:\ 0 \to 2\pi, \end{array}\right\} \tag{57}$$

which picks out all points in coordinate space.

Just as the 3-D Cartesian basis,

$$\langle x_1', x_2', x_3'| = \langle x_1'|\langle x_2'|\langle x_3'|, \tag{58}$$

is a direct product of three Hilbert spaces, we expect that the spherical basis,

$$\langle r,\theta,\phi| = \langle r|\langle\theta|\langle\phi|, \tag{59}$$

is also a direct product of separate Hilbert spaces. And just as we have completeness in each Cartesian subspace,

$$\left.\begin{array}{l} 1_{x_1} = \int_{-\infty}^{\infty} dx_1'\,|x_1'\rangle\langle x_1'|, \\ 1_{x_2} = \int dx_2'\,|x_2'\rangle\langle x_2'|, \\ 1_{x_3} = \int dx_3'\,|x_3'\rangle\langle x_3'|, \end{array}\right\} \tag{60}$$

we demand that

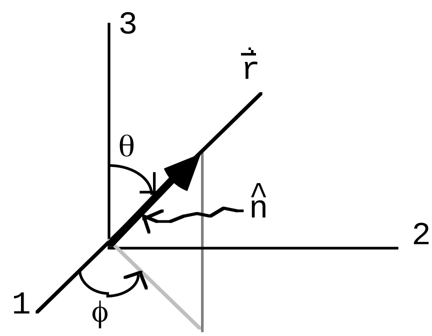
$$\left.\begin{aligned} 1_r &= \int_0^\infty dr r^2 |r><r|, \\ 1_\theta &= \int_0^\pi d\theta \sin\theta\, |\theta><\theta|, \\ 1_\phi &= \int_0^{2\pi} d\phi |\phi><\phi|, \end{aligned}\right\} \qquad (61)$$

so that

$$1 = 1_1 \cdot 1_\theta \cdot 1_\phi = \int d^3r |r,\theta,\phi><r,\theta,\phi| \ . \qquad (62)$$

We will label the angular position as

$$|\hat{n}> \equiv |\theta,\phi>. \qquad (63)$$



where $\hat{n}$ is a unit vector pointing in the $\vec{r}$ direction. Of course, there are many other bases possible, corresponding to cylindrical coordinates, elliptical coordinates, etc. It's clear that we have to be consistent in a given problem to stick with an initial choice, but other than this one is free to switch between various bases in order to simplify derivations and expressions. I will generally use $|\vec{x}>$ to denote a Cartesian basis and $|\vec{r}>$ to denote a spherical one.

Let us now introduce the quantum mechanical operator representing <u>orbital</u> angular momentum* :

$$\vec{L} \equiv \vec{x} \times \vec{p}. \tag{64}$$

Component-wise, we have

$$\left.\begin{aligned} L_1 &= x_2p_3 - x_3p_2, \\ L_2 &= x_3p_1 - x_1p_3, \\ L_3 &= x_1p_2 - x_2p_1. \end{aligned}\right\} \tag{65}$$

Notice that since $[x_i,p_j] = 0$ $(i \neq j)$, the order of the operators in (65) does not matter. Also notice that

$$\vec{L}^{+} = \vec{L}, \tag{66}$$

i.e., it is Hermitian and therefore has real eigenvalues.

The various L_i do not commute. To see this, consider

$$\begin{aligned} [L_1,L_2] &= [x_2p_3 - x_3p_2, x_3p_1 - x_1p_3] \\ &= [x_2p_3,x_3p_1] + [x_3p_2,x_1p_3] \\ &= x_2p_1[p_3,x_3] + p_2x_1[x_3,p_3] \\ &= i\hbar(x_1p_2 - x_2p_1) = i\hbar L_3. \end{aligned} \tag{67}$$

Likewise

$$[L_1,L_3] = -i\hbar L_2, \tag{68}$$

$$[L_2,L_3] = i\hbar L_1. \tag{69}$$

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* This is surely the classical form of the angular momentum, but an equivalent classical form is $\vec{L} = -\vec{p} \times \vec{x}$. Luckily, both of these produce the same <u>quantum</u> <u>mechanical</u> operator since only orthogonal components of $\vec{x}$, $\vec{p}$ are multiplied together. This is not always the case, however, and sometimes gives rise to "operator-ordering ambiguities".

It can be confirmed that

$$[L_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} L_k \ . \qquad (70)$$

is the general statement. (ε_{ijk} is the usual permutation symbol which is completely antisymmetric). This shows that the three components, L_i, are mutually incompatible observables. A quantum mechanical state can not, for example, be in an eigenstate of <u>both</u> L_1 <u>and</u> L_2. (There is one exception to this satement that we will discuss.) This is distinctly different from <u>linear</u> momentum for which we have seen

$$[p_i, p_j] = 0, \qquad (71)$$

for all i,j.

We will now try to find the effect of the L_i on a state $|\vec{x}'\rangle$. Consider

$$\left(1 - i \left(\frac{\delta\phi}{\hbar} \right) L_3\right)|\vec{x}'\rangle = \left(1 - i \left(\frac{\delta\phi}{\hbar} \right)(p_2 x_1' - p_1 x_2')\right)|\vec{x}'\rangle, \qquad (72)$$

where $\delta\phi$ is a positive, infinetismal quantity. Remember that

$$e^{i\vec{x}''\cdot\vec{p}/\hbar}|\vec{x}'\rangle = |\vec{x}' + \vec{x}''\rangle. \qquad (73)$$

Let's choose $\vec{x}'' = (-\delta x'',0,0)$ where $\delta x''$ is also a positive, infinitesimal quantity. Then (73) implies that

$$\left(1 + i \frac{\delta x''}{\hbar} p_1\right)|\vec{x}'\rangle = |x_1' - \delta x'', x_2', x_3'\rangle. \qquad (74)$$

Likewise for $\vec{x}'' = (0,\delta x'',0)$ we get

$$\left(1 - i\,\frac{\delta x''}{\hbar}\,p_2\right)|\vec{x}'> \;=\; |x_1', x_2' + \delta x'', x_3'>. \qquad (75)$$

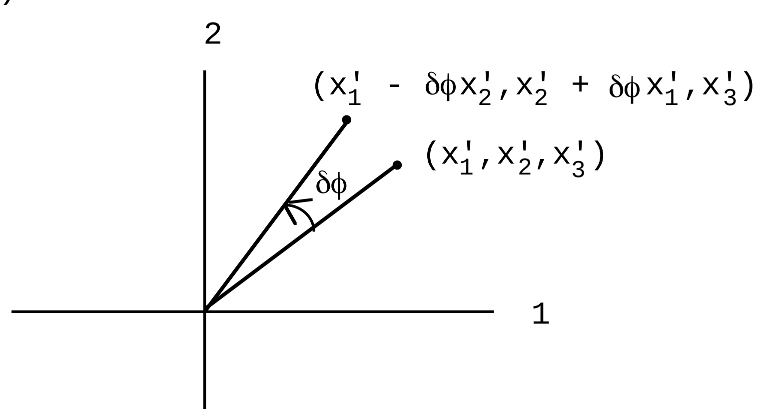
Since we may write

$$\left(1 - i\left(\frac{\delta\phi}{\hbar}\right) L_3\right) = \left(1 - i\left(\frac{\delta\phi}{\hbar}\right) x_1' p_2\right)\left(1 + i\left(\frac{\delta\phi}{\hbar}\right) x_2' p_1\right), \qquad (76)$$

(because $\delta\phi$ is infinetismal) we get that

$$\left(1 - i\left(\frac{\delta\phi}{\hbar}\right) L_3\right) |\vec{x}'> \;=\; |x_1' - \delta\phi x_2', x_2' + \delta\phi x_1', x_3'> \qquad (77)$$

The right hand side of (77) reveals that a rotation about the 3-axis has been performed. (See the following figure.) We are adopting the convention that this represents an <u>active</u> rotation of the physical system itself (rather than a passive rotation of the coordinate system in the opposite direction.) The rotation shown is defined to have $\delta\phi > 0$.



I have used the Cartesian basis to make these conclusions. In terms of a spherical basis, the effect of this operator is clearly

$$\left(1 - i\left(\frac{\delta\phi}{\hbar}\right) L_3\right) |r,\theta,\phi> \;=\; |r,\theta,\phi + \delta\phi>. \qquad (78)$$

Since $\delta\phi$ is infinitesimal, we have

$$|r,\theta,\phi + \delta\phi> = |r,\theta,\phi> + \delta\phi \frac{\partial}{\partial\phi} |r,\theta,\phi>. \qquad (79)$$

Matching the coefficient of $\delta\phi$ on both sides of (78), we conclude that

$$L_3|r,\theta,\phi> = i\hbar \frac{\partial}{\partial\phi} |r,\theta,\phi>, \qquad (80)$$

or since r and θ play no role here, that

$$L_3|\phi> = i\hbar \frac{\partial}{\partial\phi} |\phi>. \qquad (81)$$

Equivalently,

$$<\phi|L_3 = -i\hbar \frac{\partial}{\partial\phi} <\phi|. \qquad (82)$$

Finite relations can also be produced using L_3. Any finite rotation, ϕ, can always be imagined to consist of N identical partial rotations by an amount $\frac{\phi}{N}$. But in the limit $N \to \infty$ each of these partial rotations becomes infinitesimal. Thus, a finite rotation is accomplished by

$$\lim_{N\to\infty} \left(1 - i \left(\frac{\phi/N}{\hbar}\right) L_3 \right)^N .$$

Applying the formula

$$\lim_{N\to\infty} \left(1 + \frac{x}{N}\right)^N = e^x, \qquad (83)$$

to the above gives

$$\lim_{N\to\infty}\left(1 - i\left(\frac{\phi/N}{\hbar}\right) L_3\right)^N = e^{-iL_3\phi/\hbar}, \tag{84}$$

as the operator which performs finite rotations about the third axis. That is

$$e^{-iL_3\phi'/\hbar}|r,\theta,\phi> = |r,\theta,\phi + \phi'>. \tag{85}$$

Since L_3 is Hermitian, we recognize $e^{\pm iL_3\phi/\hbar}$ as a unitary operator. L_3 is called the generator of rotations about the third axis.

We will now find the effect of L_1 and L_2 on the $<\vec{r}|$ basis by a more cookbook-type approach. We have that

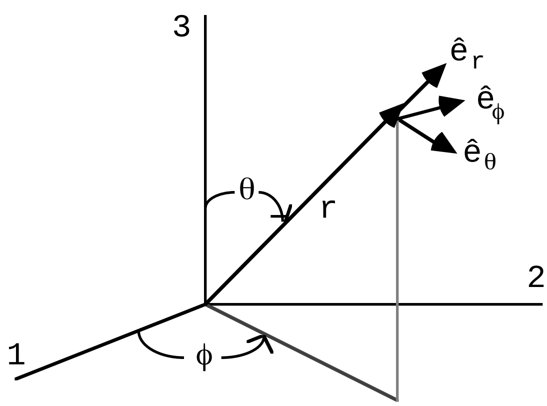
$$<\vec{r}|\vec{L} = <\vec{r}|\vec{x} \times \vec{p} = <\vec{r}|\vec{r} \times \vec{p}$$

$$= \vec{r} \times (<\vec{r}|\vec{p}) = \vec{r} \times \left(\frac{\hbar}{i}\vec{\nabla}_r <\vec{r}|\right). \tag{86}$$

Now since our basis is spherical, the gradient operator must be stated in spherical variables (which is symbolized by $\vec{\nabla}_r$):

$$\vec{\nabla}_r = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r \sin\theta}\frac{\partial}{\partial\phi} + \hat{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}, \tag{87}$$

where $\hat{e}_r$, $\hat{e}_\phi$ and $\hat{e}_\theta$ are unit vectors pointing in the instantaneous r, ϕ and θ directions.



The picture informs us that

$$\left.\begin{aligned} \hat{e}_r \times \hat{e}_\theta &= \hat{e}_\phi \ , \\ \hat{e}_\theta \times \hat{e}_\phi &= \hat{e}_r \ , \\ \hat{e}_\phi \times \hat{e}_r &= \hat{e}_\theta \ , \end{aligned}\right\} \tag{88}$$

so that

$$\langle \vec{r} | \vec{L} = \frac{\hbar}{i} \left[\hat{e}_\phi \frac{\partial}{\partial\theta} - \hat{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial\phi} \right] \langle \vec{r} | . \tag{89}$$

The $\hat{e}_r$, $\hat{e}_\theta$ and $\hat{e}_\phi$ can be related to unit vectors along $\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$, in the above figure by

$$\hat{e}_r = \sin\theta \cos\phi \ \hat{e}_1 + \sin\theta \sin\phi \ \hat{e}_2 + \cos\theta \ \hat{e}_3, \tag{90}$$

$$\hat{e}_\phi = -\sin\phi \ \hat{e}_1 + \cos\phi \ \hat{e}_2 \ . \tag{91}$$

$$\hat{e}_\theta = \cos\theta \cos\phi \ \hat{e}_1 + \cos\theta \sin\phi \ \hat{e}_2 - \sin\theta \ \hat{e}_3, \tag{92}$$

so when the basis in (89) is expressed in terms of the $\hat{e}_i$, we find

$$\langle \vec{r} | L_1 = \frac{\hbar}{i} \left(-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right) \langle \vec{r} | , \tag{93}$$

$$\langle \vec{r} | L_2 = \frac{\hbar}{i} \left(\cos\phi \frac{\partial}{\partial\theta} - \sin\phi \cot\theta \frac{\partial}{\partial\phi} \right) \langle \vec{r} | , \tag{94}$$

$$\langle \vec{r} | L_3 = \frac{\hbar}{i} \frac{\partial}{\partial\phi} \langle \vec{r} | . \tag{95}$$

Eq$^{\underline{n}}$ (95) is, of course, consistent with (82) above. We can also show from the above that

$$\langle \vec{r}|\vec{L}^2 = \langle \vec{r}| \left(L_1^2 + L_2^2 + L_3^2 \right)$$

$$= -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right] \langle \vec{r}|, \quad (96)$$

$$\equiv L_{op}^2 \langle \vec{r}|. \quad (97)$$

where we have defined the differential operator (as opposed to the Hilbert space operator, $\vec{L}^2$)

$$L_{op}^2 = -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right]. \quad (98)$$

Apart from an overall factor of $-\frac{1}{r^2\hbar^2}$, this is just seen to be the angular part of the $\vec{\nabla}_r^2$ operator. Eq$\underline{\text{n}}$s (93) - (95) could also have been stated in terms of the angular basis $\langle \hat{n}|$ since the purely radial part of the basis plays no role in these considerations. These results will be useful in a moment.

I will now prove a useful identity for $\vec{L}^2$. We know that

$$L_i = \sum_{j,k} \varepsilon_{ijk} x_j p_k, \quad (99)$$

where the order of the operators x_j, p_k does not matter since $[x_j, p_k] = 0$ for $j \neq k$. Therefore,

$$\vec{L}^2 = \sum_i L_i^2 = \sum_i \left(\sum_{j,k} \varepsilon_{ijk} x_j p_k \sum_{\ell,m} \varepsilon_{i\ell m} x_\ell p_m \right)$$

$$= \sum_{j,k,\ell,m} \left(\sum_i \varepsilon_{ijk} \varepsilon_{i\ell m} \right) x_j p_k x_\ell p_m. \quad (100)$$

One has

$$\sum_i \varepsilon_{ijk}\varepsilon_{i\ell m} = (\delta_{km}\delta_{j\ell} - \delta_{k\ell}\delta_{jm}), \qquad (101)$$

so that we may write

$$\vec{L}^2 = \sum_{j,k,\ell,m}\Big(\delta_{j\ell}\delta_{km}x_j\overbrace{(x_\ell p_k - i\hbar\delta_{\ell k})}^{p_k x_\ell}p_m - \delta_{k\ell}\delta_{jm}x_j p_k\underbrace{(p_m x_\ell + i\hbar\delta_{m\ell})}_{x_\ell p_m}\Big) \qquad (102)$$

or

$$\vec{L}^2 = \vec{x}^2\vec{p}^2 - 2i\hbar\vec{x}\cdot\vec{p} - (\vec{x}\cdot\vec{p})(\vec{p}\cdot\vec{x}). \qquad (103)$$

But (can you show it?)

$$\vec{p}\cdot\vec{x} = \vec{x}\cdot\vec{p} - 3i\hbar, \qquad (104)$$

so

$$\vec{L}^2 = \vec{x}^2\vec{p}^2 - (\vec{x}\cdot\vec{p})^2 + i\hbar\vec{x}\cdot\vec{p}. \qquad (105)$$

Notice that if $\vec{x}$ and $\vec{p}$ were regarded as numbers, the last term in (105) would not be present.

Now we can try to construct the differential equation implied by

$$H|a'\rangle = E_{a'}|a'\rangle, \qquad (106)$$

in a problem with spherical symmetry, $H = \frac{\vec{p}^2}{2m} + V(r)$. Project both sides of (106) into the spherical basis $\langle\vec{r}|$:

$$\langle\vec{r}|H|a'\rangle = E_{a'}\langle\vec{r}|a'\rangle, \qquad (107)$$

$$\Rightarrow \langle\vec{r}|\frac{\vec{p}^2}{2m}|a'\rangle + V(r)\langle\vec{r}|a'\rangle = E_{a'}\langle\vec{r}|a'\rangle, \qquad (108)$$

where $u_{a'}(\vec{r}) = \langle\vec{r}|a'\rangle$. We now have from (105) that

$$\langle\vec{r}|\vec{x}^2\vec{p}^2|a'\rangle = \langle\vec{r}|\vec{L}^2|a'\rangle + \langle\vec{r}|(\vec{x}\cdot\vec{p})^2|a'\rangle - i\hbar\,\langle\vec{r}|\vec{x}\cdot\vec{p}|a'\rangle. \qquad (109)$$

We have that

$$\langle\vec{r}|\vec{x}\cdot\vec{p}|a'\rangle = \vec{r}\cdot(\langle\vec{r}|\vec{p}|a'\rangle) = \vec{r}\cdot\left(\frac{\hbar}{i}\vec{\nabla}_r\langle\vec{r}|a'\rangle\right). \qquad (110)$$

with $\vec{\nabla}_r$ given by (87) above. Therefore

$$\langle\vec{r}|\vec{x}\cdot\vec{p}|a'\rangle = \frac{\hbar}{i}\,r\,\frac{\partial}{\partial r}\langle\vec{r}|a'\rangle = \frac{\hbar}{i}\,r\,\frac{\partial}{\partial r}u_{a'}(\vec{r}). \qquad (111)$$

Likewise

$$\langle\vec{r}|(\vec{x}\cdot\vec{p})^2|a'\rangle = \langle\vec{r}|(\vec{x}\cdot\vec{p})(\vec{x}\cdot\vec{p})|a'\rangle$$

$$= \left(\frac{\hbar}{i}\,r\,\frac{\partial}{\partial r}\right)\left(\frac{\hbar}{i}\,r\,\frac{\partial}{\partial r}\right)\langle\vec{r}|a'\rangle$$

$$= -\hbar^2\left(r^2\frac{\partial^2}{\partial r^2} + r\frac{\partial}{\partial r}\right)u_{a'}(\vec{r}), \qquad (112)$$

and

$$\langle\vec{r}|\vec{x}^2\vec{p}^2|a'\rangle = r^2\langle\vec{r}|\vec{p}^2|a'\rangle. \qquad (113)$$

Using (111), (112) and (113) in (109), we find that (dividing by r^2)

$$\langle\vec{r}|\vec{p}^2|a'\rangle = -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)u_{a'}(\vec{r}) + \frac{1}{r^2}\langle\vec{r}|\vec{L}^2|a'\rangle. \qquad (114)$$

Now using (97), we get

$$\langle \vec{r}|\vec{p}^{\,2}|a'\rangle = \left[-\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L_{op}^2}{r^2}\right] u_{a'}(\vec{r}). \qquad (115)$$

Since

$$\langle \vec{r}|\vec{p}^{\,2}|a'\rangle = -\hbar^2\,\vec{\nabla}_r^2\, u_{a'}(\vec{r}), \qquad (116)$$

all we have really accomplished in (115) is to find an explicit expression for the $\vec{\nabla}_r^2$ operator in spherical coordinates (in an especially interesting way, however.) So, using (98):

$$\vec{\nabla}_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right). \qquad (117)$$

Therefore, returning to (108), we have the explicit radial Schrödinger equation:

$$\left[-\frac{\hbar^2}{2mr^2}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \left(\frac{\vec{L}_{op}}{\hbar}\right)^2\right) + V(r)\right] u_{a'}(\vec{r}) = E_{a'}u_{a'}(\vec{r}). \qquad (118)$$

We could now proceed in a standard way to separate variables in (118) and find the eigenvalues and eigenvectors of the angular part of the problem using purely differential operator techniques (See, for example, Merzbacher, p.178 and on). Instead, let us proceed by considering what the set of quantum numbers {a'} above consists of. Notice

$$\left.\begin{aligned} \langle \vec{r}'|V(r)\vec{L} &= V(r')\langle \vec{r}'|\vec{L} = V(r')\vec{L}_{op}\langle \vec{r}'| \,, \\ \langle \vec{r}'|\vec{L}V(r) &= \vec{L}_{op}V(r')\langle \vec{r}'| = V(r')\vec{L}_{op}\langle \vec{r}'|. \end{aligned}\right\} \qquad (119)$$

Therefore

$$[\vec{L},V(r)] = 0. \qquad (120)$$

Also we have that

$$\left[\vec{p}^{\,2},L_j\right] = \left[\sum_i p_i^2, \sum_{k,\ell} \varepsilon_{jk\ell} x_k p_\ell\right] = \sum_{i,k,\ell} \left[p_i^2, x_k p_\ell\right] \varepsilon_{jk\ell}. \qquad (121)$$

Now

$$[p_i^2, x_k p_\ell] = p_i[p_i, x_k p_\ell] + [p_i, x_k p_\ell]p_i$$

$$= p_i(x_k\underbrace{[p_i,p_\ell]}_{0} + \underbrace{[p_i,x_k]}_{\frac{\hbar}{i}\delta_{ik}}p_\ell) + (x_k\underbrace{[p_i,p_\ell]}_{0} + \underbrace{[p_i,x_k]}_{\frac{\hbar}{i}\delta_{ik}}p_\ell)p_i \qquad (122)$$

so that

$$[p_i^2, x_k p_\ell] = 2\,\frac{\hbar}{i}\, p_i p_\ell \delta_{ik}. \qquad (123)$$

Using this in (121) gives

$$[\vec{p}^{\,2},L_j] = \sum_{i,k,\ell} \varepsilon_{jk\ell}\, 2\,\frac{\hbar}{i}\, p_1 p_\ell \delta_{ik} = 2\,\frac{\hbar}{i} \sum_{k,\ell} \varepsilon_{jk\ell}\, p_k p_\ell. \qquad (124)$$

Notice in (124) we have an object which is symmetric in two summed indices (k,ℓ) multiplied into an object which is antisymmetric in the same two indices. The result is zero. We can see this in general as follows. Let's say we have the 2 index objects A_{ij} and B_{ij} and that

$$\left.\begin{array}{l} A_{ij} = -A_{ji}\ , \\ \text{and} \\ B_{ij} = B_{ji}\ . \end{array}\right\} \qquad (125)$$

Then we have

$$\sum_{i,j} A_{ij}B_{ij} = - \sum_{i,j} A_{ji}B_{ji} \ . \qquad (126)$$

But since we are free to rename our indices, this means

$$\sum_{i,j} A_{ij}B_{ij} = - \sum_{i,j} A_{ij}B_{ij} \ . \qquad (127)$$

Anything which is equal to minus itself is zero, and so it is for the right hand side of (124):

$$[\vec{p}^2, \vec{L}] = 0. \qquad (128)$$

so since $H = \frac{\vec{p}^2}{2m} + V(r)$, (120) and (128) imply

$$[H, \vec{L}] = 0. \qquad (129)$$

Thus the $\vec{L}$ gives rise to good quantum numbers (See discussion in Ch.4). Eq$\underline{n}$ (129) implies of course that

$$[H, \vec{L}^2] = 0. \qquad (130)$$

What's more

$$[\vec{L}^2, L_i] = \left[\sum_j L_j^2, L_i\right] = \sum_j (L_j[L_j, L_i] + [L_j, L_i]L_j), \qquad (131)$$

and using (70) above we get

$$[\vec{L}^2, L_i] = i\hbar \sum_{j,k} \varepsilon_{jik}(L_jL_k + L_kL_j). \qquad (132)$$

This is again a situation in which a sum over two indices (j,k) is being performed on a symmetric object $[(L_jL_k + L_kL_j)]$ and an antisymmetric one (ε_{jik}). Therefore

$$[\vec{L}^2, \vec{L}] = 0. \qquad (133)$$

Now one of the theorems I talked about, and partially proved in Ch.4, said essentially that: ($A = A^+$, $B = B^+$)

A,B possess a common complete set of orthonormal eigenkets $\Leftrightarrow [A,B] = 0$.

Therefore from (129), (130) and (133) I may choose to characterize the set of quantum numbers {a'} in (118) (which is just an explicit version of (106) in a spherical basis) as eigenvalues of the set,

$$\{H, \vec{L}^2, L_3\} \ .$$

I could not, for example, add L_1 or L_2 to this list since $[L_{1,2}, L_3] \neq 0$. I did not have to choose L_3 in the above set; L_1 or L_2 would have done just as well. However, the choice of L_3 is simpler and conventional. The above represent a complete set for a spinless particle subjected to a spherically symmetric potential. (This is very nearly the case for an electron in the hydrogen atom.)

Thus, given the above choice of commuting observables, we take

$$|a'\rangle = |n,a,b\rangle, \tag{134}$$

where n is a radial quantum number which depends on the nature of the potential (more about this later), and "a" and "b" are eigenvalues of $\vec{L}^2$ and L_3:

$$\vec{L}^2|a,b\rangle = \hbar^2 a|a,b\rangle, \tag{135}$$

$$L_3|a,b\rangle = \hbar b|a,b\rangle, \tag{136}$$

where factors of $\hbar$ have been inserted for convenience. (a and b are real since $\vec{L}^2$ and L_3 are Hermitian.)

Let us find the eigenvalues and eigenvectors of $\vec{L}^2$ and L_3. Let us introduce

$$L_\pm = L_1 \pm iL_2, \tag{137}$$

$$L_+^+ = L_- \text{ . (not Hermitian)} \tag{138}$$

We can now show that

$$[L_+,L_-] = 2\hbar L_3, \tag{139}$$

$$[L_3,L_\pm] = \pm\hbar L_\pm . \tag{140}$$

Also

$$[\vec{L}^2,L_\pm] = 0 \tag{141}$$

is obvious. Now consider

$$\begin{aligned} L_3(L_\pm|a,b\rangle) &= L_\pm(L_3 \pm \hbar)|a,b\rangle \\ &= \hbar(b \pm 1)(L_\pm |a,b\rangle), \end{aligned} \tag{142}$$

and

$$\vec{L}^2(L_\pm|a,b\rangle) = L_\pm\hbar^2 a|a,b\rangle = \hbar^2 a(L_\pm|a,b\rangle). \tag{143}$$

Therefore, the $L_\pm$ are ladder operators in the "b" space; they raise or lower the value of this quantum number by one unit (similar to the operators A and A^+ in the harmonic oscillator problem.). The conclusion is that

$$L_\pm|a,b\rangle = C_\pm|a,b \pm 1\rangle, \tag{144}$$

or

$$\langle a,b|L_\mp = C_\pm^*\langle a,b \pm 1|, \tag{145}$$

where the $C_\pm$ are unknown constants.

Now we have that

$$\begin{aligned} L_-L_+ &= (L_1 - iL_2)(L_1 + iL_2) \\ &= L_1^2 + L_2^2 + i[L_1,L_2] \\ &= \vec{L}^2 - L_3^2 - \hbar L_3 \end{aligned} \tag{146}$$

so that

$$\begin{aligned} L_-L_+|a,b\rangle &= (\hbar^2 a - \hbar^2 b^2 - \hbar(\hbar b))|a,b\rangle \\ &= \hbar^2[a - b(b + 1)]|a,b\rangle \end{aligned} \tag{147}$$

But since

$$\langle a,b|L_-L_+|a,b\rangle = |C_+|^2, \tag{148}$$

we have

$$|C_+|^2 = \hbar^2[a - b(b + 1)]. \tag{149}$$

We <u>choose</u> the arbitrary phase to be such that

$$C_+ = \hbar\sqrt{a - b(b + 1)} \quad . \tag{150}$$

Likewise

$$L_+L_- = \vec{L}^2 - L_3^2 + \hbar L_3 \ , \tag{151}$$

so that

$$L_+L_-|a,b> = \hbar^2[a - b(b - 1)]|a,b> , \tag{152}$$

and since

$$|C_-|^2 = <a,b|L_+L_-|a,b>, \tag{153}$$

we have

$$|C_-|^2 = \hbar^2[a - b(b - 1)], \tag{154}$$

so

$$C_- = e^{i\phi}\hbar\sqrt{a - b(b - 1})), \tag{155}$$

where ϕ is an unknown phase. Actually ϕ is fixed from our previous choice for C_+ in (150). To see this consider

$$L_+[L_-|a,b> = e^{i\phi}\hbar\sqrt{a - b(b - 1}) |a,b - 1>] , \tag{156}$$

$$\Rightarrow \quad L_+L_-|a,b> = e^{i\phi}\hbar^2\sqrt{a - b(b - 1}) \sqrt{a - (b - 1)}b |a,b>$$

$$= e^{i\phi}\hbar^2[a - b(b - 1)]|a,b> . \tag{157}$$

Comparing (157) with (152) implies that $e^{i\phi} = 1$. Therefore, we have found that

$$L_\pm|a,b> = \hbar\sqrt{a - b(b \pm 1}) |a,b \pm 1> . \tag{158}$$

Now, what are the allowed values of a and b? We can easily show that the expectation value of the square of a Hermitian operator is always nonnegative. Therefore since

$$L_1^2 + L_2^2 = \vec{L}^2 - L_3^2, \tag{159}$$

we have

$$(L_1^2 + L_2^2)|a,b\rangle = \hbar^2(a - b^2)|a,b\rangle, \qquad (160)$$

and since, when multiplying on the left by $\langle a,b|$, the left hand side of (160) is guaranteed to be nonnegative, we have that

$$a - b^2 \geq 0. \qquad (161)$$

Now we know that the $L_\pm$ raise or lower the value of "b" in $|a,b\rangle$ by ±1 unit while keeping the value of "a" unchanged. Hence, for a fixed "a" value, we have

$$-\sqrt{a} \leq b \leq \sqrt{a}. \qquad (162)$$

Therefore, for a given "a" value there is a largest value of "b"; let us call this b_{max} (b_{max} does not necessarily equal $\sqrt{a}$ since there may exist more restrictive conditions. (162) only shows b is bounded.) Thus by definition we must have

$$L_+|a,b_{max}\rangle = 0. \qquad (163)$$

Likewise call the minimum value of b, for a given "a", b_{min}. Therefore

$$L_-|a,b_{min}\rangle = 0. \qquad (164)$$

From (146) and (151) we have

$$L_\mp L_\pm = \vec{L}^2 - L_3(L_3 \pm \hbar). \qquad (165)$$

Thus, applying (165) to (163) and (164), we find

$$\left.\begin{aligned} L_-L_+|a,b_{max}\rangle &= \hbar^2[a - b_{max}(b_{max} + 1)]|a,b_{max}\rangle = 0, \\ L_+L_-|a,b_{min}\rangle &= \hbar^2[a - b_{min}(b_{min} - 1)]|a,b_{min}\rangle = 0. \end{aligned}\right\} \quad (166)$$

The equations (166) together imply that

$$b_{max}(b_{max} + 1) = b_{min}(b_{min} - 1) \ , \qquad (167)$$

or

$$(b_{max} + b_{min})(b_{max} - b_{min} + 1) = 0. \qquad (168)$$

But since $b_{max} \geq b_{min}$, we get that

$$b_{max} = -b_{min}. \qquad (169)$$

Let us say it takes 2ℓ steps (2ℓ is a positive or zero integer) to go from $b = b_{min}$ to $b = b_{max}$ in steps of one:

$$b_{max} = b_{min} + 2\ell, \qquad (170)$$

where the possible ℓ values are

$$\ell = 0 \overset{X}{\tfrac{1}{2}},1,\overset{X}{\tfrac{3}{2}},... \qquad (171)$$

(The reason for the "X" above $\ell = \frac{1}{2},\frac{3}{2},...$ will be discussed shortly). Then because $b_{min} = -b_{max}$, we have

$$b_{max} = \ell, \qquad (172)$$

and from either of Eq$\underline{\text{n}}$s (166), we get

$$a = \ell(\ell + 1). \qquad (173)$$

So, for a given ℓ value, we have the possible "b" values:

$$\left.\begin{array}{l} b = b_{min}, b_{min} + 1, \ldots, b_{max} - 1, b_{max} \\ \text{or} \\ b = -\ell, -\ell + 1, \ldots, \ell - 1, \ell \end{array}\right\} \qquad (174)$$

It is more conventional to relabel "b" as "m", called the "magnetic quantum number." As an example, let us choose $\ell=3$. Then m can take on $2\ell + 1 = 7$ values:

$$\ell = 3 \left\{ \begin{array}{lll} \underline{\quad\quad} & m = 3 & \downarrow L_- \\ \underline{\quad\quad} & \quad 2 & \\ \underline{\quad\quad} & \quad 1 & \\ \underline{\quad\quad} & \quad 0 & \\ \underline{\quad\quad} & \; -1 & \\ \underline{\quad\quad} & \; -2 & \\ \underline{\quad\quad} & \; -3 & \uparrow L_+ \end{array} \right.$$

There is a subtlety involved in the labeling of the eigenstates of $\vec{L}^2$ and L_3. Since $\vec{L}^2$ and L_3 commute (and therefore are simultaneously measurable), we may regard the state $|\ell,m\rangle$ as a type of direct product, which would seem to imply that

$$|\ell,m\rangle \stackrel{?}{=} |\ell\rangle \otimes |m\rangle .$$

However, because $\vec{L}^2$ does not project entirely into θ space (see (93) and (94) above), the value of m enters the eigenvalue equation for $\vec{L}^2$ (see Eq$\underline{^n}$ (188) below). Therefore, we will define*

$$|\ell,m\rangle \equiv \underset{\substack{\text{projects into}\\ \theta \text{ space}}}{|\ell(m)\rangle} \otimes \underset{\substack{\text{projects into}\\ \phi \text{ space}}}{|m\rangle},$$

---

* Technically speaking, these states are <u>separable</u> but not true direct products.

$|\ell,m\rangle$ is just a way of labelling the more proper object on the right hand side. The $\ell(m)$ notation is supposed to indicate that "ℓ" is the quantum number associated with the θ eigenvalue equation, but that "m" enters this equation as a parameter. The same sort of subtlety affects the labeling of the Hilbert space description of the radial eigenstates; that is, the value of ℓ enters the radial eigenvalue equation (see Eq$\underline{\text{n}}$ (253) below), and we shall define

$$|n,\ell,m\rangle \equiv |n(\ell)\rangle \otimes |\ell,m\rangle.$$

These Hilbert spaces are such that

$$\begin{aligned}\langle r,\theta,\phi|n,\ell,m\rangle &= \langle r|n(\ell)\rangle\langle\theta|\ell(m)\rangle\langle\phi|m\rangle \\ &= u_{n\ell}(r)u_{\ell m}(\theta)u_m(\phi).\end{aligned}$$

The eigenvalue equations for $u_m(\phi)$, $u_{\ell m}(\theta)$ and $u_{n\ell}(r)$ are given by (180), (188) and (253) below, respectively.

Let us relabel our states as

$$|a,b\rangle \to |\ell,m\rangle. \tag{175}$$

We have therefore found the eigenvalues of $\vec{L}^2$ and L_3 as

$$\vec{L}^2|\ell,m\rangle = \hbar^2\ell(\ell+1)|\ell,m\rangle, \tag{176}$$

$$L_3|\ell,m\rangle = \hbar m|\ell,m\rangle, \tag{177}$$

and

$$L_\pm|\ell,m\rangle = \hbar\sqrt{(\ell \mp m)(\ell \pm m + 1)}\;|\ell,m \pm 1\rangle. \tag{178}$$

Actually, "half-integer" values of $\ell (\ell = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots)$ are not allowed. One way to see this is as follows. The eigenvalue equation for L_3 is

$$L_3|m\rangle = m\hbar|m\rangle. \qquad (179)$$

Projecting both sides of (179) into $\langle\phi|$ and calling $U_m(\phi) = \langle\phi|m\rangle$, we get

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi} u_m(\phi) = m\hbar u_m(\phi). \qquad (180)$$

The solution to (180) is

$$u_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \qquad (181)$$

which is normalized so that

$$\int_0^{2\pi} d\phi |u_m|^2 = 1 . \qquad (182)$$

Now consider half-integer values of ℓ. From (181) it would seem that

$$\langle\phi|m\rangle = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \qquad (183)$$

where m is also required, by (174), to take on half-integer values. Therefore given (183) we have

$$\langle\phi + 2\pi|m\rangle = -\frac{1}{\sqrt{2\pi}} e^{im\phi} . \qquad (184)$$

But $\langle\phi|$ and $\langle\phi + 2\pi|$ pick out the <u>same</u> point in coordinate space. Therefore, the spatial wavefunctions of half-integer

ℓ are not single valued, a condition we must require for the transformation between the $|\phi>$ and $|m>$ bases.

There are other arguments as to why half-integer ℓ values are not allowed. The end result is to limit ℓ to the values

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

and m to

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

($2\ell + 1$ values) for each ℓ.

Now we know the eigenvalues of $\vec{L}^2$ and L_3. We would like to find the explicit eigenvectors also. We write (the $Y_{\ell m}$ are called "spherical harmonics")

$$\begin{aligned} Y_{\ell m}(\theta,\phi) &\equiv <\theta,\phi|\ell,m> \\ &= <\theta|\ell(m)> <\phi|m> \\ &\equiv u_{\ell m}(\theta)u_m(\phi). \end{aligned} \tag{185}$$

The eigenvalue equation for $u_m(\phi)$ is written down in (180), and it's normalized solution is (181). The eigenvalue equation for $u_{\ell m}(\theta)$ comes from

$$\vec{L}^2|\ell,m> = \hbar^2\ell(\ell + 1)|\ell,m>. \tag{186}$$

We have to start out with $|\ell,m>$ in (186) (and <u>not</u> $|\ell(m)>$) since we don't know the effect of $\vec{L}^2$ on $<\theta|$ but only on $<\theta,\phi|$ from (97) and (98).

Projected into $<\theta,\phi|$ space (using (97) and (98) above gives

$$- \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right] u_{\ell m}(\theta) u_m(\phi)$$

$$= \ell(\ell + 1) u_{\ell m}(\theta) u_m(\phi), \qquad (187)$$

or, making the replacement $\frac{\partial^2}{\partial\phi^2} \rightarrow -m^2$ from (180), and then dividing both sides by $u_m(\phi)$, we get

$$- \left[\frac{-m^2}{\sin^2\theta} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right] u_{\ell m}(\theta) = \ell(\ell + 1) u_{\ell m}(\theta). \qquad (188)$$

The solution to this equation determines the eignevectors $u_{\ell m}(\theta)$.

Rather than trying to solve (188) directly, we will generate the solutions by operator techniques, using the ladder operators $L_\pm$. We can construct all of the $|\ell,m\rangle$ by considering $|\ell,\ell\rangle$ and then applying L_- $(\ell - m)$ times:

$$(L_-)^{\ell-m}|\ell,\ell\rangle = \hbar\sqrt{2\ell}\,(L_-)^{(\ell-m)-1}|\ell,\ell - 1\rangle$$
$$= \hbar^2\sqrt{2\ell}\,\sqrt{(2\ell - 1)2}\,(L_-)^{(\ell-m)-2}|\ell,\ell - 2\rangle$$
$$= \hbar^3\sqrt{2\ell}\,\sqrt{(2\ell - 1)2}\,\sqrt{(2\ell - 2)3}(L_-)^{(\ell-m)-3}|\ell,\ell - 3\rangle, \quad (189)$$

or, in general, after $(\ell - m)$ applications of L_-:

$$(L_-)^{(\ell-m)}|\ell,\ell\rangle$$

$$= (\hbar)^{\ell-m}\underbrace{\sqrt{2\ell}\,\sqrt{(2\ell - 1)2}\ldots\sqrt{(2\ell - (\ell - m - 1))(\ell - m)}}_{(\ell - m \text{ factors})}\,|\ell,m\rangle.$$

(190)

Let's look at some of the individual pieces that make up the overall factor in (190). We recognize the combination,

$$(2\ell)(2\ell-1)\ldots\underbrace{(2\ell-(\ell-m-1))}_{(\ell+m+1)}$$

in (190), which we can write as

$$\frac{(2\ell)(2\ell-1)\ldots(2)(1)}{(\ell+m)(\ell+m-1)\ldots(2)(1)} = \frac{(2\ell)!}{(\ell+m)!}\,. \tag{191}$$

We also have the combination

$$(1)(2)\ldots(\ell-m) = (\ell-m)!\,. \tag{192}$$

Therefore, we may write (190) as

$$(L_-)^{\ell-m}|\ell,\ell\rangle = (\hbar)^{\ell-m}\sqrt{\frac{(2\ell)!(\ell-m)!}{(\ell+m)!}}\;|\ell,m\rangle, \tag{193}$$

or, solving for $|\ell,m\rangle$:

$$|\ell,m\rangle = \frac{1}{(\hbar)^{\ell-m}}\sqrt{\frac{(\ell+m)!}{(2\ell)!(\ell-m)!}}\;(L_-)^{\ell-m}|\ell,\ell\rangle. \tag{194}$$

I remind you of the effect of L_1 and L_2 (compare with (93) and (94); here I am using the $\langle\hat{n}| = \langle\theta,\phi|$ notation):

$$\langle\hat{n}|L_1 = \frac{\hbar}{i}\left(-\sin\phi\,\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\,\frac{\partial}{\partial\phi}\right)\langle\hat{n}|, \tag{195}$$

$$\langle\hat{n}|L_2 = \frac{\hbar}{i}\left(\cos\phi\,\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\,\frac{\partial}{\partial\phi}\right)\langle\hat{n}|. \tag{196}$$

So therefore

$<\hat{n}|L_+ =$

$$\frac{\hbar}{i}\left(\underbrace{(-\sin\phi + i\cos\phi)}_{ie^{i\phi}}\frac{\partial}{\partial\theta} - \underbrace{(\cos\phi + i\sin\phi)}_{e^{i\phi}}\cot\theta\,\frac{\partial}{\partial\phi}\right)<\hat{n}|, \quad (197)$$

or

$$<\hat{n}|L_+ = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\phi}\right)<\hat{n}|. \quad (198)$$

Also

$<\hat{n}|L_- =$

$$\frac{\hbar}{i}\left((-\sin\phi - i\cos\phi)\,\frac{\partial}{\partial\theta} - (\cos\phi - i\sin\phi)\cot\theta\,\frac{\partial}{\partial\phi}\right)<\hat{n}|. \quad (199)$$

or

$$<\hat{n}|L_- = -\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\,\frac{\partial}{\partial\phi}\right)<\hat{n}|. \quad (200)$$

Now consider

$$<\hat{n}|L_-|\ell,m> = -\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\,\frac{\partial}{\partial\phi}\right)<\hat{n}|\ell,m>. \quad (201)$$

where $<\hat{n}|\ell,m> = Y_{\ell m}(\hat{n})$. We know that

$$Y_{\ell m}(\theta,\phi) = u_{\ell m}(\theta)\,\frac{1}{\sqrt{2\pi}}\,e^{im\phi}, \quad (202)$$

where $m = 0,\pm1,\pm2,...,\pm\ell$ ($2\ell + 1$ values). Therefore

$$\langle \hat{n}|L_-|\ell,m\rangle = -\frac{\hbar}{\sqrt{2\pi}}\, e^{i(m-1)\phi}\left(\frac{d}{d\theta} + m\cot\theta\right) u_{\ell m}(\theta). \qquad (203)$$

Consider the identity:

$$(\sin\theta)^{1-m} \frac{d}{d\cos\theta}\,[(\sin\theta)^m F(\theta)]$$

$$= (\sin\theta)^{1-m} \underbrace{\frac{d\theta}{d\cos\theta}}_{-\frac{1}{\sin\theta}}\; \underbrace{\frac{d}{d\theta}[(\sin\theta)^m F(\theta)]}_{(\sin\theta)^m \frac{dF(\theta)}{d\theta} + m(\sin\theta)^{m-1}\cos\theta\, F(\theta)}$$

$$= -\left(\frac{d}{d\theta} + m\cot\theta\right) F(\theta). \qquad (204)$$

But the right hand side of (204) is the same as the structure in (203), so we may make the replacement

$$\langle \hat{n}|L_-|\ell,m\rangle =$$

$$\frac{\hbar}{\sqrt{2\pi}}\, e^{i(m-1)\phi} \sin(\theta)^{1-m} \frac{d}{d\cos\theta}\,[(\sin\theta)^m u_{\ell m}(\theta)]. \qquad (205)$$

Now consider

$$\langle \hat{n}|L_-L_-|\ell,m\rangle = -\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\,\frac{\partial}{\partial\phi}\right)\langle \hat{n}|L_-|\ell,m\rangle$$

$$= \frac{-(\hbar)^2}{\sqrt{2\pi}}\, e^{i(m-2)\phi}\left(\frac{d}{d\theta} + (m-1)\cot\theta\right)$$

$$\cdot \left[(\sin\theta)^{1-m} \frac{d}{d\cos\theta}\Big((\sin\theta)^m u_{\ell m}(\theta)\Big)\right]. \qquad (206)$$

Employing (204) again in (206) (with $m \to m-1$) gives

$$< \hat{n}|(L_-)^2|\ell,m>$$

$$= \frac{(\hbar)^2}{\sqrt{2\pi}} \; e^{i(m-2)\phi}(\sin\theta)^{2-m} \frac{d^2}{d\cos\theta^2}\left[(\sin\theta)^m u_{\ell m}(\theta)\right]. \quad (207)$$

Seeing the pattern that seems to have developed, we may now prove by induction that

$$< \hat{n}|(L_-)^k|\ell,m>$$

$$= \frac{(\hbar)^k}{\sqrt{2\pi}} \; e^{i(m-k)\phi}(\sin\theta)^{k-m} \left(\frac{d}{d\cos\theta}\right)^k \left[(\sin\theta)^m u_{\ell m}(\theta)\right]. \quad (208)$$

Let's set $m = \ell$ and $k = \ell - m$ in (208):

$$< \hat{n}|(L_-)^{\ell-m}|\ell,\ell>$$

$$= \frac{(\hbar)^{\ell-m}}{\sqrt{2\pi}} \; e^{im\phi}(\sin\theta)^{-m} \left(\frac{d}{d\cos\theta}\right)^{\ell-m} \left[(\sin\theta)^\ell u_{\ell\ell}(\theta)\right]. \quad (209)$$

But from (194)

$$< \hat{n}|\ell,m> = (\hbar)^{m-\ell}\sqrt{\frac{(\ell+m)!}{(2\ell)!(\ell-m)!}} \; < \hat{n}|(L_-)^{\ell-m}|\ell,\ell>, \quad (210)$$

and so we find ($Y_{\ell m}(\hat{n}) \equiv < \hat{n}|\ell,m>$)

$$Y_{\ell m}(\theta,\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}\sqrt{\frac{(\ell+m)!}{(2\ell)!(\ell-m)!}} \; (\sin\theta)^{-m}\left(\frac{d}{d\cos\theta}\right)^{\ell-m}$$

$$\left[(\sin\theta)^\ell u_{\ell\ell}(\theta)\right]. \quad (211)$$

Therefore, we will have a general expression for <u>all</u> the $Y_{\ell m}(\hat{n})$ if we can find the explicit expression for $u_{\ell\ell}(\theta)$. Now remember that

$$L_+|\ell,\ell\rangle = 0, \tag{212}$$

so that

$$\langle\hat{n}|L_+|\ell,\ell\rangle = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi}\right) \underbrace{\langle\hat{n}|\ell,\ell\rangle}_{\frac{e^{i\ell\phi}}{\sqrt{2\pi}} u_{\ell\ell}(\theta)}, \tag{213}$$

which gives us the first order differential equation:

$$\left[\frac{d}{d\theta} - \ell \cot\theta\right] u_{\ell\ell}(\theta) = 0. \tag{214}$$

It's easy to check that the solution to (214) is

$$u_{\ell\ell}(\theta) = C_\ell (\sin\theta)^\ell . \tag{215}$$

(Do it.) C_ℓ is an unknown constant which is determined by the normalization condition

$$\int d\Omega_{\hat{n}} \left| u_{\ell\ell}(\theta) \frac{e^{i\ell\phi}}{\sqrt{2\pi}} \right|^2 = 1. \tag{216}$$

(Eq<u>n</u> (216) can be viewed as saying the probability of seeing the particle somewhere in angular space is unity.)
Explicitly, this gives

$$|C_\ell|^2 \int_0^\pi d\theta \sin\theta \sin^{2\ell}\theta = 1, \tag{217}$$

or

$$|C_\ell|^2 \int_{-1}^{1} d(\cos\theta)\sin^{2\ell}\theta = 1, \ . \tag{218}$$

Setting

$$x = \cos\theta \tag{219}$$

we then get

$$|C_\ell|^2 \int_{-1}^{1}(dx)(1 - x^2)^\ell = 1. \tag{220}$$

The integral in (220) can be done by parts (this will be a homework problem) to yield

$$|C_\ell|^2 \left(2 \frac{(2^\ell \ell!)^2}{(2\ell + 1)!}\right) = 1. \tag{221}$$

It is conventional to choose the phase such that

$$C_\ell = \frac{(-1)^\ell}{2^\ell \ell!} \sqrt{\frac{(2\ell + 1)!}{2}} \ , \tag{222}$$

and so

$$u_{\ell\ell}(\theta) = \frac{(-1)^\ell}{2^\ell \ell!} \sqrt{\frac{(2\ell + 1)!}{2}} \sin^\ell \theta \ . \tag{223}$$

Using (223) in (211) now gives the general result

$$Y_{\ell m}(\theta,\phi) = \frac{(-1)^\ell e^{im\phi}}{2^\ell \ell!} \sqrt{\frac{(2\ell + 1)(\ell + m)!}{4\pi(\ell - m)!}} \ (\sin\theta)^{-m}$$

$$\times \left(\frac{d}{d\cos\theta}\right)^{\ell-m}[(\sin\theta)^{2\ell}]. \tag{224}$$

Because of the normalization of the spherical basis, Eq$^{\underline{n}}$(62), we have

$$<\ell',m'|\left[\int d\Omega_{\hat{n}}|\hat{n}><\hat{n}| = 1\right]|\ell,m>, \tag{225}$$

which means that

$$\int d\Omega_{\hat{n}} Y^{*}_{\ell'm'}(\hat{n})Y_{\ell m}(\hat{n}) = \delta_{\ell\ell'}\delta_{mm'} \ . \tag{226}$$

Eq$^{\underline{n}}$ (226) is completeness for spherical harmonics in angular space. We also have

$$<\hat{n}|\left[\sum_{\ell,m}|\ell,m><\ell,m| = 1\right]|\hat{n}'> , \tag{227}$$

or

$$\sum_{\ell,m} Y_{\ell m}(\hat{n})Y^{*}_{\ell m}(\hat{n}') = <\hat{n}|\hat{n}'>, \tag{228}$$

which expresses completeness of the $|\ell,m>$ basis states. The $<\hat{n}|\hat{n}'>$ is a <u>spherical</u> Dirac delta function. We can get an explicit form for it by requiring that

$$1_{\hat{n}} = \int d\Omega_{\hat{n}}|\hat{n}><\hat{n}|\int d\Omega_{\hat{n}'}|\hat{n}'><\hat{n}'|,$$

$$= \int d\Omega_{\hat{n}}d\Omega_{\hat{n}'}|\hat{n}><\hat{n}|\hat{n}'><\hat{n}'|,$$

$$= \int d(\cos\theta)d(\cos\theta')d\phi d\phi'|\theta,\phi><\theta,\phi|\theta',\phi'><\theta',\phi'|. \tag{229}$$

Comparing this with the original expression

$$1_{\hat{n}} = \int d(\cos\theta)d\phi|\theta,\phi><\theta,\phi| \ , \qquad (230)$$

means that we may take

$$<\hat{n}|\hat{n}'> = \delta(\cos\theta - \cos\theta')\delta(\phi - \phi'). \qquad (231)$$

[Using the delta function rule (see Jackson, p.30)

$$\delta(f(x)) = \sum_i \frac{1}{\left|\frac{df}{dx}(x_i)\right|}\delta(x - x_i),$$

where the sum is over the simple zeros of f(x), located at $x = x_i$, we may write

$$\delta(\cos\theta - \cos\theta') = \frac{1}{\sin\theta'}\delta(\theta - \theta'),$$

where both θ and θ' are assumed to be in the range from 0 to π.] Therefore

$$\sum_{\ell=0}^{\infty}\sum_{m=\ell}^{\ell} Y_{\ell m}(\theta,\phi)Y^{*}_{\ell m}(\theta',\phi') = \delta(\cos\theta - \cos\theta')\delta(\phi - \phi'). \qquad (232)$$

[Notice we haven't really proven either (226) or (232); the proofs require more sophisticated analysis.] A useful connection is

$$Y_{\ell 0}(\theta,\phi) = \frac{(-1)^{\ell}}{2^{\ell}\ell!}\sqrt{\frac{(2\ell + 1)}{4\pi}}\left(\frac{d}{d\cos\theta}\right)^{\ell}(\sin\theta)^{2\ell}$$

$$= \sqrt{\frac{(2\ell + 1)}{4\pi}} \quad P_\ell(\cos\theta), \tag{233}$$

where $P_\ell(x)$ is called a "Legendre polynomial." (Notice that when m = 0, there is no ϕ dependence in $Y_{\ell 0}(\theta,\phi)$.) By definition then

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2 - 1)^\ell \ . \tag{234}$$

I am not going to go through all of the explicit steps, but in the same way that I showed (194) to be true by operating $(\ell - m)$ times with L_- on $|\ell,\ell>$ to give $|\ell,m>$, we can also start at the other end and operate $(\ell + m)$ times with L_+ on $|\ell,-\ell>$ to give $|\ell,m>$. The result is

$$|\ell,m> = (\hbar)^{-(\ell+m)} \sqrt{\frac{(\ell - m)!}{(2\ell)!(\ell + m)!}} \quad (L_+)^{\ell+m} \ |\ell,-\ell>. \tag{235}$$

We can also show that

$$<\hat{n}|(L_+)^{\ell+m} \ |\ell,-\ell> = \frac{(\hbar)^{(\ell+m)}}{\sqrt{2\pi}} \ (-1)^{\ell+m} \ e^{im\phi}$$

$$\cdot \ (\sin\theta)^m \left(\frac{d}{d\cos\theta}\right)^{\ell+m} \Big[(\sin\theta)^\ell \ u_{\ell -\ell}(\theta)\Big]. \tag{236}$$

From our earlier $Y_{\ell m}(\theta,\phi)$ expression, (224), we can show that

$$Y_{\ell -\ell}(\theta,\phi) = \frac{e^{-i\ell\phi}}{2^\ell \ell!} \sqrt{\frac{(2\ell + 1)!}{4\pi}} \quad (\sin\theta)^\ell \ , \tag{237}$$

from which we can identify

$$u_{\ell\,-\ell}(\theta) = \frac{1}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{2}}\ (\sin\theta)^\ell\ . \tag{238}$$

(Notice that unlike (223) there is no factor of $(-1)^\ell$ here.)

The above steps then lead in the same manner as before to the alternate expression

$$Y_{\ell m}(\theta,\phi) = \frac{(-1)^{m+\ell}e^{im\phi}}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\ (\sin\theta)^m \cdot \left(\frac{d}{d\cos\theta}\right)^{\ell+m}\left[(\sin\theta)^{2\ell}\right]\ . \tag{239}$$

You should now go back to Eq$\underline{\text{n}}$ (224) and carefully compare it to (239) above.) By using the expression (224) when $m \geq 0$ and the expression (239) when $m \leq 0$, one may also write, for example

$$Y_{\ell m}(\theta,\phi) = \frac{(-1)^{(m-|m|)/2}(-1)^\ell}{2^\ell \ell!}\ e^{im\phi}\sqrt{\frac{(2\ell+1)(\ell+|m|)!}{4\pi(\ell-|m|)!}} \times (\sin\theta)^{-|m|}\left(\frac{d}{d\cos\theta}\right)^{\ell-|m|}\left[(\sin\theta)^{2\ell}\right]\ . \tag{240}$$

We can read off from (240) the symmetry property

$$(-1)^m Y_{\ell\,-m}(\theta,-\phi) = Y_{\ell m}(\theta,\phi)\ , \tag{241}$$

but since

$$Y^*_{\ell m}(\theta,\phi) = Y_{\ell m}(\theta,-\phi)\ , \tag{242}$$

we may write (241) as

$$(-1)^m Y^*_{\ell\,-m}(\theta,\phi) = Y_{\ell m}(\theta,\phi)\ . \qquad (243)$$

We can tie this discussion into the parity operator (introduced in Chapter 3) for which, by definition

$$<\hat{n}|\mathbb{P} = <-\hat{n}|\ , \qquad (244)$$

where we may take

$$<\hat{n}| = \begin{cases} <\pi - \theta, \phi + \pi|, \text{ if } \phi < \pi \\ <\pi - \theta, \phi - \pi|, \text{ if } \phi \geq \pi \end{cases}\ . \qquad (245)$$

Now we have that

$$\begin{aligned} \cos(\pi - \theta) &= -\cos\theta, \\ \sin(\pi - \theta) &= \sin\theta, \end{aligned} \qquad (246)$$

which helps us to see from (240) that

$$Y_{\ell m}(\pi - \theta, \phi \pm \pi) = Y_{\ell m}(\theta,\phi)\underbrace{e^{\pm im\pi}(-1)^{\ell-|m|}}_{(-1)^{\ell}}. \qquad (247)$$

Therefore

$$<\hat{n}|\mathbb{P}\,|\ell,m> = <-\hat{n}|\ell,m> = (-1)^{\ell}<\hat{n}|\ell,m>. \qquad (248)$$

Since (248) is true for all $<\hat{n}|$, we have that

$$\mathbb{P}\,|\ell,m> = (-1)^{\ell}|\ell,m>\ . \qquad (249)$$

The words that go with Eq$\underline{\text{n}}$ (249) say "the parity of the state $|\ell,m>$ is $(-1)^{\ell}$."

We now return to the Schrödinger equation in spherical coordinates, Eqn (118). We now know that

$$u_{a'}(\vec{r}) = u_{n\ell}(r)Y_{\ell m}(\theta,\phi), \tag{250}$$

and also that

$$L_{op}^2 \langle \hat{n}|\ell,m\rangle = \langle \hat{n}|\vec{L}^2|\ell,m\rangle = \hbar^2\ell(\ell + 1)\langle \hat{n}|\ell,m\rangle, \tag{251}$$

or

$$L_{op}^2 Y_{\ell m}(\theta,\phi) = \hbar^2\ell(\ell + 1)Y_{\ell m}(\theta,\phi), \tag{252}$$

so that (118) is equivalent to

$$\left[- \frac{\hbar^2}{2mr^2}\left(\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \ell(\ell + 1)\right) + V(r)\right]u_{n\ell}(r) = E_{n\ell}u_{n\ell}(r). \tag{253}$$

Notice that the magnetic quantum number, m, does not enter in (253). This equation determines the energy levels of the system; therefore, the energies are independent of m for a problem with spherical symmetry and we have a $2\ell + 1$ fold degeneracy (at least) of each energy level labeled by $(n\ell)$. Also note that, as stated earlier, ℓ enters this equation simply as a *parameter*; the *quantum number* determined by this equation is "n". In the next chapter we will examine solutions to (253) for various forms for the potential V(r).

Problems

1. Answer the question in the notes, bottom of page 6.9.

2. Using expressions (93)-(95) of the notes, show that (96) is true.

3.(a) Given an operator U with the properties

$$[\vec{L}^2,U] = 0$$
$$[L_3,U] = -\ell\hbar U,$$

show that

$$U|\ell,\ell\rangle = \text{const.}|\ell,0\rangle.$$

(b) Given an operator V with the properties

$$[L_+,V] = 0$$
$$[L_3,V] = \hbar V,$$

show that

$$V|\ell,\ell\rangle = \text{const.}|\ell+1,\ell+1\rangle.$$

(c) Given an operator W with the properties,

$$[L_-,W] = 0,$$
$$[L_3,W] = -\hbar W,$$

find:

$$W|\ell,-\ell\rangle = ?$$

4. Show Eq.(139) and Eq.(140) of the text (Ch.6).

5. Do the integral in Eq.(220) of Ch.6 of the notes.

6. Using Eq.(224) of Ch.6, write out the explicit forms for the spherical harmonics:

$$Y_{00},\ Y_{11},\ Y_{10},\ Y_{1-1}.$$

7. Prove: The expectation value of the square of a Hermitian operator is nonnegative. (I used this on p.6.27 of the notes. This is essentially a one-line proof.)

8. Prove Eq.(208) of Ch.6 by induction. (That is, assume it is true for k, and use this to show it then holds for the k+1 case.)

Other Problems

9. The wavefunction of a bound particle is given by

$$\Psi(\vec{r},0) = xz\Psi(r),$$

where $r = |\vec{r}|$.

(a) If $\vec{L}^2$ is measured at t = 0, what value is found?

(b) What possible values of L_z will measurement find at t = 0, and with what probability will they occur? [Hint: See Table 9.1, p.369, of Liboff.]

10.(a) Evaluate:

$$[L_3,\phi] = ?$$

(ϕ is an operator whose eigenvalue is the spherical azimuthal angle:

$$\phi|\phi'\rangle = \phi'|\phi'\rangle.)$$

(b) Apply (a) to evaluate the quantity:

$$e^{-iL_3\phi'/\hbar}\ \phi\ e^{iL_3\phi'/\hbar} = ?$$

(ϕ' is a number.) [If you can't figure out part (a), I will give you the answer, but you will then get no credit for (a).]

Other problems

11. Assume a particle has an orbital angular momentum with $L_3' = \hbar m$ and $(\vec{L}^2)' = \hbar^2 \ell(\ell + 1)$. Show that in this state:

(a) $$\langle L_x \rangle = \langle L_y \rangle = 0,$$

(b) $$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \frac{1}{2}\hbar^2(\ell(\ell + 1) - m^2).$$

12. Can one measure a particle's momentum, $\vec{p}$, and angular momentum, $\vec{L}$, along the same coordinate axis simultaneously? What quantity must I compute in order to answer this question? Compute it!