12

Rotational Invariance and Angular Momentum

In the last chapter on symmetries, rotational invariance was not discussed, not because it is unimportant, but because it is all too important and deserves a chapter on its own. The reason is that most of the problems we discuss involve a single particle (which may be the reduced mass) in an external potential, and whereas translational invariance of H implies that the particle is free, rotational invariance of H leaves enough room for interesting dynamics. We first consider two dimensions and then move on to three.

12.1. Translations in Two Dimensions

Although we are concerned mainly with rotations, let us quickly review translations in two dimensions. By a straightforward extension of the arguments that led to Eq. (11.2.14) from Eq. (11.2.13), we may deduce that the generators of infinitesimal translations along the x and y directions are, respectively,

$$P_x \xrightarrow[\text{basis}]{\text{coordinate}} -i\hbar \frac{\partial}{\partial x} \tag{12.1.1}$$

$$P_y \xrightarrow[\text{basis}]{\text{coordinate}} -i\hbar \frac{\partial}{\partial y} \tag{12.1.2}$$

In terms of the *vector operator* $\mathbf{P}$, which represents momentum,

$$\mathbf{P} = P_x \mathbf{i} + P_y \mathbf{j} \tag{12.1.3}$$

P_x and P_y are the dot products of $\mathbf{P}$ with the unit vector ($\mathbf{i}$ or $\mathbf{j}$) in the direction of the translation. Since there is nothing special about these two directions, we conclude that in general,

$$\hat{n}\cdot\mathbf{P}\equiv P_{\hat{n}} \tag{12.1.4}$$

is the generator of translations in the direction of the unit vector $\hat{n}$. Finite translation operators are found by exponentiation. Thus $T(\mathbf{a})$, which translates by $\mathbf{a}$, is given by

$$T(\mathbf{a})=e^{-iaP_{\hat{a}}/\hbar}=e^{-ia\hat{a}\cdot\mathbf{P}/\hbar}=e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar} \tag{12.1.5}$$

where $\hat{a}=\mathbf{a}/a$.

The Consistency Test. Let us now ask if the translation operators we have constructed have the right laws of combination, i.e., if

$$T(\mathbf{b})T(\mathbf{a})=T(\mathbf{a}+\mathbf{b}) \tag{12.1.6}$$

or equivalently if

$$e^{-i\mathbf{b}\cdot\mathbf{P}/\hbar}e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}=e^{-i(\mathbf{a}+\mathbf{b})\cdot\mathbf{P}/\hbar} \tag{12.1.7}$$

This amounts to asking if P_x and P_y may be treated as c numbers in manipulating the exponentials. The answer is yes, since in view of Eqs. (12.1.1) and (12.1.2), the operators commute

$$[P_x, P_y]=0 \tag{12.1.8}$$

and their q number nature does not surface here. The commutativity of P_x and P_y reflects the commutativity of translations in the x and y directions.

*Exercise 12.1.1.** Verify that $\hat{a}\cdot\mathbf{P}$ is the generator of infinitesimal translations along $\mathbf{a}$ by considering the relation

$$\langle x, y|I-\frac{i}{\hbar}\delta\mathbf{a}\cdot\mathbf{P}|\psi\rangle=\psi(x-\delta a_x, y-\delta a_y)$$

12.2. Rotations in Two Dimensions

Classically, the effect of a rotation $\phi_0\mathbf{k}$, i.e., by an angle ϕ_0 about the z axis (counterclockwise in the x–y plane) has the following effect on the state of a particle:

$$\begin{bmatrix}x\\y\end{bmatrix}\to\begin{bmatrix}\bar{x}\\\bar{y}\end{bmatrix}=\begin{bmatrix}\cos\phi_0 & -\sin\phi_0\\\sin\phi_0 & \cos\phi_0\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix} \tag{12.2.1}$$

$$\begin{bmatrix}p_x\\p_y\end{bmatrix}\to\begin{bmatrix}\bar{p}_x\\\bar{p}_y\end{bmatrix}=\begin{bmatrix}\cos\phi_0 & -\sin\phi_0\\\sin\phi_0 & \cos\phi_0\end{bmatrix}\begin{bmatrix}p_x\\p_y\end{bmatrix} \tag{12.2.2}$$

Let us denote the operator that rotates these two-dimensional vectors by $R(\phi_0\mathbf{k})$. It is represented by the 2×2 matrix in Eqs. (12.2.1) and (12.2.2). Just as $T(\mathbf{a})$ is the operator in Hilbert space associated with the translation $\mathbf{a}$, let $U[R(\phi_0\mathbf{k})]$ be the operator associated with the rotation $R(\phi_0\mathbf{k})$. In the active transformation picture‡

$$|\psi\rangle \underset{U[R]}{\longrightarrow} |\psi_R\rangle = U[R]|\psi\rangle \tag{12.2.3}$$

The rotated state $|\psi_R\rangle$ must be such that

$$\langle X\rangle_R = \langle X\rangle \cos\phi_0 - \langle Y\rangle \sin\phi_0 \tag{12.2.4a}$$

$$\langle Y\rangle_R = \langle X\rangle \sin\phi_0 + \langle Y\rangle \cos\phi_0 \tag{12.2.4b}$$

$$\langle P_x\rangle_R = \langle P_x\rangle \cos\phi_0 - \langle P_y\rangle \sin\phi_0 \tag{12.2.5a}$$

$$\langle P_y\rangle_R = \langle P_x\rangle \sin\phi_0 + \langle P_y\rangle \cos\phi_0 \tag{12.2.5b}$$

where

$$\langle X\rangle_R = \langle \psi_R|X|\psi_R\rangle$$

and

$$\langle X\rangle = \langle \psi|X|\psi\rangle, \text{ etc.}$$

In analogy with the translation problem, we define the action of $U[R]$ on position eigenkets:

$$U[R]|x, y\rangle = |x\cos\phi_0 - y\sin\phi_0,\ x\sin\phi_0 + y\cos\phi_0\rangle \tag{12.2.6}$$

As in the case of translations, this equation is guided by more than just Eq. (12.2.4), which specifies how $\langle X\rangle$ and $\langle Y\rangle$ transform: in omitting a possible phase factor $g(x, y)$, we are also ensuring that $\langle P_x\rangle$ and $\langle P_y\rangle$ transform as in Eq. (12.2.5).

One way to show this is to keep the phase factor and use Eqs. (12.2.5a) and (12.2.5b) to eliminate it. We will take the simpler route of dropping it from the outset and proving at the end that $\langle P_x\rangle$ and $\langle P_y\rangle$ transform according to Eq. (12.2.5).

Explicit Construction of $U[R]$

Let us now construct $U[R]$. Consider first an infinitesimal rotation $\varepsilon_z\mathbf{k}$. In this case we set

$$U[R(\varepsilon_z\mathbf{k})] = I - \frac{i\varepsilon_z L_z}{\hbar} \tag{12.2.7}$$

‡ We will suppress the rotation angle when it is either irrelevant or obvious.

where L_z, *the generator of infinitesimal rotations*, is to be determined. Starting with Eq. (12.2.6), which becomes to first order in ε_z

$$U[R]|x, y\rangle = |x - y\varepsilon_z, x\varepsilon_z + y\rangle \tag{12.2.8}$$

it can be shown that

$$\langle x, y|I - \frac{i\varepsilon_z L_z}{\hbar}|\psi\rangle = \psi(x + y\varepsilon_z, y - x\varepsilon_z) \tag{12.2.9}$$

*Exercise 12.2.1.** Provide the steps linking Eq. (12.2.8) to Eq. (12.2.9). [Hint: Recall the derivation of Eq. (11.2.8) from Eq. (11.2.6).]

Expanding both sides to order ε_z

$$\langle x, y|I|\psi\rangle - \frac{i\varepsilon_z}{\hbar}\langle x, y|L_z|\psi\rangle = \psi(x, y) + \frac{\partial\psi}{\partial x}(y\varepsilon_z) + \frac{\partial\psi}{\partial y}(-x\varepsilon_z)$$

$$\langle x, y|L_z|\psi\rangle = \left[x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)\right]\psi(x, y)$$

So

$$L_z \xrightarrow[\text{basis}]{\text{coordinate}} x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right) \tag{12.2.10}$$

or in the abstract

$$L_z = XP_y - YP_x \tag{12.2.11}$$

Let us verify that $\langle P_x\rangle$ and $\langle P_y\rangle$ transform according to Eq. (12.2.5). Since

$$L_z \xrightarrow[\text{basis}]{\text{momentum}} \left(i\hbar\frac{\partial}{\partial p_x}p_y - i\hbar\frac{\partial}{\partial p_y}p_x\right) \tag{12.2.12}$$

it is clear that

$$\frac{-i\varepsilon_z}{\hbar}\langle p_x, p_y|L_z|\psi\rangle = \frac{\partial\psi}{\partial p_x}(p_y\varepsilon_z) + \frac{\partial\psi}{\partial p_y}(-p_x\varepsilon_z) \tag{12.2.13}$$

Thus $I - i\varepsilon_z L_z/\hbar$ rotates the momentum space wave function $\psi(p_x, p_y)$ by ε_z in momentum space, and as a result $\langle P_x\rangle$ and $\langle P_y\rangle$ transform just as $\langle X\rangle$ and $\langle Y\rangle$ do, i.e., in accordance with Eq. (12.2.5).

We could have also derived Eq. (12.2.11) for L_z by starting with the passive transformation equations for an infinitesimal rotation:

$$U^\dagger[R]XU[R]=X-Y\varepsilon_z \tag{12.2.14a}$$

$$U^\dagger[R]YU[R]=X\varepsilon_z+Y \tag{12.2.14b}$$

$$U^\dagger[R]P_xU[R]=P_x-P_y\varepsilon_z \tag{12.2.15a}$$

$$U^\dagger[R]P_yU[R]=P_x\varepsilon_z+P_y \tag{12.2.15b}$$

By feeding Eq. (12.2.7) into the above we can deduce that

$$[X, L_z]=-i\hbar Y \tag{12.2.16a}$$

$$[Y, L_z]=i\hbar X \tag{12.2.16b}$$

$$[P_x, L_z]=-i\hbar P_y \tag{12.2.17a}$$

$$[P_y, L_z]=i\hbar P_x \tag{12.2.17b}$$

These commutation relations suffice to fix L_z as XP_y-YP_x.

Exercise 12.2.2. Using these commutation relations (and your keen hindsight) derive $L_z=XP_y-YP_x$. At least show that Eqs. (12.2.16) and (12.2.17) are consistent with $L_z=XP_y-YP_x$.

The finite rotation operator $U[R(\phi_0\mathbf{k})]$ is

$$U[R(\phi_0\mathbf{k})]=\lim_{N\to\infty}\left(I-\frac{i}{\hbar}\frac{\phi_0}{N}L_z\right)^N=\exp(-i\phi_0 L_z/\hbar) \tag{12.2.18}$$

Given

$$L_z \xrightarrow[\text{basis}]{\text{coordinate}} x\left(-i\hbar\frac{\partial}{\partial y}\right)-y\left(-i\hbar\frac{\partial}{\partial x}\right)$$

it is hard to see that $e^{-i\phi_0 L_z/\hbar}$ indeed rotates the state by the angle ϕ_0. For one thing, expanding the exponential is complicated by the fact that $x(-i\hbar\partial/\partial y)$ and $y(-i\hbar\partial/\partial x)$ do not commute. So let us consider an alternative form for L_z. It can be shown, by changing to polar coordinates, that

$$L_z \xrightarrow[\text{basis}]{\text{coordinate}} -i\hbar\frac{\partial}{\partial\phi} \tag{12.2.19}$$

This result can also be derived more directly by starting with the requirement that under an infinitesimal rotation $\varepsilon_z\mathbf{k}$, $\psi(x, y) = \psi(\rho, \phi)$ becomes $\psi(\rho, \phi - \varepsilon_z)$.

*Exercise 12.2.3.** Derive Eq. (12.2.19) by doing a coordinate transformation on Eq. (12.2.10), and also by the direct method mentioned above.

Now it is obvious that

$$\exp(-i\phi_0 L_z/\hbar) \xrightarrow[\text{basis}]{\text{coordinate}} \exp\left(-\phi_0 \frac{\partial}{\partial\phi}\right) \tag{12.2.20}$$

rotates the state by an angle ϕ_0 about the z axis, for

$$\exp(-\phi_0 \partial/\partial\phi)\psi(\rho, \phi) = \psi(\rho, \phi - \phi_0)$$

by Taylor's theorem. It is also obvious that $U[R(\phi_0'\mathbf{k})]U[R(\phi_0\mathbf{k})] = U[R((\phi_0 + \phi_0')\mathbf{k})]$. Thus the rotation operators have the right law of combination.

Physical Interpretation of L_z. We identify L_z as the angular momentum operator, since (i) it is obtained from $l_z = xp_y - yp_x$ by the usual substitution rule (Postulate II), and (ii) it is the generator of infinitesimal rotations about the z axis. L_z is conserved in a problem with rotational invariance: if

$$U^\dagger[R]H(X, P_x;\ Y, P_y)U[R] = H(X, P_x;\ Y, P_y) \tag{12.2.21}$$

it follows (by choosing an infinitesimal rotation) that

$$[L_z, H] = 0 \tag{12.2.22}$$

Since X, P_x, Y, and P_y respond to the rotation as do their classical counterparts [Eqs. (12.2.14) and (12.2.15)] and H is the same function of these operators as $\mathscr{H}$ is of the corresponding classical variables, H is rotationally invariant whenever $\mathscr{H}$ is.

Besides the conservation of $\langle L_z \rangle$, Eq. (12.2.22) also implies the following:

(1) An experiment and its rotated version will give the same result if H is rotationally invariant.
(2) There exists a common basis for L_z and H. (We will spend a lot of time discussing this basis as we go along.)

The Consistency Check. Let us now verify that our rotation and translation operators combine as they should. In contrast to pure translations or rotations, which have a simple law of composition, the combined effect of translations and rotations is nothing very simple. We seem to be facing the prospect of considering every possible combination of rotations and translations, finding their net effect, and then verifying that the product of the corresponding quantum operators equals the operator corresponding to the result of all the transformations. Let us take one small step in this direction, which will prove to be a giant step toward our goal.

Consider the following product of four infinitesimal operations:

$$U[R(-\varepsilon_z\mathbf{k})]T(-\boldsymbol{\varepsilon})U[R(\varepsilon_z\mathbf{k})]T(\boldsymbol{\varepsilon})$$

where $\boldsymbol{\varepsilon}=\varepsilon_x\mathbf{i}+\varepsilon_y\mathbf{j}$. By subjecting a point in the x–y plane to these four operations we find

$$\begin{bmatrix} x \\ y \end{bmatrix} \xrightarrow[\boldsymbol{\varepsilon}]{} \begin{bmatrix} x+\varepsilon_x \\ y+\varepsilon_y \end{bmatrix} \xrightarrow[R(\varepsilon_z\mathbf{k})]{} \begin{bmatrix} (x+\varepsilon_x)-(y+\varepsilon_y)\varepsilon_z \\ (x+\varepsilon_x)\varepsilon_z+(y+\varepsilon_y) \end{bmatrix}$$
$$\xrightarrow[-\boldsymbol{\varepsilon}]{} \begin{bmatrix} x-(y+\varepsilon_y)\varepsilon_z \\ (x+\varepsilon_x)\varepsilon_z+y \end{bmatrix} \xrightarrow[R(-\varepsilon_z\mathbf{k})]{} \begin{bmatrix} x-\varepsilon_y\varepsilon_z \\ y+\varepsilon_x\varepsilon_z \end{bmatrix} \tag{12.2.23}$$

i.e., that the net effect is a translation by $-\varepsilon_y\varepsilon_z\mathbf{i}+\varepsilon_x\varepsilon_z\mathbf{j}$.‡ In the above, we have ignored terms involving ε_x^2, ε_y^2, ε_z^2, and beyond. We do, however, retain the $\varepsilon_x\varepsilon_z$ and $\varepsilon_y\varepsilon_z$ terms since they contain the first germ of noncommutativity. Note that although these are second-order terms, they are fully determined in our approximation, i.e. unaffected by the second-order terms that we have ignored. Equation (12.2.23) imposes the following restriction on the quantum operators:

$$U[R(-\varepsilon_z\mathbf{k})]T(-\boldsymbol{\varepsilon})U[R(\varepsilon_z\mathbf{k})]T(\boldsymbol{\varepsilon})=T(-\varepsilon_y\varepsilon_z\mathbf{i}+\varepsilon_x\varepsilon_z\mathbf{j}) \tag{12.2.24}$$

or

$$\left(I+\frac{i}{\hbar}\varepsilon_z L_z\right)\left[I+\frac{i}{\hbar}(\varepsilon_x P_x+\varepsilon_y P_y)\right]\left(I-\frac{i}{\hbar}\varepsilon_z L_z\right)\left[I-\frac{i}{\hbar}(\varepsilon_x P_x+\varepsilon_y P_y)\right]$$
$$=I+\frac{i}{\hbar}\varepsilon_y\varepsilon_z P_x-\frac{i}{\hbar}\varepsilon_x\varepsilon_z P_y \tag{12.2.25}$$

By matching coefficients (you should do this) we can deduce the following constraints:

$$[P_x, L_z]=-i\hbar P_y$$
$$[P_y, L_z]=i\hbar P_x$$

which are indeed satisfied by the generators [Eq. (12.2.17)].

So our operators have passed this test. But many other tests are possible. How about the coefficients of terms such as $\varepsilon_x\varepsilon_z^2$, or more generally, how about finite

‡ Note that if rotations and translations commuted, the fourfold product would equal I, as can be seen by rearranging the factors so that the two opposite rotations and the two opposite translations cancel each other. The deviation from this result of I is a measure of noncommutativity. Given two symmetry operations that do not commute, the fourfold product provides a nice characterization of their noncommutativity. As we shall see, this characterization is complete.

rotations? How about tests other than the fourfold product, such as one involving 14 translations and six rotations interlaced?

There is a single answer to all these equations: there is no need to conduct any further tests. Although it is beyond the scope of this book to explain why this is so, it is not hard to explain when it is time to stop testing. We can stop the tests when all possible commutators between the generators have been considered. In the present case, given the generators P_x, P_y, and L_z, the possible commutators are $[P_x, L_z]$, $[P_y, L_z]$, and $[P_x, P_y]$. We have just finished testing the first two. Although the third was tested implicitly in the past, let us do it explicitly again. If we convert the law of combination

$$\begin{bmatrix} x \\ y \end{bmatrix} \xrightarrow[\varepsilon_x \mathbf{i}]{} \begin{bmatrix} x+\varepsilon_x \\ y \end{bmatrix} \xrightarrow[\varepsilon_y \mathbf{j}]{} \begin{bmatrix} x+\varepsilon_x \\ y+\varepsilon_y \end{bmatrix} \xrightarrow[-\varepsilon_x \mathbf{i}]{} \begin{bmatrix} x \\ y+\varepsilon_y \end{bmatrix} \xrightarrow[-\varepsilon_y \mathbf{j}]{} \begin{bmatrix} x \\ y \end{bmatrix} \tag{12.2.26}$$

into the operator constraint

$$T(-\varepsilon_y \mathbf{j})T(-\varepsilon_x \mathbf{i})T(\varepsilon_y \mathbf{j})T(\varepsilon_x \mathbf{i})=I \tag{12.2.27}$$

we deduce that

$$[P_x, P_y]=0$$

which of course is satisfied by the generators P_x and P_y. [Although earlier on, we did not consider the fourfold product, Eq. (12.2.27), we did verify that the arguments of the T operators combined according to the laws of vector analysis. Equation (12.2.26) is just a special case which brings out the commutativity of P_x and P_y.]

When I say that there are no further tests to be conducted, I mean the following:

(1) Every consistency test will reduce to just another relation between the *commutators* of the generators.

(2) This relation will be automatically satisfied if the generators pass the tests we have finished conducting. The following exercise should illustrate this point.

*Exercise 12.2.4.** Rederive the equivalent of Eq. (12.2.23) keeping terms of order $\varepsilon_x \varepsilon_z^2$. (You may assume $\varepsilon_y=0$.) Use this information to rewrite Eq. (12.2.24) to order $\varepsilon_x \varepsilon_z^2$. By equating coefficients of this term deduce the constraint

$$-2L_z P_x L_z + P_x L_z^2 + L_z^2 P_x = \hbar^2 P_x$$

This seems to conflict with statement (1) made above, but not really, in view of the identity

$$-2\Lambda\Omega\Lambda + \Omega\Lambda^2 + \Lambda^2\Omega \equiv [\Lambda, [\Lambda, \Omega]]$$

Using the identify, verify that the new constraint coming from the $\varepsilon_x \varepsilon_z^2$ term is satisfied given the commutation relations between P_x, P_y, and L_z.

Vector Operators

We call $\mathbf{V} = V_x\mathbf{i} + V_y\mathbf{j}$ a vector operator if V_x and V_y transform as components of a vector under a passive transformation generated by $U[R]$:

$$U^{\dagger}[R]V_i U[R] = \sum_j R_{ij} V_j$$

where R_{ij} is the 2×2 rotation matrix appearing in Eq. (12.2.1). Examples of $\mathbf{V}$ are $\mathbf{P} = P_x\mathbf{i} + P_y\mathbf{j}$ and $\mathbf{R} = X\mathbf{i} + Y\mathbf{j}$ [see Eqs. (12.2.14) and (12.2.15)]. Note the twofold character of a vector operator such as $\mathbf{P}$: on the one hand, its components are operators in Hilbert space, and on the other, it transforms as a vector in $\mathbb{V}^2(R)$.

The same definition of a vector operator holds in three dimensions as well, with the obvious difference that R_{ij} is a 3×3 matrix.

12.3. The Eigenvalue Problem of L_z

We have seen that in a rotationally invariant problem, H and L_z share a common basis. In order to exploit this fact we must first find the eigenfunctions of L_z. We begin by writing

$$L_z|l_z\rangle = l_z|l_z\rangle \tag{12.3.1}$$

in the coordinate basis:

$$-i\hbar\frac{\partial\psi_{l_z}(\rho,\phi)}{\partial\phi} = l_z\,\psi_{l_z}(\rho,\phi) \tag{12.3.2}$$

The solution to this equation is

$$\psi_{l_z}(\rho,\phi) = R(\rho)\,e^{il_z\phi/\hbar} \tag{12.3.3}$$

where $R(\rho)$ is an arbitrary function normalizable with respect to $\int_0^\infty \rho\,d\rho$.‡ We shall have more to say about $R(\rho)$ in a moment. But first note that l_z seems to be arbitrary: it can even be complex since ϕ goes only from 0 to 2π. (Compare this to the eigenfunctions $e^{ipx/\hbar}$ of linear momentum, where we could argue that p had to be real to keep $|\psi|$ bounded as $|x|\to\infty$.) The fact that complex eigenvalues enter the answer, signals that we are overlooking the Hermiticity constraint. Let us impose it. The condition

$$\langle\psi_1|L_z|\psi_2\rangle = \langle\psi_2|L_z|\psi_1\rangle^* \tag{12.3.4}$$

‡ This will ensure that ψ is normalizable with respect to

$$\iint dx\,dy = \int_0^\infty\int_0^{2\pi}\rho\,d\rho\,d\phi$$

becomes in the coordinate basis

$$\int_0^\infty \int_0^{2\pi} \psi_1^* \left(-i\hbar \frac{\partial}{\partial\phi}\right)\psi_2 \rho \, d\rho \, d\phi = \left[\int_0^\infty \int_0^{2\pi} \psi_2^* \left(-i\hbar \frac{\partial}{\partial\phi}\right)\psi_1 \rho \, d\rho \, d\phi\right]^* \tag{12.3.5}$$

If this requirement is to be satisfied for all ψ_1 and ψ_2, one can show (upon integrating by parts) that it is enough if each ψ obeys

$$\psi(\rho, 0) = \psi(\rho, 2\pi) \tag{12.3.6}$$

If we impose this constraint on the L_z eigenfunctions, Eq. (12.3.3), we find

$$1 = e^{2\pi i l_z/\hbar} \tag{12.3.7}$$

This forces l_z not merely to be real, but also to be an integral multiple of $\hbar$:

$$l_z = m\hbar, \qquad m = 0, \pm 1, \pm 2, \ldots \tag{12.3.8}$$

One calls m the *magnetic quantum number*. Notice that $l_z = m\hbar$ implies that ψ is a single-valued function of ϕ. (However, see Exercise 12.3.2.)

Exercise 12.3.1. Provide the steps linking Eq. (12.3.5) to Eq. (12.3.6).

Exercise 12.3.2. Let us try to deduce the restriction on l_z from another angle. Consider a superposition of two allowed l_z eigenstates:

$$\psi(\rho, \phi) = A(\rho)\, e^{i\phi l_z/\hbar} + B(\rho)\, e^{i\phi l'_z/\hbar}$$

By demanding that upon a 2π rotation we get the same physical state (not necessarily the same state vector), show that $l_z - l'_z = m\hbar$, where m is an integer. By arguing on the grounds of symmetry that the allowed values of l_z must be symmetric about zero, show that these values are *either* $\ldots, 3\hbar/2, \hbar/2, -\hbar/2, -3\hbar/2, \ldots$ or $\ldots, 2\hbar, \hbar, 0, -\hbar, -2\hbar, \ldots$. It is not possible to restrict l_z any further this way. □

Let us now return to the arbitrary function $R(\rho)$ that accompanies the eigenfunctions of L_z. Its presence implies that the eigenvalue $l_z = m\hbar$ does not nail down a unique state in Hilbert space but only a subspace $\mathbb{V}_m$. The dimensionality of this space is clearly infinite, for the space of all normalizable functions R is infinite dimensional. The natural thing to do at this point is to introduce some operator that commutes with L_z and whose simultaneous eigenfunctions with L_z pick out a unique basis in each $\mathbb{V}_m$. We shall see in a moment that the Hamiltonian in a rotationally invariant problem does just this. Physically this means that a state is not uniquely specified by just its angular momentum (which only fixes the angular part of the wave function), but it can be specified by its energy and angular momentum in a rotationally invariant problem.

It proves convenient to introduce the functions

$$\Phi_m(\phi)=(2\pi)^{-1/2}\,e^{im\phi} \qquad (12.3.9)$$

which would have been nondegenerate eigenfunctions of L_z if the ρ coordinate had not existed. These obey the orthonormality condition

$$\int_0^{2\pi}\Phi_m^*(\phi)\Phi_{m'}(\phi)\,d\phi=\delta_{mm'} \qquad (12.3.10)$$

It will be seen that these functions play an important role in problems with rotational invariance.

*Exercise 12.3.3.** A particle is described by a wave function

$$\psi(\rho,\phi)=A\,e^{-\rho^2/2\Delta^2}\cos^2\phi$$

Show (by expressing $\cos^2\phi$ in terms of Φ_m) that

$$P(l_z=0)=2/3$$

$$P(l_z=2\hbar)=1/6$$

$$P(l_z=-2\hbar)=1/6$$

(Hint: Argue that the radial part $e^{-\rho^2/2\Delta^2}$ is irrelevant here.)

*Exercise 12.3.4.** A particle is described by a wave function

$$\psi(\rho,\phi)=A\,e^{-\rho^2/2\Delta^2}\left(\frac{\rho}{\Delta}\cos\phi+\sin\phi\right)$$

Show that

$$P(l_z=\hbar)=P(l_z=-\hbar)=\tfrac{1}{2}$$

Solutions to Rotationally Invariant Problems

Consider a problem where $V(\rho,\phi)=V(\rho)$. The eigenvalue equation for H is

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+V(\rho)\right]\psi_E(\rho,\phi)=E\psi_E(\rho,\phi) \qquad (12.3.11)$$

(We shall use μ to denote the mass, since m will denote the angular momentum quantum number.) Since $[H,L_z]=0$ in this problem, we seek simultaneous eigenfunctions of H and L_z. We have seen that the most general eigenfunction of L_z with eigenvalue $m\hbar$ is of the form

$$\psi_m(\rho, \phi) = R(\rho)(2\pi)^{-1/2}e^{im\phi} = R(\rho)\Phi_m(\phi)$$

where $R(\rho)$ is undetermined. In the present case R is determined by the requirement that

$$\psi_{Em}(\rho, \phi) = R_{Em}(\rho)\Phi_m(\phi) \tag{12.3.12}$$

be an eigenfunction of H as well, with eigenvalue E, i.e., that ψ_{Em} satisfy Eq. (12.3.11). Feeding the above form into Eq. (12.3.11), we get the *radial equation* that determines $R_{Em}(\rho)$ and the allowed values for E:

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{m^2}{\rho^2}\right) + V(\rho)\right]R_{Em}(\rho) = ER_{Em}(\rho) \tag{12.3.13}$$

As we change the potential, only the *radial part* of the wave function, R, changes; the angular part Φ_m is unchanged. Thus the functions $\Phi_m(\phi)$, which were obtained by pretending ρ does not exist, provide the angular part of the wave function in the eigenvalue problem of any rotationally invariant Hamiltonian.

*Exercise 12.3.5**. Note that the angular momentum seems to generate a repulsive potential in Eq. (12.3.13). Calculate its gradient and identify it as the centrifugal force.

Exercise 12.3.6. Consider a particle of mass μ constrained to move on a circle of radius a. Show that $H = L_z^2/2\mu a^2$. Solve the eigenvalue problem of H and interpret the degeneracy.

Exercise 12.3.7. (The Isotropic Oscillator).* Consider the Hamiltonian

$$H = \frac{P_x^2 + P_y^2}{2\mu} + \frac{1}{2}\mu\omega^2(X^2 + Y^2)$$

(1) Convince yourself $[H, L_z] = 0$ and reduce the eigenvalue problem of H to the radial differential equation for $R_{Em}(\rho)$.

(2) Examine the equation as $\rho \to 0$ and show that

$$R_{Em}(\rho) \underset{\rho\to 0}{\longrightarrow} \rho^{|m|}$$

(3) Show likewise that up to powers of ρ

$$R_{Em}(\rho) \underset{\rho\to\infty}{\longrightarrow} e^{-\mu\omega\rho^2/2\hbar}$$

So assume that $R_{Em}(\rho) = \rho^{|m|}\, e^{-\mu\omega\rho^2/2\hbar}U_{Em}(\rho)$.

(4) Switch to dimensionless variables $\varepsilon = E/\hbar\omega$, $y = (\mu\omega/\hbar)^{1/2}\rho$.

(5) Convert the equation for R into an equation for U. (I suggest proceeding in two stages: $R = y^{|m|}f, f = e^{-y^2/2}U$.) You should end up with

$$U'' + \left[\left(\frac{2|m|+1}{y}\right) - 2y\right]U' + (2\varepsilon - 2|m| - 2)U = 0$$

(6) Argue that a power series for U of the form

$$U(y) = \sum_{r=0}^{\infty} C_r y^r$$

will lead to a *two-term* recursion relation.

(7) Find the relation between C_{r+2} and C_r. Argue that the series must terminate at some finite r if the $y \to \infty$ behavior of the solution is to be acceptable. Show $\varepsilon = r + |m| + 1$ leads to termination after r terms. Now argue that r is necessarily even—i.e., $r = 2k$. (Show that if r is odd, the behavior of R as $\rho \to 0$ is not $\rho^{|m|}$.) So finally you must end up with

$$E = (2k + |m| + 1)\hbar\omega, \qquad k = 0, 1, 2, \ldots$$

Define $n = 2k + |m|$, so that

$$E_n = (n+1)\hbar\omega$$

(8) For a given n, what are the allowed values of $|m|$? Given this information show that for a given n, the degeneracy is $n+1$. Compare this to what you found in Cartesian coordinates (Exercise 10.2.2).

(9) Write down all the normalized eigenfunctions corresponding to $n = 0, 1$.

(10) Argue that the $n = 0$ function *must* equal the corresponding one found in Cartesian coordinates. Show that the two $n = 2$ solutions are linear combinations of their counterparts in Cartesian coordinates. Verify that the parity of the states is $(-1)^n$ as you found in Cartesian coordinates.

*Exercise 12.3.8.** Consider a particle of charge q in a vector potential

$$\mathbf{A} = \frac{B}{2}(-y\mathbf{i} + x\mathbf{j})$$

(1) Show that the magnetic field is $\mathbf{B} = B\mathbf{k}$.

(2) Show that a classical particle in this potential will move in circles at an angular frequency $\omega_0 = qB/\mu c$.

(3) Consider the Hamiltonian for the corresponding quantum problem:

$$H = \frac{[P_x + qYB/2c]^2}{2\mu} + \frac{[P_y - qXB/2c]^2}{2\mu}$$

Show that $Q = (cP_x + qYB/2)/qB$ and $P = (P_y - qXB/2c)$ are canonical. Write H in terms of P and Q and show that allowed levels are $E = (n + 1/2)\hbar\omega_0$.

(4) Expand H out in terms of the original variables and show

$$H = H\left(\frac{\omega_0}{2}, \mu\right) - \frac{\omega_0}{2} L_z$$

where $H(\omega_0/2, \mu)$ is the Hamiltonian for an isotropic two-dimensional harmonic oscillator of mass μ and frequency $\omega_0/2$. Argue that the same basis that diagonalized $H(\omega_0/2, \mu)$ will diagonalize H. By thinking in terms of this basis, show that the allowed levels for H are $E = (k + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2})\hbar\omega_0$, where k is any integer and m is the angular momentum. Convince yourself that you get the same levels from this formula as from the earlier one $[E = (n + 1/2)\hbar\omega_0]$. We shall return to this problem in Chapter 21.

12.4. Angular Momentum in Three Dimensions

It is evident that as we pass from two to three dimensions, the operator L_z picks up two companions L_x and L_y which generate infinitesimal rotations about the x and y axes, respectively. So we have

$$L_x = YP_z - ZP_y \tag{12.4.1a}$$

$$L_y = ZP_x - XP_z \tag{12.4.1b}$$

$$L_z = XP_y - YP_x \tag{12.4.1c}$$

As usual, we subject these to the consistency test. It may be verified, (Exercise 12.4.2), that if we take a point in three-dimensional space and subject it to the following rotations: $R(\varepsilon_x \mathbf{i})$, $R(\varepsilon_y \mathbf{j})$, $R(-\varepsilon_x \mathbf{i})$ and lastly $R(-\varepsilon_y \mathbf{j})$, it ends up rotated by $-\varepsilon_x\varepsilon_y \mathbf{k}$. In other words

$$R(-\varepsilon_y \mathbf{j})R(-\varepsilon_x \mathbf{i})R(\varepsilon_y \mathbf{j})R(\varepsilon_x \mathbf{i}) = R(-\varepsilon_x\varepsilon_y \mathbf{k}) \tag{12.4.2}$$

It follows that the quantum operators $U[R]$ must satisfy

$$U[R(-\varepsilon_y \mathbf{j})]U[R(-\varepsilon_x \mathbf{i})]U[R(\varepsilon_y \mathbf{j})]U[R(\varepsilon_x \mathbf{i})] = U[R(-\varepsilon_x\varepsilon_y \mathbf{k})] \tag{12.4.3}$$

If we write each U to order ε and match coefficients of $\varepsilon_x\varepsilon_y$, we will find

$$[L_x, L_y] = i\hbar L_z \tag{12.4.4a}$$

By considering two similar tests involving $\varepsilon_y\varepsilon_z$ and $\varepsilon_z\varepsilon_x$, we can deduce the constraints

$$[L_y, L_z] = i\hbar L_x \tag{12.4.4b}$$

$$[L_z, L_x] = i\hbar L_y \tag{12.4.4c}$$

You may verify that the operators in Eq. (12.4.1) satisfy these constraints. So they are guaranteed to generate finite rotation operators that obey the right laws of combination.

The three relations above may be expressed compactly as one vector equation

$$\mathbf{L}\times\mathbf{L}=i\hbar\mathbf{L} \tag{12.4.5}$$

Yet another way to write the commutation relations is

$$[L_i, L_j]=i\hbar\sum_{k=1}^{3}\varepsilon_{ijk}L_k \tag{12.4.6}$$

In this equation, i and j run from 1 to 3, L_1, L_2, and L_3 stand for L_x, L_y, and L_z, respectively,‡ and ε_{ijk} are the components of an antisymmetric tensor of rank 3, with the following properties:

(1) They change sign when any two indices are exchanged. Consequently no two indices can be equal.
(2) $\varepsilon_{123}=1$.

This fixes all other components. For example,

$$\varepsilon_{132}=-1, \qquad \varepsilon_{312}=(-1)(-1)=+1 \tag{12.4.7}$$

and so on. In short, ε_{ijk} is $+1$ for any cyclic permutation of the indices in ε_{123} and -1 for the others. (The relation

$$\mathbf{c}=\mathbf{a}\times\mathbf{b} \tag{12.4.8}$$

between three vectors from $\mathbb{V}^3(R)$ may be written in component form as

$$c_i=\sum_{j=1}^{3}\sum_{k=1}^{3}\varepsilon_{ijk}a_jb_k \tag{12.4.9}$$

Of course $\mathbf{a}\times\mathbf{a}$ is zero if $\mathbf{a}$ is a vector whose components are numbers, but not zero if it is an operator such as $\mathbf{L}$.)

*Exercise 12.4.1.** (1) Verify that Eqs. (12.4.9) and Eq. (12.4.8) are equivalent, given the definition of ε_{ijk}.

(2) Let U_1, U_2, and U_3 be three energy eigenfunctions of a single particle in some potential. Construct the wave function $\psi_A(x_1, x_2, x_3)$ of three fermions in this potential, one of which is in U_1, one in U_2, and one in U_3, using the ε_{ijk} tensor.

*Exercise 12.4.2.** (1) Verify Eq. (12.4.2) by first constructing the 3×3 matrices corresponding to $R(\varepsilon_x\mathbf{i})$ and $R(\varepsilon_y\mathbf{j})$, to order ε.

(2) Provide the steps connecting Eqs. (12.4.3) and (12.4.4a).

‡ We will frequently let the indices run over 1, 2, and 3 instead of x, y, and z.

(3) Verify that L_x and L_y defined in Eq. (12.4.1) satisfy Eq. (12.4.4a). The proof for other commutators follows by cyclic permutation.

We next define the total angular momentum operator squared

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{12.4.10}$$

It may be verified (by you) that

$$[L^2, L_i] = 0, \qquad i = x, y, \text{ or } z \tag{12.4.11}$$

Finite Rotation Operators. Rotations about a given axis commute. So a finite rotation may be viewed as a sequence of infinitesimal rotations about the same axis. What is the operator that rotates by angle $\boldsymbol{\theta}$, i.e., by an amount θ about an axis parallel to $\hat{\theta}$? If $\boldsymbol{\theta} = \theta_x \mathbf{i}$, then clearly

$$U[R(\theta_x \mathbf{i})] = e^{-i\theta_x L_x/\hbar}$$

The same goes for $\boldsymbol{\theta}$ along the unit vectors $\mathbf{j}$ and $\mathbf{k}$. What if $\boldsymbol{\theta}$ has some arbitrary direction? We conjecture that $L_{\hat{\theta}} \equiv \hat{\theta} \cdot \mathbf{L}$ (where $\hat{\theta} = \boldsymbol{\theta}/\theta$) is the generator of infinitesimal rotations about that axis and that

$$\begin{aligned} U[R(\boldsymbol{\theta})] &= \lim_{N\to\infty} \left(I - \frac{i}{\hbar}\frac{\theta}{N}\hat{\theta}\cdot\mathbf{L}\right)^N = e^{-i\theta\hat{\theta}\cdot\mathbf{L}/\hbar} \\ &= e^{-\boldsymbol{\theta}\cdot\mathbf{L}/\hbar} \end{aligned} \tag{12.4.12}$$

Our conjecture is verified in the following exercise.

*Exercise 12.4.3.** We would like to show that $\hat{\theta}\cdot\mathbf{L}$ generates rotations about the axis parallel to $\hat{\theta}$. Let $\delta\boldsymbol{\theta}$ be an infinitesimal rotation parallel to $\boldsymbol{\theta}$.

(1) Show that when a vector $\mathbf{r}$ is rotated by an angle $\delta\boldsymbol{\theta}$, it changes to $\mathbf{r} + \delta\boldsymbol{\theta} \times \mathbf{r}$. (It might help to start with $\mathbf{r} \perp \delta\boldsymbol{\theta}$ and then generalize.)

(2) We therefore demand that (to first order, as usual)

$$\psi(\mathbf{r}) \xrightarrow[U[R(\delta\boldsymbol{\theta})]]{} \psi(\mathbf{r} - \delta\boldsymbol{\theta}\times\mathbf{r}) = \psi(\mathbf{r}) - (\delta\boldsymbol{\theta}\times\mathbf{r})\cdot\boldsymbol{\nabla}\psi$$

Comparing to $U[R(\delta\boldsymbol{\theta})] = I - (i\,\delta\theta/\hbar)L_{\hat{\theta}}$, show that $L_{\hat{\theta}} = \hat{\theta}\cdot\mathbf{L}$.

*Exercise 12.4.4.** Recall that $\mathbf{V}$ is a vector operator if its components V_i transform as

$$U^\dagger[R]V_i U[R] = \sum_j R_{ij} V_j \tag{12.4.13}$$

(1) For an infinitesimal rotation $\delta\boldsymbol{\theta}$, show, on the basis of the previous exercise, that

$$\sum_j R_{ij} V_j = V_i + (\delta\boldsymbol{\theta} \times \mathbf{V})_i = V_i + \sum_j \sum_k \varepsilon_{ijk} (\delta\theta)_j V_k$$

(2) Feed in $U[R] = 1 - (i/\hbar)\delta\boldsymbol{\theta}\cdot\mathbf{L}$ into the left-hand side of Eq. (12.4.13) and deduce that

$$[V_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} V_k \tag{12.4.14}$$

This is as good a definition of a vector operator as Eq. (12.4.13). By setting $\mathbf{V} = \mathbf{L}$, we can obtain the commutation rules among the L's.

If the Hamiltonian is invariant under arbitrary rotations,

$$U^\dagger[R] H U[R] = H \tag{12.4.15}$$

it follows (upon considering infinitesimal rotations around the x, y, and z axes) that

$$[H, L_i] = 0 \tag{12.4.16}$$

and from it

$$[H, L^2] = 0 \tag{12.4.17}$$

Thus L^2 and all three components of $\mathbf{L}$ are conserved. It does not, however, follow that there exists a basis common to H and all three L's. This is because the L's do not commute with each other. So the best one can do is find a basis common to H, L^2, and one of the L's, usually chosen to be L_z.

We now examine the eigenvalue problem of the commuting operators L^2 and L_z. When this is solved, we will turn to the eigenvalue problem of H, L^2, and L_z.

12.5. The Eigenvalue Problem of L^2 and L_z

There is a close parallel between our approach to this problem and that of the harmonic oscillator. Recall that in that case we (1) solved the eigenvalue problem of H in the coordinate basis; (2) solved the problem in the energy basis directly, using the a and $a^\dagger$ operators, the commutation rules, and the positivity of H; (3) obtained the coordinate wave function $\psi_n(y)$ given the results of part (2), by the following trick. We wrote

$$a|0\rangle = 0$$

in the coordinate basis as

$$\left(y + \frac{\partial}{\partial y}\right)\psi_0(y) = 0$$

which immediately gave us $\psi_0(y) \sim e^{-y^2/2}$, up to a normalization that could be easily determined.

Given the normalized eigenfunction $\psi_0(y)$, we got $\psi_n(y)$ by the application of the (differential) operator $(a^\dagger)^n/(n!)^{1/2} \to (y - \partial/\partial y)^n/(2^n n!)^{1/2}$.

In the present case we omit part (1), which involves just one more bout with differential equations and is not particularly enlightening.

Let us now consider part (2). It too has many similarities with part (2) of the oscillator problem.‡ We begin by assuming that there exists a basis $|\alpha, \beta\rangle$ common to L^2 and L_z:

$$L^2|\alpha\beta\rangle = \alpha|\alpha\beta\rangle \tag{12.5.1}$$

$$L_z|\alpha\beta\rangle = \beta|\alpha\beta\rangle \tag{12.5.2}$$

We now define *raising and lower operators*

$$L_\pm = L_x \pm iL_y \tag{12.5.3}$$

which satisfy

$$[L_z, L_\pm] = \pm\hbar L_\pm \tag{12.5.4}$$

and of course (since L^2 commutes with L_x and L_y)

$$[L^2, L_\pm] = 0 \tag{12.5.5}$$

Equations (12.5.4) and (12.5.5) imply that $L_\pm$ raise/lower the eigenvalue of L_z by $\hbar$, while leaving the eigenvalue of L^2 alone. For example,

$$\begin{aligned} L_z(L_+|\alpha\beta\rangle) &= (L_+L_z + \hbar L_+)|\alpha\beta\rangle \\ &= (L_+\beta + \hbar L_+)|\alpha\beta\rangle \\ &= (\beta + \hbar)(L_+|\alpha\beta\rangle) \end{aligned} \tag{12.5.6}$$

and

$$L^2L_+|\alpha\beta\rangle = L_+L^2|\alpha\beta\rangle = \alpha L_+|\alpha\beta\rangle \tag{12.5.7}$$

From Eqs. (12.5.6) and (12.5.7) it is clear that $L_+|\alpha\beta\rangle$ is proportional to the normalized eigenket $|\alpha, \beta+\hbar\rangle$:

$$L_+|\alpha\beta\rangle = C_+(\alpha, \beta)|\alpha, \beta+\hbar\rangle \tag{12.5.8a}$$

‡ If you have forgotten the latter, you are urged to refresh your memory at this point.

It can similarly be shown that

$$L_-|\alpha\beta\rangle = C_-(\alpha, \beta)|\alpha, \beta - \hbar\rangle \tag{12.5.8b}$$

The existence of $L_\pm$ implies that given an eigenstate $|\alpha\beta\rangle$ there also exist eigenstates $|\alpha, \beta+\hbar\rangle$, $|\alpha, \beta+2\hbar\rangle, \ldots$; and $|\alpha, \beta-\hbar\rangle$, $|\alpha, \beta-2\hbar\rangle, \ldots$. This clearly signals trouble, for classical intuition tells us that the z component of angular momentum cannot take arbitrarily large positive or negative values for a given value of the square of the total angular momentum; in fact classically $|l_z| \le (l^2)^{1/2}$.

Quantum mechanically we have

$$\langle\alpha\beta|L^2 - L_z^2|\alpha\beta\rangle = \langle\alpha\beta|L_x^2 + L_y^2|\alpha\beta\rangle \tag{12.5.9}$$

which implies

$$\alpha - \beta^2 \ge 0$$

(since $L_x^2 + L_y^2$ is positive definite) or

$$\alpha \ge \beta^2 \tag{12.5.10}$$

Since β^2 is bounded by α, it follows that there must exist a state $|\alpha\beta_{\text{max}}\rangle$ such that it cannot be raised:

$$L_+|\alpha\beta_{\text{max}}\rangle = 0 \tag{12.5.11}$$

Operating with L_- and using $L_-L_+ = L^2 - L_z^2 - \hbar L_z$, we get

$$(L^2 - L_z^2 - \hbar L_z)|\alpha\beta_{\text{max}}\rangle = 0$$

$$(\alpha - \beta_{\text{max}}^2 - \hbar\beta_{\text{max}})|\alpha\beta_{\text{max}}\rangle = 0$$

$$\alpha = \beta_{\text{max}}(\beta_{\text{max}} + \hbar) \tag{12.5.12}$$

Starting with $|\alpha\beta_{\text{max}}\rangle$ let us operate k times with L_-, till we reach a state $|\alpha\beta_{\text{min}}\rangle$ that cannot be lowered further without violating the inequality (12.5.10):

$$L_-|\alpha\beta_{\text{min}}\rangle = 0$$

$$L_+L_-|\alpha\beta_{\text{min}}\rangle = 0$$

$$(L^2 - L_z^2 + \hbar L_z)|\alpha\beta_{\text{min}}\rangle = 0$$

$$\alpha = \beta_{\text{min}}(\beta_{\text{min}} - \hbar) \tag{12.5.13}$$

A comparison of Eqs. (12.5.12) and (12.5.13) shows (as is to be expected)

$$\beta_{\text{min}} = -\beta_{\text{max}} \tag{12.5.14}$$

Table 12.1. Some Low-Angular-Momentum States

(Angular momentum) $k/2$	β_{max}	α	$\lvert\alpha\beta\rangle$
0	0	0	$\lvert 0, 0\rangle$
1/2	$\hbar/2$	$(1/2)(3/2)\hbar^2$	$\lvert(3/4)\hbar^2, \hbar/2\rangle$ $\lvert(3/4)\hbar^2, -\hbar/2\rangle$
1	$\hbar$	$(1)(2)\hbar^2$	$\lvert 2\hbar^2, \hbar\rangle$ $\lvert 2\hbar^2, 0\rangle$ $\lvert 2\hbar^2, -\hbar\rangle$
3/2			
⋮	⋮	⋮	⋮

Since we got to $|\alpha\beta_{min}\rangle$ from $|\alpha\beta_{max}\rangle$ in k steps of $\hbar$ each, it follows that

$$\beta_{max}-\beta_{min}=2\beta_{max}=\hbar k$$

$$\beta_{max}=\frac{\hbar k}{2}, \qquad k=0, 1, 2, \ldots \tag{12.5.15a}$$

$$\alpha=(\beta_{max})(\beta_{max}+\hbar)=\hbar^2\left(\frac{k}{2}\right)\left(\frac{k}{2}+1\right) \tag{12.5.15b}$$

We shall refer to $(k/2)=(\beta_{max}/\hbar)$ as the *angular momentum of the state*. Notice that unlike in classical physics, β_{max}^2 is less than α, the square of the magnitude of angular momentum, except when $\alpha=\beta_{max}=0$, i.e., in a state of zero angular momentum.

Let us now take a look at a few of the low-angular-momentum states listed in Table 12.1.

At this point the astute reader raises the following objection.

A.R.: I am disturbed by your results for odd k. You seem to find that L_z can have half-integral eigenvalues (in units of $\hbar$). But you just convinced us in Section 12.3 that L_z has only integral eigenvalues m (in units of $\hbar$). Where did you go wrong?

R.S.: Nowhere, but your point is well taken. The extra (half-integral) eigenvalues arise because we have solved a more general problem than that of L_x, L_y, L_z, and L^2 (although we didn't intend to). Notice that nowhere in the derivation did we use the explicit expressions for the L's [Eq. (12.4.1)] and in particular $L_z\to -i\hbar\partial/\partial\phi$. (Had we done so, we would have gotten only integral eigenvalues as you expect.) We relied instead on just the commutation relations, $\mathbf{L}\times\mathbf{L}=i\hbar\mathbf{L}$. Now, these commutation relations reflect the law of combinations of infinitesimal rotations in three dimensions and must be satisfied by the three generators of rotations whatever the nature of the wave functions they rotate. We have so far considered just scalar wave functions $\psi(x, y, z)$, which assign a complex number (scalar) to each point. Now, there can be particles in nature for which the wave function is more complicated, say a vector field $\boldsymbol{\Psi}(x, y, z)=\psi_x(x, y, z)\mathbf{i}+\psi_y(x, y, z)\mathbf{j}+\psi_z(x, y, x)\mathbf{k}$. The response of such a wave function to rotations is more involved. Whereas in the scalar case the effect of rotation by $\delta\boldsymbol{\theta}$ is to take the number assigned to each point (x, y, z)

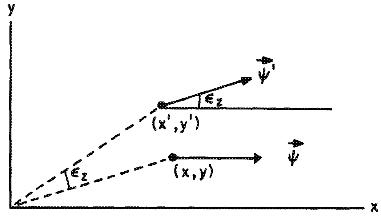


Figure 12.1. The effect of the infinitesimal rotations by ε_z on a vector ψ in two dimensions is to (1) first reassign it to the rotated point (x', y') (2) and then rotate the vector itself by the infinitesimal angle. The differential operator L_z does the first part while a 2×2 spin matrix S_z does the second.

and reassign it to the rotated point (x', y', z'), in the vector case the vector at (x, y, z) (i) must itself be rotated by $\delta\boldsymbol{\theta}$ and (ii) then reassigned to (x', y', z'). (A simple example from two dimensions is given in Fig. 12.1.) The differential operators L_x, L_y, and L_z will only do part (ii) but not part (i), which has to be done by 3×3 matrices S_x, S_y, and S_z which shuffle the components ψ_x, ψ_y, ψ_z of $\boldsymbol{\Psi}$. In such cases, the generators of infinitesimal rotations will be of the form

$$J_i = L_i + S_i$$

where L_i does part (2) and S_i does part (1) (see Exercise 12.5.1 for a concrete example). One refers to L_i as the *orbital angular* momentum, S_i as the *spin angular momentum* (or simply spin), and J_i as the *total angular momentum*. We do not yet know what J_i or S_i look like in these general cases, but we do know this: the J_i's must obey the same commutation rules as the L_i's, for the commutation rules reflect the law of combination of rotations and must be obeyed by any triplet of generators (the consistency condition), whatever be the nature of wave function they rotate. So in general we have

$$\mathbf{J}\times\mathbf{J} = i\hbar\mathbf{J} \tag{12.5.16}$$

with $\mathbf{L}$ as a special case when the wave function is a scalar. So our result, which followed from just the commutation relations, applies to the problem of arbitrary $\mathbf{J}$ and not just $\mathbf{L}$. Thus the answer to the question raised earlier is that unlike L_z, J_z is not restricted to have integral eigenvalues. But our analysis tells us, who know very little about spin, that S_z can have only integral or half-integral eigenvalues if the commutation relations are to be satisfied. Of course, our analysis doesn't imply that there *must* exist particles with spin integral or half integral—but merely reveals the possible variety in wave functions. But the old maxim—if something can happen, it will—is true here and nature does provide us with particles that possess spin—i.e., particles whose wave functions are more complicated than scalars. We will study them in Chapter 14 on spin.

*Exercise 12.5.1.** Consider a vector field $\boldsymbol{\Psi}(x, y)$ in two dimensions. From Fig. 12.1 it follows that under an infinitesimal rotation $\varepsilon_z\mathbf{k}$,

$$\psi_x \to \psi'_x(x, y) = \psi_x(x + y\varepsilon_z, y - x\varepsilon_z) - \psi_y(x + y\varepsilon_z, y - x\varepsilon_z)\varepsilon_z$$

$$\psi_y \to \psi'_y(x, y) = \psi_x(x + y\varepsilon_z, y - x\varepsilon_z)\varepsilon_z + \psi_y(x + y\varepsilon_z, y - x\varepsilon_z)$$

Show that (to order ε_z)

$$\begin{bmatrix}\psi'_x\\ \psi'_y\end{bmatrix}=\left(\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}-\frac{i\varepsilon_z}{\hbar}\begin{bmatrix}L_z & 0\\ 0 & L_z\end{bmatrix}-\frac{i\varepsilon_z}{\hbar}\begin{bmatrix}0 & -i\hbar\\ i\hbar & 0\end{bmatrix}\right)\begin{bmatrix}\psi_x\\ \psi_y\end{bmatrix}$$

so that

$$\begin{aligned}J_z&=L_z^{(1)}\otimes I^{(2)}+I^{(1)}\otimes S_z^{(2)}\\ &=L_z+S_z\end{aligned}$$

where $I^{(2)}$ is a 2×2 identity matrix with respect to the vector components, $I^{(1)}$ is the identity operator with respect to the argument (x, y) of $\Psi(x, y)$. This example only illustrates the fact that $J_z=L_z+S_z$ if the wave function is not a scalar. An example of half-integral eigenvalues will be provided when we consider spin in a later chapter. (In the present example, S_z has eigenvalues $\pm\hbar$.)

Let us return to our main discussion. To emphasize the generality of the results we have found, we will express them in terms of J's rather than L's and also switch to a more common notation. Here is a summary of what we have found. The eigenvectors of the operators J^2 and J_z are given by

$$J^2|jm\rangle=j(j+1)\hbar^2|jm\rangle, \qquad j=0, 1/2, 1, 3/2, \ldots \tag{12.5.17a}$$

$$J_z|jm\rangle=m\hbar|jm\rangle, \qquad m=j, j-1, j-2, \ldots, -j \tag{12.5.17b}$$

We shall call j the angular momentum of the state. Note that in the above m can be an integer or half-integer depending on j.

The results for the restricted problem $\mathbf{J}=\mathbf{L}$ that we originally set out to solve are contained in Eq. (12.5.17): we simply ignore the states with half-integral m and j. To remind us in these cases that we are dealing with $\mathbf{J}=\mathbf{L}$, we will denote these states by $|lm\rangle$. They obey

$$L^2|lm\rangle=l(l+1)\hbar^2|lm\rangle, \qquad l=0, 1, 2, \ldots \tag{12.5.18a}$$

$$L_z|lm\rangle=m\hbar|lm\rangle, \qquad m=l, l-1, \ldots, -l \tag{12.5.18b}$$

Our problem has not been fully solved: we have only found the eigenvalues—the eigenvectors aren't fully determined yet. (As in the oscillator problem, finding the eigenvectors means finding the matrices corresponding to the basic operators whose commutation relations are given.) Let us continue our analysis in terms of the J's. If we rewrite Eq. (12.5.8) in terms of $J_\pm$, j, and m (instead of $L_\pm$, α, and β), we get

$$J_\pm|jm\rangle=C_\pm(j, m)|j, m\pm 1\rangle \tag{12.5.19}$$

where $C_\pm(j, m)$ are yet to be determined. We will determine them now.

If we take the adjoint of

$$J_+|jm\rangle = C_+(j, m)|j, m+1\rangle$$

we get

$$\langle jm|J_- = C_+^*(j, m)\langle j, m+1|$$

Equating the inner product of the objects on the left-hand side to the product of the objects on the right-hand side, we obtain

$$\begin{aligned}\langle jm|J_-J_+|jm\rangle &= |C_+(j, m)|^2\langle j, m+1|j, m+1\rangle \\ &= |C_+(j, m)|^2 \\ \langle jm|J^2 - J_z^2 - \hbar J_z|jm\rangle &= |C_+(j, m)|^2\end{aligned}$$

or

$$\begin{aligned}|C_+(j, m)|^2 &= j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \\ &= \hbar^2(j-m)(j+m+1)\end{aligned}$$

or‡

$$C_+(j, m) = \hbar[(j-m)(j+m+1)]^{1/2}$$

It can likewise be shown that

$$C_-(j, m) = \hbar[(j+m)(j-m+1)]^{1/2}$$

so that finally

$$J_\pm|jm\rangle = \hbar[(j\mp m)(j\pm m+1)]^{1/2}|j, m\pm 1\rangle \tag{12.5.20}$$

Notice that when $J_\pm$ act on $|j, \pm j\rangle$ they kill the state, so that each family with a given angular momentum j has only $2j+1$ states with eigenvalues $j\hbar$, $(j-1)\hbar, \ldots, -(j\hbar)$ for J_z.

Equation (12.5.20) brings us to the end of our calculation, for we can write down the matrix elements of J_x and J_y in this basis:

$$\begin{aligned}\langle j'm'|J_x|jm\rangle &= \langle j'm'|\frac{J_+ + J_-}{2}|jm\rangle \\ &= \frac{\hbar}{2}\{\delta_{jj'}\delta_{m',m+1}[(j-m)(j+m+1)]^{1/2} + \delta_{jj'}\delta_{m',m-1} \\ &\quad \times [(j+m)(j-m+1)]^{1/2}\}\end{aligned} \tag{12.5.21a}$$

‡ There can be an overall phase factor in front of C_+. We choose it to be unity according to standard convention.

$$\langle j'm'|J_y|jm\rangle = \langle j'm'|\frac{J_+ - J_-}{2i}|jm\rangle$$

$$= \frac{\hbar}{2i}\{\delta_{jj'}\delta_{m',m+1}[(j-m)(j+m+1)]^{1/2} - \delta_{jj'}\delta_{m',m-1} \times [(j+m)(j-m+1)]^{1/2}\} \quad (12.5.21\text{b})$$

Using these (or our mnemonic based on images) we can write down the matrices corresponding to J^2, J_z, J_x, and J_y in the $|jm\rangle$ basis‡:

$$J^2 \rightarrow \begin{array}{c|ccccccc} j'm' \backslash jm & (0,0) & (\frac{1}{2},\frac{1}{2}) & (\frac{1}{2},-\frac{1}{2}) & (1,1) & (1,0) & (1,-1) & \cdots \\ \hline (0,0) & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ (\frac{1}{2},\frac{1}{2}) & 0 & \frac{3}{4}\hbar^2 & 0 & 0 & 0 & 0 & \\ (\frac{1}{2},-\frac{1}{2}) & 0 & 0 & \frac{3}{4}\hbar^2 & 0 & 0 & 0 & \\ (1,1) & 0 & 0 & 0 & 2\hbar^2 & 0 & 0 & \\ (1,0) & 0 & 0 & 0 & 0 & 2\hbar^2 & 0 & \\ (1,-1) & 0 & 0 & 0 & 0 & 0 & 2\hbar^2 & \\ & \vdots & & & & & & \ddots \end{array} \quad (12.5.22)$$

J_z is also diagonal with elements $m\hbar$.

$$J_x \rightarrow \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \hbar/2 & 0 & 0 & 0 & \\ 0 & \hbar/2 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \\ 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \hbar/2^{1/2} & \\ 0 & 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \\ \vdots & & & & & & \ddots \end{bmatrix} \quad (12.5.23)$$

$$J_y \rightarrow \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -i\hbar/2 & 0 & 0 & 0 & \\ 0 & i\hbar/2 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & -i\hbar/2^{1/2} & 0 & \\ 0 & 0 & 0 & i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} & \\ 0 & 0 & 0 & 0 & i\hbar/2^{1/2} & 0 & \\ \vdots & & & & & & \ddots \end{bmatrix} \quad (12.5.24)$$

Notice that although J_x and J_y are not diagonal in the $|jm\rangle$ basis, they are *block diagonal*: they have no matrix elements between one value of j and another. This is

‡ The quantum numbers j and m do not fully label a state; a state is labeled by $|\alpha jm\rangle$, where α represents the remaining labels. In what follows, we suppress α but assume it is the same throughout.

because $J_\pm$ (out of which they are built) do not change j when they act on $|jm\rangle$. Since the J's are all block diagonal, the blocks do not mix when we multiply them. *In particular when we consider a commutation relation such as* $[J_x, J_y]=i\hbar J_z$, *it will be satisfied within each block.* If we denote the $(2j+1)\times(2j+1)$ block in J_i, corresponding to a certain j, by $J_i^{(j)}$, then we have

$$[J_x^{(j)}, J_y^{(j)}]=i\hbar J_z^{(j)}, \qquad j=0, \tfrac{1}{2}, 1, \ldots \tag{12.5.25}$$

Exercise 12.5.2. (1) Verify that the 2×2 matrices $J_x^{(1/2)}$, $J_y^{(1/2)}$, and $J_z^{(1/2)}$ obey the commutation rule $[J_x^{(1/2)}, J_y^{(1/2)}]=i\hbar J_z^{(1/2)}$.

(2) Do the same for the 3×3 matrices $J_i^{(1)}$.

(3) Construct the 4×4 matrices and verify that

$$[J_x^{(3/2)}, J_y^{(3/2)}]=i\hbar J_z^{(3/2)}$$

*Exercise 12.5.3.** (1) Show that $\langle J_x\rangle=\langle J_y\rangle=0$ in a state $|jm\rangle$.

(2) Show that in these states

$$\langle J_x^2\rangle=\langle J_y^2\rangle=\tfrac{1}{2}\hbar^2[j(j+1)-m^2]$$

(use symmetry arguments to relate $\langle J_x^2\rangle$ to $\langle J_y^2\rangle$).

(3) Check that $\Delta J_x \cdot \Delta J_y$ from part (2) satisfies the inequality imposed by the uncertainty principle [Eq. (9.2.9)].

(4) Show that the uncertainty bound is saturated in the state $|j, \pm j\rangle$.

Finite Rotations‡

Now that we have explicit matrices for the generators of rotations, J_x, J_y, and J_z, we can construct the matrices representing $U[R]$ by exponentiating $(-i\boldsymbol{\theta}\cdot\mathbf{J}/\hbar)$. But this is easier said than done. The matrices J_i are infinite dimensional and exponentiating them is not practically possible. But the situation is not as bleak as it sounds for the following reason. First note that since J_i are block diagonal, so is the linear combination $\boldsymbol{\theta}\cdot\mathbf{J}$, and so is its exponential. Consequently, *all* rotation operators $U[R]$ will be represented by block diagonal matrices. The $(2j+1)$-dimensional block at a given j is denoted by $D^{(j)}[R]$. The block diagonal form of the rotation matrices implies (recall the mnemonic of images) that any vector $|\psi_j\rangle$ in the subspace $\mathbb{V}_j$ spanned by the $(2j+1)$ vectors $|jj\rangle, \ldots, |j-j\rangle$ goes into another element $|\psi_j'\rangle$ of $\mathbb{V}_j$. Thus to rotate $|\psi_j\rangle$, we just need the matrix $D^{(j)}$. More generally, if $|\psi\rangle$ has components only in $\mathbb{V}_0, \mathbb{V}_1, \mathbb{V}_2, \ldots, \mathbb{V}_j$, we need just the first $(j+1)$ matrices $D^{(j)}$. What makes the situation hopeful is that it is possible, in practice, to evaluate these if j is small. Let us see why. Consider the series representing $D^{(j)}$:

$$D^{(j)}[R(\boldsymbol{\theta})]=\exp\left[-\frac{i\boldsymbol{\theta}\cdot\mathbf{J}^{(j)}}{\hbar}\right]=\sum_0^\infty\left(\frac{-i\theta}{\hbar}\right)^n(\hat{\theta}\cdot\mathbf{J}^{(j)})^n\frac{1}{n!}$$

‡ The material from here to the end of Exercise 12.5.7 may be skimmed over in a less advanced course.

It can be shown (Exercise 12.5.4) that $(\hat{\theta}\cdot\mathbf{J}^{(j)})^n$ for $n>2j$ can be written as a linear combination of the first $2j$ powers of $\hat{\theta}\cdot\mathbf{J}^{(j)}$. Consequently the series representing $D^{(j)}$ may be reduced to

$$D^{(j)}=\sum_0^{2j} f_n(\theta)(\hat{\theta}\cdot\mathbf{J}^{(j)})^n$$

It is possible, in practice, to find closed expressions for $f_n(\theta)$ in terms of trigonometric functions, for modest values of j (see Exercise 12.5.5). For example,

$$D^{(1/2)}[R]=\cos\left(\frac{\theta}{2}\right)-\frac{2i}{\hbar}\hat{\theta}\cdot\mathbf{J}^{(1/2)}\sin\left(\frac{\theta}{2}\right)$$

Let us return to the subspaces $\mathbb{V}_j$. Since they go into themselves under arbitrary rotations, they are called *invariant subspaces.* The physics behind the invariance is simple: each subspace contains states of a definite magnitude of angular momentum squared $j(j+1)\hbar^2$, and a rotation cannot change this. Formally it is because $[J^2, U[R]]=0$ and so $U[R]$ cannot change the eigenvalue of J^2.

The invariant subspaces have another feature: they are *irreducible.* This means that $\mathbb{V}_j$ itself does not contain *invariant subspaces.* We prove this by showing that any invariant subspace $\bar{\mathbb{V}}_j$ of $\mathbb{V}_j$ is as big as the latter. Let $|\psi\rangle$ be an element of $\bar{\mathbb{V}}_j$. Since we haven't chosen a basis yet, let us choose one such that $|\psi\rangle$ is one of the basis vectors, and furthermore, such that it is the basis vector $|jj\rangle$, up to a normalization factor, which is irrelevant in what follows. (What if we had already chosen a basis $|jj\rangle,\ldots,|j,-j\rangle$ generated by the operators J_i? Consider any unitary transformation U which converts $|jj\rangle$ into $|\psi\rangle$ and a different triplet of operators J_i' defined by $J_i'=UJ_iU^\dagger$. The primed operators have the same commutation rules and hence eigenvalues as the J_i. The eigenvectors are just $|jm\rangle'=U|jm\rangle$, with $|jj\rangle'=|\psi\rangle$. In the following analysis we drop all primes.)

Let us apply an infinitesimal rotation $\delta\boldsymbol{\theta}$ to $|\psi\rangle$. This gives

$$\begin{aligned}|\psi'\rangle&=U[R(\delta\boldsymbol{\theta})]|jj\rangle\\&=[I-(i/\hbar)(\delta\boldsymbol{\theta}\cdot\mathbf{J})]|jj\rangle\\&=[I-(i/2\hbar)(\delta\theta_+J_-+\delta\theta_-J_++2\delta\theta_zJ_z)]|jj\rangle\end{aligned}$$

where

$$\delta\theta_\pm=(\delta\theta_x\pm i\delta\theta_y)$$

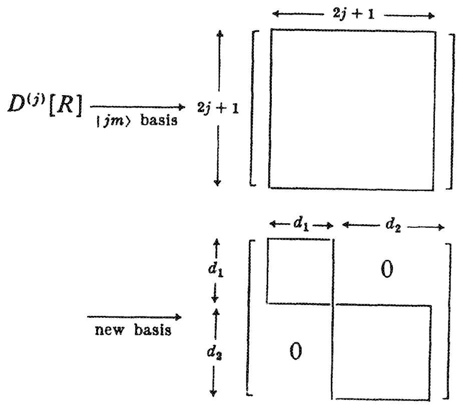
Since $J_+|jj\rangle=0$, $J_z|jj\rangle=j\hbar|jj\rangle$, and $J_-|jj\rangle=\hbar(2j)^{1/2}|j,j-1\rangle$, we get

$$|\psi'\rangle=(1-ij\delta\theta_z)|jj\rangle-\tfrac{1}{2}i(2j)^{1/2}\delta\theta_+|j,j-1\rangle$$

Since $\bar{\mathbb{V}}_j$ is assumed to be invariant under any rotation, $|\psi'\rangle$ also belongs to $\bar{\mathbb{V}}_j$. Subtracting $(1-ij\delta\theta_z)|jj\rangle$, which also belongs to $\bar{\mathbb{V}}_j$, from $|\psi'\rangle$, we find that $|j,j-1\rangle$ also belongs to $\bar{\mathbb{V}}_j$. By considering more of such rotations, we can easily establish that the $(2j+1)$ orthonormal vectors, $|jj\rangle$, $|j,j-1\rangle,\ldots,|j,-j\rangle$ all belong to $\bar{\mathbb{V}}_j$.

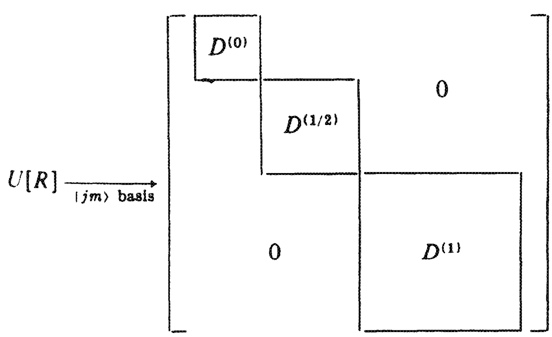
Thus $\bar{\mathbb{V}}_j$ has the same dimensionality as $\mathbb{V}_j$. Thus $\mathbb{V}_j$ has no invariant subspaces. (In a technical sense, $\mathbb{V}_j$ is its own subspace and is invariant. We are concerned here with subspaces of smaller dimensionality.)

The irreducibility of $\mathbb{V}_j$ means that we cannot, by a change of basis within $\mathbb{V}_j$, further block diagonalize all the $D^{(j)}$. We show that if this were not true, then a contradiction would arise. Let it be possible to block diagonalize *all* the $D^{(j)}$, say, as follows:



(The boxed regions are generally nonzero). It follows that $\mathbb{V}_j$ contains two invariant subspaces of dimensionalities d_1 and d_2, respectively. (For example, any vector with just the first d_1 components nonzero will get rotated into another such vector. Such vectors form a d_1-dimensional subspace.) We have seen this is impossible.

The block diagonal matrices representing the rotation operators $U[R]$ are said to provide an *irreducible* (*matrix*) *representation* of these operators. For the set of all rotation operators, the elements of which do not generally commute with each other, this irreducible form is the closest one can come to simultaneous diagonalization. All this is summarized schematically in the sketch below, where the boxed regions represent the blocks, $D^{(0)}$, $D^{(1)}$, . . . etc. The unboxed regions contain zeros.



Consider next the matrix representing a rotationally invariant Hamiltonian in this basis. Since $[H, \mathbf{J}]=0$, H has the same form as J^2, which also commutes with all the generators, namely,

(1) H is diagonal, since $[H, J^2]=0$, $[H, J_z]=0$.
(2) Within each block, H has the same eigenvalue E_j, since $[H, J_\pm]=0$.

It follows from (2) that $\mathbb{V}_j$ is an eigenspace of H with eigenvalue E_j, i.e., all states of a given j are degenerate in a rotationally invariant problem. Although the same result is true classically, the relation between degeneracy and rotational invariance is different in the two cases. Classically, if we are given two states with the same magnitude of angular momentum but different orientation, we argue that they are degenerate because

(1) One may be rotated into the other.
(2) This rotation does not change the energy.

Quantum mechanically, given two elements of $\mathbb{V}_j$, it is not always true that they may be rotated into each other (Exercise 12.5.6). However, we argue as follows:

(1) One may be reached from the other (in general) by the combined action of $J_\pm$ and $U[R]$.
(2) These operators commute with H.

In short, rotational invariance is the cause of degeneracy in both cases, but the degenerate states are not always rotated versions of each other in the quantum case (Exercises 12.5.6 and 12.5.7).

*Exercise 12.5.4.** (1) Argue that the eigenvalues of $J_x^{(j)}$ and $J_y^{(j)}$ are the same as those of $J_z^{(j)}$, namely, $j\hbar$, $(j-1)\hbar, \ldots, (-j\hbar)$. Generalize the result to $\hat{\theta}\cdot\mathbf{J}^{(j)}$.

(2) Show that

$$(J-j\hbar)[J-(j-1)\hbar][J-(j-2)\hbar]\cdots(J+j\hbar)=0$$

where $J\equiv\hat{\theta}\cdot\mathbf{J}^{(j)}$. (Hint: In the case $J=J_z$ what happens when both sides are applied to an arbitrary eigenket $|jm\rangle$? What about an arbitrary superpositions of such kets?)

(3) It follows from (2) that J^{2j+1} is a linear combination of $J^0, J^1, \ldots, J^{2j}$. Argue that the same goes for J^{2j+k}, $k=1, 2, \ldots$.

Exercise 12.5.5. (Hard). Using results from the previous exercise and Eq. (12.5.23), show that

(1) $D^{(1/2)}[R]=\exp(-i\hat{\theta}\cdot\mathbf{J}^{(1/2)}/\hbar)=\cos(\theta/2)I^{(1/2)}-(2i/\hbar)\sin(\theta/2)\hat{\theta}\cdot\mathbf{J}^{(1/2)}$

(2) $D^{(1)}[R]=\exp(-i\theta_x J_x^{(1)}/\hbar)=(\cos\theta_x-1)\left(\dfrac{J_x^{(1)}}{\hbar}\right)^2-i\sin\theta_x\left(\dfrac{J_x^{(1)}}{\hbar}\right)+I^{(1)}$

Exercise 12.5.6. Consider the family of states $|jj\rangle, \ldots, |jm\rangle, \ldots, |j, -j\rangle$. One refers to them as states of the same magnitude but different orientation of angular momentum. If ones takes this remark literally, i.e., in the classical sense, one is led to believe that one may rotate these into each other, as is the case for classical states with these properties. Consider, for instance, the family $|1, 1\rangle$, $|1, 0\rangle$, $|1, -1\rangle$. It may seem, for example, that the state with zero angular momentum along the z axis, $|1, 0\rangle$, may be obtained by rotating $|1, 1\rangle$ by some suitable ($\frac{1}{2}\pi$?) angle about the x axis. Using $D^{(1)}[R(\theta_x \mathbf{i})]$ from part (2) in the last exercise show that

$$|1, 0\rangle \neq D^{(1)}[R(\theta_x \mathbf{i})]|1, 1\rangle \quad \text{for any } \theta_x$$

The error stems from the fact that classical reasoning should be applied to $\langle \mathbf{J} \rangle$, which responds to rotations like an ordinary vector, and not direcly to $|jm\rangle$, which is a vector in Hilbert space. Verify that $\langle \mathbf{J} \rangle$ responds to rotations like its classical counterpart, by showing that $\langle \mathbf{J} \rangle$ in the state $D^{(1)}[R(\theta_x \mathbf{i})]|1, 1\rangle$ is $\hbar[-\sin\theta_x \mathbf{j} + \cos\theta_x \mathbf{k}]$.

It is not too hard to see why we can't always satisfy

$$|jm'\rangle = D^{(j)}[R]|jm\rangle$$

or more generally, for two normalized kets $|\psi_j'\rangle$ and $|\psi_j\rangle$, satisfy

$$|\psi_j'\rangle = D^{(j)}[R]|\psi_j\rangle$$

by any choice of R. These abstract equations imply $(2j+1)$ linear, complex relations between the components of $|\psi_j'\rangle$ and $|\psi_j\rangle$ that can't be satisfied by varying R, which depends on only three parameters, θ_x, θ_y, and θ_z. (Of course one can find a unitary matrix in $\mathbb{V}_j$ that takes $|jm\rangle$ into $|jm'\rangle$ or $|\psi_j\rangle$ into $|\psi_j'\rangle$, but it will not be a *rotation* matrix corresponding to $U[R]$.)

Exercise 12.5.7: Euler Angles. Rather than parametrize an arbitrary rotation by the angle $\boldsymbol{\theta}$, which describes a *single* rotation by θ about an axis parallel to $\boldsymbol{\theta}$, we may parametrize it by three angles, γ, β, and α called *Euler angles*, which define three successive rotations:

$$U[R(\alpha, \beta, \gamma)] = e^{-i\alpha J_z/\hbar}\, e^{-i\beta J_y/\hbar}\, e^{-i\gamma J_z/\hbar}$$

(1) Construct $D^{(1)}[R(\alpha, \beta, \gamma)]$ explicitly as a product of three 3×3 matrices. (Use the result from Exercise 12.5.5 with $J_x \to J_y$.)

(2) Let it act on $|1, 1\rangle$ and show that $\langle \mathbf{J} \rangle$ in the resulting state is

$$\langle \mathbf{J} \rangle = \hbar(\sin\beta\cos\alpha \mathbf{i} + \sin\beta\sin\alpha \mathbf{j} + \cos\beta \mathbf{k})$$

(3) Show that for no value of α, β, and γ can one rotate $|1, 1\rangle$ into just $|1, 0\rangle$.

(4) Show that one can always rotate any $|1, m\rangle$ into a linear combination that involves $|1, m'\rangle$, i.e.,

$$\langle 1, m'|D^{(1)}[R(\alpha, \beta, \gamma)]|1, m\rangle \neq 0$$

for some α, β, γ and any m, m'.

(5) To see that one can occasionally rotate $|jm\rangle$ into $|jm'\rangle$, verify that a $180°$ rotation about the y axis applied to $|1, 1\rangle$ turns it into $|1, -1\rangle$.

Angular Momentum Eigenfunctions in the Coordinate Basis

We now turn to step (3) outlined at the beginning of this section, namely, the construction of the eigenfunctions of L^2 and L_z in the coordinate basis, given the information on the kets $|lm\rangle$.

Consider the states corresponding to a given l. The "topmost" state $|ll\rangle$ satisfies

$$L_+|ll\rangle = 0 \tag{12.5.26}$$

If we write the operator $L_\pm = L_x \pm iL_y$ in spherical coordinates we find

$$L_\pm \xrightarrow[\text{basis}]{\text{coordinate}} \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\,\frac{\partial}{\partial\phi}\right) \tag{12.5.27}$$

Exercise 12.5.8 (Optional). Verify that

$$L_x \xrightarrow[\text{basis}]{\text{coordinate}} i\hbar\left(\sin\phi\,\frac{\partial}{\partial\theta} + \cos\phi\cot\theta\,\frac{\partial}{\partial\phi}\right)$$

$$L_y \xrightarrow[\text{basis}]{\text{coordinate}} i\hbar\left(-\cos\phi\,\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\,\frac{\partial}{\partial\phi}\right)$$

If we denote by $\psi_l^l(r, \theta, \phi)$ the eigenfunction corresponding to $|ll\rangle$, we find that it satisfies

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\phi}\right)\psi_l^l(r, \theta, \phi) = 0 \tag{12.5.28}$$

Since ψ_l^l is an eigenfunction of L_z with eigenvalue $l\hbar$, we let

$$\psi_l^l(r, \theta, \phi) = U_l^l(r, \theta)\, e^{il\phi} \tag{12.5.29}$$

and find that

$$\left(\frac{\partial}{\partial\theta} - l\cot\theta\right)U_l^l = 0 \tag{12.5.30}$$

$$\frac{dU_l^l}{U_l^l} = l\,\frac{d(\sin\theta)}{\sin\theta}$$

or

$$U_l^l(r, \theta) = R(r)(\sin\theta)^l \tag{12.5.31}$$

where $R(r)$ is an arbitrary (normalizable) function of r. When we address the eigenvalue problem of rotationally invariant Hamiltonians, we will see that H will nail down R if we seek simultaneous eigenfunctions of H, L^2, and L_z. But first let us introduce, as we did in the study of L_z in two dimensions, the function that would have been the unique, nondegenerate solution in the absence of the radial coordinate:

$$Y_l^l(\theta, \phi) = (-1)^l \left[\frac{(2l+1)!}{4\pi}\right]^{1/2} \frac{1}{2^l l!} (\sin\theta)^l e^{il\phi} \tag{12.5.32}$$

Whereas the phase factor $(-1)^l$ reflects our convention, the others ensure that

$$\int |Y_l^l|^2 \, d\Omega \equiv \int_{-1}^{1} \int_0^{2\pi} |Y_l^l|^2 \, d(\cos\theta) \, d\phi = 1 \tag{12.5.33}$$

We may obtain Y_l^{l-1} by using the lowering operator. Since

$$L_-|ll\rangle = \hbar[(l+l)(1)]^{1/2}|l, l-1\rangle = \hbar(2l)^{1/2}|l, l-1\rangle$$

$$Y_l^{l-1}(\theta, \phi) = \frac{1}{(2l)^{1/2}} \frac{(-1)}{\hbar} \left[\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta \frac{\partial}{\partial\phi}\right)\right] Y_l^l \tag{12.5.34}$$

We can keep going in this manner until we reach Y_l^{-1}. The result is, for $m \geq 0$,

$$Y_l^m(\theta, \phi) = (-1)^l \left[\frac{(2l+1)!}{4\pi}\right]^{1/2} \frac{1}{2^l l!} \left[\frac{(l+m)!}{(2l)!(l-m)!}\right]^{1/2} e^{im\phi} (\sin\theta)^{-m}$$
$$\times \frac{d^{l-m}}{d(\cos\theta)^{l-m}} (\sin\theta)^{2l} \tag{12.5.35}$$

For $m < 0$, see Eq. (12.5.40). These functions are called *spherical harmonics* and satisfy the orthonormality condition

$$\int Y_l^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \, d\Omega = \delta_{ll'} \delta_{mm'}$$

Another route to the Y_l^m is the direct solution of the L^2, L_z eigenvalue problem in the coordinate basis where

$$L^2 \to (-\hbar^2)\left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}\right) \tag{12.5.36}$$

and of course

$$L_z \to -i\hbar \frac{\partial}{\partial\phi}$$

If we seek common eigenfunctions of the form‡ $f(\theta)\, e^{im\phi}$, which are regular between $\theta = 0$ and π, we will find that L^2 has eigenvalues of the form $l(l+1)\hbar^2$, $l = 0, 1, 2, \ldots,$

‡ We neglect the function $R(r)$ that can tag along as a spectator.

where $l \geq |m|$. The Y_l^m functions are mutually orthogonal because they are *nondegenerate* eigenfunctions of L^2 *and* L_z, which are Hermitian on single-valued functions of θ and ϕ.

Exercise 12.5.9. Show that L^2 above is Hermitian in the sense

$$\int \psi_1^*(L^2\psi_2)\, d\Omega = \left[\int \psi_2^*(L^2\psi_1)\, d\Omega\right]^*$$

The same goes for L_z, which is insensitive to θ and is Hermitian with respect to the ϕ integration.

We may expand any $\psi(r, \theta, \phi)$ in terms of $Y_l^m(\theta, \phi)$ *using r-dependent coefficients* [consult Eq. (10.1.20) for a similar expansion]:

$$\psi(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_l^m(r) Y_l^m(\theta, \phi) \tag{12.5.37a}$$

where

$$C_l^m(r) = \int Y_l^{m*}(\theta, \phi)\psi(r, \theta, \phi)\, d\Omega \tag{12.5.37b}$$

If we compute $\langle \psi | L^2 | \psi \rangle$ and interpret the result as a weighted average, we can readily see (assuming ψ is normalized to unity) that

$$P(L^2 = l(l+1)\hbar^2, L_z = m\hbar) = \int_0^\infty |C_l^m(r)|^2 r^2\, dr \tag{12.5.38}$$

It is clear from the above that C_l^m is the amplitude to find the particle at a radial distance r with angular momentum (l, m).‡ The expansion Eq. (12.5.37a) tells us how to rotate any $\psi(r, \theta, \phi)$ by an angle $\boldsymbol{\theta}$ (in principle):

(1) We construct the block diagonal matrices, $\exp(-i\boldsymbol{\theta}\cdot\mathbf{L}^{(l)}/\hbar)$.

(2) Each block will rotate the C_l^m into linear combination of each other, i.e., under the action of $U[R]$, the coefficients $C_l^m(r)$, $m = 1, l-1, \ldots, -l$; will get mixed with each other by $D_{m'm}^{(l)}$.

In practice, one can explicitly carry out these steps only if ψ contains only Y_l^m's with small l. A concrete example will be provided in one of the exercises.

‡ Note that r is just the eigenvalue of the operator $(X^2 + Y^2 + Z^2)^{1/2}$ which commutes with L^2 and L_z.

Here are the first few Y_l^m functions:

$$\begin{aligned}
Y_0^0 &= (4\pi)^{-1/2} \\
Y_1^{\pm 1} &= \mp (3/8\pi)^{1/2} \sin\theta\, e^{\pm i\phi} \\
Y_1^0 &= (3/4\pi)^{1/2} \cos\theta \\
Y_2^{\pm 2} &= (15/32\pi)^{1/2} \sin^2\theta\, e^{\pm 2i\phi} \\
Y_2^{\pm 1} &= \mp (15/8\pi)^{1/2} \sin\theta \cos\theta\, e^{\pm i\phi} \\
Y_2^0 &= (5/16\pi)^{1/2}(3\cos^2\theta - 1)
\end{aligned} \tag{12.5.39}$$

Note that

$$Y_l^{-m} = (-1)^m (Y_l^m)^* \tag{12.5.40}$$

Closely related to the spherical harmonics are the *associated Legendre polynomials* P_l^m (with $0 \le m \le l$) defined by

$$Y_l^m(\theta, \phi) = \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2} (-1)^m e^{im\phi} P_l^m(\cos\theta) \tag{12.5.41}$$

If $m=0$, $P_l^0(\cos\theta) \equiv P_l(\cos\theta)$ is called a Legendre polynomial.

The Shape of the Y_l^m Functions. For large l, the functions $|Y_l^m|$ exhibit many classical features. For example, $|Y_l^l| \propto |\sin^l\theta|$, is almost entirely confined to the x–y plane, as one would expect of a classical particle with all its angular momentum pointing along the z axis. Likewise, $|Y_l^0|$ is, for large l, almost entirely confined to the z axis. Polar plots of these functions may be found in many textbooks.

Exercise 12.5.10. Write the differential equation corresponding to

$$L^2|\alpha\beta\rangle = \alpha|\alpha\beta\rangle$$

in the coordinate basis, using the L^2 operator given in Eq. (12.5.36). We already know $\beta = m\hbar$ from the analysis of $-i\hbar(\partial/\partial\phi)$. So assume that the simultaneous eigenfunctions have the form

$$\psi_{\alpha m}(\theta, \phi) = P_\alpha^m(\theta)\, e^{im\phi}$$

and show that P_α^m satisfies the equation

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{\alpha}{\hbar^2} - \frac{m^2}{\sin^2\theta}\right) P_\alpha^m(\theta) = 0$$

We need to show that

(1) $\frac{\alpha}{\hbar^2}=l(l+1), \qquad l=0, 1, 2, , \ldots$

(2) $|m|\leq l$

We will consider only part (1) and that too for the case $m=0$. By rewriting the equation in terms of $u=\cos\theta$, show that P_α^0 satisfies

$$(1-u^2)\frac{d^2P_\alpha^0}{du^2}-2u\frac{dP_\alpha^0}{du}+\left(\frac{\alpha}{\hbar^2}\right)P_\alpha^0=0$$

Convince yourself that a power series solution

$$P_\alpha^0=\sum_{n=0}^{\infty} C_n u^n$$

will lead to a two-term recursion relation. Show that $(C_{n+2}/C_n)\to 1$ as $n\to\infty$. Thus the series diverges when $|u|\to 1$ ($\theta\to 0$ or π). Show that if $\alpha/\hbar^2=(l)(l+1)$; $l=0, 1, 2, \ldots$, the series will terminate and be either an even or odd function of u. The functions $P_\alpha^0(u)=P_{l(l+1)\hbar^2}^0(u)\equiv P_l^0(u)\equiv P_l(u)$ are just the Legendre polynomials up to a scale factor. Determine P_0, P_1, and P_2 and compare (ignoring overall scales) with the Y_l^0 functions.

Exercise 12.5.11. Derive Y_1^1 starting from Eq.(12.5.28) and normalize it yourself. [Remember the $(-1)^l$ factor from Eq. (12.5.32).] Lower it to get Y_1^0 and Y_1^{-1} and compare it with Eq. (12.5.39).

*Exercise 12.5.12.** Since L^2 and L_z commute with Π, they should share a basis with it. Verify that under parity $Y_l^m\to(-1)^l Y_l^m$. (First show that $\theta\to\pi-\theta$, $\phi\to\phi+\pi$ under parity. Prove the result for Y_l^l. Verify that L_- does not alter the parity, thereby proving the result for all Y_l^m.)

*Exercise 12.5.13.** Consider a particle in a state described by

$$\psi=N(x+y+2z)\,e^{-\alpha r}$$

where N is a normalization factor.

(1) Show, by rewriting the $Y_1^{\pm1,0}$ functions in terms of x, y, z, and r, that

$$Y_1^{\pm1}=\mp\left(\frac{3}{4\pi}\right)^{1/2}\frac{x\pm iy}{2^{1/2}r} \qquad (12.5.42)$$

$$Y_1^0=\left(\frac{3}{4\pi}\right)^{1/2}\frac{z}{r}$$

(2) Using this result, show that for a particle described by ψ above, $P(l_z=0)=2/3$; $P(l_z=+\hbar)=1/6=P(l_z=-\hbar)$.

Exercise 12.5.14. Consider a rotation $\theta_x \mathbf{i}$. Under this

$$x \to x$$
$$y \to y \cos\theta_x - z \sin\theta_x$$
$$z \to z \cos\theta_z + y \sin\theta_x$$

Therefore we must have

$$\psi(x, y, z) \xrightarrow[U[R(\theta_x \mathbf{i})]]{} \psi_R = \psi(x, y\cos\theta_x - z\sin\theta_x, z\cos\theta_x + y\sin\theta_x)$$

Let us verify this prediction for a special case

$$\psi = Az\, e^{-r^2/a^2}$$

which must go into

$$\psi_R = A(z\cos\theta_x - y\sin\theta_x)\, e^{-r^2/a^2}$$

(1) Expand ψ in terms of Y_1^1, Y_1^0, Y_1^{-1}.

(2) Use the matrix $e^{-i\theta_x L_x/\hbar}$ to find the fate of ψ under this rotation.‡ Check your result against that anticipated above. [Hint: (1) $\psi \sim Y_1^0$, which corresponds to

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

(2) Use Eq. (12.5.42).]

12.6. Solution of Rotationally Invariant Problems

We now consider a class of problems of great practical interest: problems where $V(r, \theta, \phi) = V(r)$. The Schrödinger equation in spherical coordinates becomes

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) + V(r)\right]$$
$$\times \psi_E(r, \theta, \phi) = E\psi_E(r, \theta, \phi) \tag{12.6.1}$$

Since $[H, \mathbf{L}] = 0$ for a spherically symmetric potential, we seek simultaneous eigenfunctions of H, L^2, and L_z:

$$\psi_{Elm}(r, \theta, \phi) = R_{Elm}(r)\, Y_l^m(\theta, \phi) \tag{12.6.2}$$

Feeding in this form, and bearing in mind that the angular part of ∇^2 is just the L^2 operator in the coordinate basis [up to a factor $(-\hbar^2 r^2)^{-1}$, see Eq. (12.5.36)], we get

‡ See Exercise 12.5.5.

the *radial equation*

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\frac{l(l+1)}{r^2}\right]+V(r)\right\}R_{El}=ER_{El} \qquad (12.6.3)$$

Notice that the subscript m has been dropped: neither the energy nor the radial function depends on it. We find, as anticipated earlier, the $(2l+1)$-fold degeneracy of H.

*Exercise 12.6.1.** A particle is described by the wave function

$$\psi_E(r,\theta,\phi)=A\,e^{-r/a_0} \qquad (a_0=\text{const})$$

(1) What is the angular momentum content of the state?
(2) Assuming ψ_E is an eigenstate in a potential that vanishes as $r\to\infty$, find E. (Match leading terms in Schrödinger's equation.)
(3) Having found E, consider finite r and find $V(r)$.

At this point it becomes fruitful to introduce an auxiliary function U_{El} defined as follows:

$$R_{El}=U_{El}/r \qquad (12.6.4)$$

and which obeys the equation

$$\left\{\frac{d^2}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-V(r)-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]\right\}U_{El}=0 \qquad (12.6.5)$$

*Exercise 12.6.2.** Provide the steps connecting Eq. (12.6.3) and Eq. (12.6.5).

The equation is the same as the one-dimensional Schrödinger equation except for the following differences:

(1) The independent variable (r) goes from 0 to ∞ and not from $-\infty$ to ∞.

(2) In addition to the actual potential $V(r)$, there is the *repulsive centrifugal barrier*, $l(l+1)\hbar^2/2\mu r^2$, in all but the $l=0$ states.

(3) The boundary conditions on U are different from the one-dimensional case. We find these by rewriting Eq. (12.6.5) as an eigenvalue equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}\equiv D_l(r)U_{El}=EU_{El} \qquad (12.6.6)$$

and demanding that the functions U_{El} be such that D_l is Hermitian with respect to them. In other words, if U_1 and U_2 are two such functions, then we demand that

$$\int_0^\infty U_1^*(D_l U_2)\,dr = \left[\int_0^\infty U_2^*(D_l U_1)\,dr\right]^* \equiv \int_0^\infty (D_l U_1)^* U_2\,dr \qquad (12.6.7a)$$

This reduces to the requirement

$$\left(U_1^* \frac{dU_2}{dr} - U_2 \frac{dU_1^*}{dr}\right)\Bigg|_0^\infty = 0 \qquad (12.6.7b)$$

Exercise 12.6.3. Show that Eq. (12.6.7b) follows from Eq. (12.6.7a).

Now, a necessary condition for

$$\int_0^\infty |R_{El}|^2 r^2\,dr = \int_0^\infty |U_{El}|^2\,dr$$

to be normalizable to unity or the Dirac delta function is that

$$U_{El} \underset{r\to\infty}{\longrightarrow} 0 \qquad (12.6.8a)$$

or

$$U_{El} \underset{r\to\infty}{\longrightarrow} e^{ikr} \qquad (12.6.8b)$$

the first corresponding to bound states and the second to unbound states. In either case, the expression in the brackets in Eq. (12.6.7b) vanishes at the upper limit‡ and the Hermiticity of D_l hinges on whether or not

$$\left[U_1^* \frac{dU_2}{dr} - U_2 \frac{dU_1^*}{dr}\right]_0 = 0 \qquad (12.6.9)$$

Now this condition is satisfied if

$$U \underset{r\to 0}{\longrightarrow} c, \qquad c = \text{const} \qquad (12.6.10)$$

‡ For the oscillating case, we must use the limiting scheme described in Section 1.10.

If c is nonzero, then

$$R \sim \frac{U}{r} \sim \frac{c}{r}$$

diverges at the origin. This in itself is not a disqualification, for R is still square integrable. The problem with $c \neq 0$ is that the corresponding total wave function‡

$$\psi \sim \frac{c}{r} Y_0^0$$

does not satisfy Schrödinger's equation at the origin. This is because of the relation

$$\nabla^2(1/r) = -4\pi\delta^3(\mathbf{r}) \tag{12.6.11}$$

the proof of which is taken up in Exercise 12.6.4. Thus unless $V(r)$ contains a delta function at the origin (which we assume it does not) the choice $c \neq 0$ is untenable. Thus we deduce that

$$U_{El} \xrightarrow[r\to 0]{} 0 \tag{12.6.12}$$

*Exercise 12.6.4.** (1) Show that

$$\delta^3(\mathbf{r}-\mathbf{r}') \equiv \delta(x-x')\delta(y-y')\delta(z-z') = \frac{1}{r^2 \sin\theta}\,\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi')$$

(consider a test function).

(2) Show that

$$\nabla^2(1/r) = -4\pi\delta^3(\mathbf{r})$$

(Hint: First show that $\nabla^2(1/r)=0$ if $r \neq 0$. To see what happens at $r=0$, consider a small sphere centered at the origin and use Gauss's law and the identity $\nabla^2\phi = \nabla\cdot\nabla\phi$).§

General Properties of U_{El}

We have already discussed some of the properties of U_{El} as $r\to 0$ or ∞. We shall try to extract further information on U_{El} by analyzing the equation governing it in these limits, without making detailed assumptions about $V(r)$. Consider first the limit $r\to 0$. Assuming $V(r)$ is less singular than r^{-2}, the equation is dominated by the

‡ As we will see in a moment, $l \neq 0$ is incompatible with the requirement that $\psi(\mathbf{r})\to r^{-1}$ as $r\to 0$. Thus the angular part of ψ has to be $Y_0^0 = (4\pi)^{-1/2}$.

§ Or compare this equation to Poisson's equation in electrostatics $\nabla^2\phi = -4\pi\rho$. Here $\rho = \delta^3(\mathbf{r})$, which represents a unit point charge at the origin. In this case we know from Coulomb's law that $\phi = 1/r$.

centrifugal barrier:

$$U_l'' \simeq \frac{l(l+1)}{r^2} U_l \qquad (12.6.13)$$

We have dropped the subscript E, since E becomes inconsequential in this limit. If we try a solution of the form

$$U_l \sim r^\alpha$$

we find

$$\alpha(\alpha - 1) = l(l+1)$$

or

$$\alpha = l+1 \quad \text{or } (-l)$$

and

$$U_l \sim \begin{cases} r^{l+1} & \text{(regular)} \\ r^{-l} & \text{(irregular)} \end{cases} \qquad (12.6.14)$$

We reject the irregular solution since it does not meet the boundary condition $U(0) = 0$. The behavior of the regular solutions near the origin is in accord with our expectation that as the angular momentum increases the particle should avoid the origin more and more.

The above arguments are clearly true only if $l \neq 0$. If $l = 0$, the centrifugal barrier is absent, and the answer may be sensitive to the potential. In the problems we will consider, $U_{l=0}$ will also behave as r^{l+1} with $l=0$. Although $U_0(r) \to 0$ as $r \to 0$, note that a particle in the $l=0$ state has a nonzero amplitude to be at the origin, since $R_0(r) = U_0(r)/r \neq 0$ at $r=0$.

Consider now the behavior of U_{El} as $r \to \infty$. If $V(r)$ does not vanish as $r \to \infty$, it will dominate the result (as in the case of the isotropic oscillator, for which $V(r) \propto r^2$) and we cannot say anything in general. So let us consider the case where $rV(r) \to 0$ as $r \to \infty$. At large r the equation becomes

$$\frac{d^2 U_E}{dr^2} = -\frac{2\mu E}{\hbar^2} U_E \qquad (12.6.15)$$

(We have dropped the subscript l since the answer doesn't depend on l.) There are now two cases:

1. $E > 0$: the particle is allowed to escape to infinity classically. We expect U_E to oscillate as $r \to \infty$.
2. $E < 0$: The particle is bound. The region $r \to \infty$ is classically forbidden and we expect U_E to fall exponentially there.

Consider the first case. The solutions to Eq. (12.6.15) are of the form

$$U_E = A\, e^{ikr} + B\, e^{-ikr}, \qquad k = (2\mu E/\hbar^2)^{1/2}$$

that is to say, the particle behaves as a free particle far from the origin.‡ Now, you might wonder why we demanded that $rV(r)\to 0$ and not simply $V(r)\to 0$ as $r\to\infty$. To answer this question, let us write

$$U_E = f(r)\, e^{\pm ikr}$$

and see if $f(r)$ tends to a constant as $r\to\infty$. Feeding in this form of U_E into Eq. (12.6.5) we find (ignoring the centrifugal barrier)

$$f'' \pm (2ik) f' - \frac{2\mu V(r)}{\hbar^2} f = 0$$

Since we expect $f(r)$ to be slowly varying as $r\to\infty$, we ignore f'' and find

$$\frac{df}{f} = \mp \frac{i}{k} \frac{\mu}{\hbar^2} V(r)\, dr$$

$$f(r) = f(r_0) \cdot \exp \mp \left[\frac{i\mu}{k\hbar^2} \int_{r_0}^{r} V(r')\, dr' \right] \tag{12.6.16}$$

where r_0 is some constant. If $V(r)$ falls faster than r^{-1}, i.e., $rV(r)\to 0$ as $r\to\infty$, we can take the limit as $r\to\infty$ in the integral and $f(r)$ approaches a constant as $r\to\infty$. If instead

$$V(r) = -\frac{e^2}{r}$$

as in the Coulomb problem,§ then

$$f(r) = f(r_0) \exp \pm \left[\frac{i\mu e^2}{k\hbar^2} \ln\left(\frac{r}{r_0}\right) \right]$$

and

$$U_E(r) \sim \exp \pm \left[i \left(kr + \frac{\mu e^2}{k\hbar^2} \ln r \right) \right] \tag{12.6.17}$$

This means that no matter how far away the particle is from the origin, it is never completely free of the Coulomb potential. If $V(r)$ falls even slower than a Coulomb potential, this problem only gets worse.

‡ Although A and B are arbitrary in this asymptotic form, their ratio is determined by the requirement that if U_E is continued inward to $r=0$, it must vanish. That there is just one free parameter in the solution (the overall scale), and not two, is because D_l is nondegenerate even for $E>0$, which in turn is due to the constraint $U_{El}(r=0)=0$; see Exercise 12.6.5.

§ We are considering the case of equal and opposite charges with an eye on the next chapter.

Consider now the case $E<0$. All the results from the $E>0$ case carry over with the change

$$k \to i\kappa, \qquad \kappa = (2\mu|E|/\hbar^2)^{1/2}$$

Thus

$$U_E \underset{r\to\infty}{\longrightarrow} A\,e^{-\kappa r} + B\,e^{+\kappa r} \tag{12.6.18}$$

Again B/A is not arbitrary if we demand that U_E continued inward vanish at $r=0$. Now, the growing exponential is disallowed. For arbitrary $E<0$, both $e^{\kappa r}$ and $e^{-\kappa r}$ will be present in U_E. Only for certain discrete values of E will the $e^{\kappa r}$ piece be absent; these will be the allowed bound state levels. (If A/B were arbitrary, we could choose $B=0$ and get a normalizable bound state for every $E<0$.)

As before, Eq. (12.6.18) is true only if $rV(r)\to 0$. In the Coulomb case we expect [from Eq. (12.6.17) with $k\to i\kappa$]

$$\begin{aligned} U_E &\sim \exp\left(\pm\frac{\mu e^2}{\kappa\hbar^2}\ln r\right)e^{\mp\kappa r} \\ &= (r)^{\pm\mu e^2/\kappa\hbar^2}\,e^{\mp\kappa r} \end{aligned} \tag{12.6.19}$$

When we solve the problem of the hydrogen atom, we will find that this is indeed the case.

When $E<0$, the energy eigenfunctions are normalizable to unity. As the operator $D_l(r)$ is nondegenerate (Exercise 12.6.5), we have

$$\int_0^\infty U_{E'l}(r)U_{El}(r)\,dr = \delta_{EE'}$$

and

$$\psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_l^m(\theta,\phi)$$

obeys

$$\iiint \psi^*_{Elm}(r,\theta,\phi)\psi_{E'l'm'}(r,\theta,\phi)r^2\,dr\,d\Omega = \delta_{EE'}\delta_{ll'}\delta_{mm'}$$

We will consider the case $E>0$ in a moment.

Exercise 12.6.5. Show that D_l is nondegenerate in the space of functions U that vanish as $r\to 0$. (Recall the proof of Theorem 15, Section 5.6.) Note that U_{El} is nondegenerate even for $E>0$. This means that E, l, and m, label a state fully in three dimensions.

The Free Particle in Spherical Coordinates‡

If we begin as usual with

$$\psi_{Elm}(r, \theta, \phi) = R_{El}(r) Y_l^m(\theta, \phi)$$

and switch to U_{El}, we end up with

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] U_{El} = 0, \qquad k^2 = \frac{2\mu E}{\hbar^2}$$

Dividing both sides by k^2, and changing to $\rho = kr$, we obtain

$$\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right] U_l = U_l \tag{12.6.20}$$

The variable k, which has disappeared, will reappear when we rewrite the answer in terms of $r = \rho/k$. This problem looks a lot like the harmonic oscillator except for the fact that we have a potential $1/\rho^2$ instead of ρ^2. So we define operators analogous to the raising and lowering operators. These are

$$d_l = \frac{d}{d\rho} + \frac{l+1}{\rho} \tag{12.6.21a}$$

and its adjoint

$$d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho} \tag{12.6.21b}$$

(Note that $d/d\rho$ is anti-Hermitian.) In terms of these, Eq. (12.6.20) becomes

$$(d_l d_l^\dagger) U_l = U_l \tag{12.6.22}$$

Now we premultiply both sides by $d_l^\dagger$ to get

$$d_l^\dagger d_l (d_l^\dagger U_l) = d_l^\dagger U_l \tag{12.6.23}$$

You may verify that

$$d_l^\dagger d_l = d_{l+1} d_{l+1}^\dagger \tag{12.6.24}$$

so that

$$d_{l+1} d_{l+1}^\dagger (d_l^\dagger U_l) = d_l^\dagger U_l \tag{12.6.25}$$

‡ The present analysis is a simplified version of the work of L. Infeld, *Phys. Rev.*, **59**, 737 (1941).

It follows that

$$d_l^\dagger U_l = c_l U_{l+1} \tag{12.6.26}$$

where c_l is a constant. We choose it to be unity, for it can always be absorbed in the normalization. We see that $d_l^\dagger$ serves as a "raising operator" in the index l. Given U_0, we can find the others.‡ From Eq. (12.6.20) it is clear that if $l=0$ there are two independent solutions:

$$U_0^A(\rho) = \sin\rho, \qquad U_0^B = -\cos\rho \tag{12.6.27}$$

The constants in front are chosen according to a popular convention. Now U_0^B is unacceptable at $\rho=0$ since it violates Eq. (12.6.12). If, however, one is considering the equation in a region that excludes the origin, U_0^B must be included. Consider now the tower of solutions built out of U_0^A and U_0^B. Let us begin with the equation

$$U_{l+1} = d_l^\dagger U_l \tag{12.6.28}$$

Now, we are really interested in the functions $R_l = U_l/\rho$.§ These obey (from the above)

$$\begin{aligned}
\rho R_{l+1} &= d_l^\dagger(\rho R_l) \\
&= \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)(\rho R_l) \\
R_{l+1} &= \left(-\frac{d}{d\rho} + \frac{l}{\rho}\right) R_l \\
&= \rho^l \left(-\frac{d}{d\rho}\right) \frac{R_l}{\rho^l}
\end{aligned}$$

or

$$\begin{aligned}
\frac{R_{l+1}}{\rho^{l+1}} &= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_l}{\rho^l} \\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^2 \frac{R_{l-1}}{\rho^{l-1}} \\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1} \frac{R_0}{\rho^0}
\end{aligned}$$

‡ In Chapter 15, we will gain some insight into the origin of such a ladder of solutions.

§ Actually we want $R_l = U_l/r = kU_l/\rho$. But the factor k may be absorbed in the normalization factors of U and R.

so that finally we have

$$R_l = (-\rho)^l \left(\frac{1}{\rho}\frac{\partial}{\partial \rho}\right)^l R_0 \tag{12.6.29}$$

Now there are two possibilities for R_0:

$$R_0^A = \frac{\sin \rho}{\rho}$$

$$R_0^B = \frac{-\cos \rho}{\rho}$$

These generate the functions

$$R_l^A \equiv j_l = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\sin \rho}{\rho}\right) \tag{12.6.30a}$$

called the *spherical Bessel functions* of order l, and

$$R_l^B \equiv n_l = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{-\cos \rho}{\rho}\right) \tag{12.6.30b}$$

called *spherical Neumann functions* of order l.‡ Here are a few of these functions:

$$\begin{aligned} j_0(\rho) &= \frac{\sin \rho}{\rho}, & n_0(\rho) &= \frac{-\cos \rho}{\rho} \\ j_1(\rho) &= \frac{\sin \rho}{\rho^2} - \frac{\cos \rho}{\rho}, & n_1(\rho) &= \frac{-\cos \rho}{\rho^2} - \frac{\sin \rho}{\rho} \\ j_2(\rho) &= \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin \rho - \frac{3\cos \rho}{\rho^2}, & n_2(\rho) &= -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\cos \rho - \frac{3\sin \rho}{\rho^2} \end{aligned} \tag{12.6.31}$$

As $\rho \to \infty$, these functions behave as

$$j_l \underset{\rho\to\infty}{\longrightarrow} \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right) \tag{12.6.32}$$

$$n_l \underset{\rho\to\infty}{\longrightarrow} -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right) \tag{12.6.32}$$

Despite the apparent singularities as $\rho \to 0$, the $j_l(l)$ functions are finite and in fact

$$j_l(\rho) \underset{\rho\to 0}{\longrightarrow} \frac{\rho^l}{(2l+1)!!} \tag{12.6.33}$$

‡ One also encounters *spherical Hankel functions* $h_l = j_l + in_l$ in some problems.

where $(2l+1)!!=(2l+1)(2l-1)(2l-3)\ldots(5)(3)(1)$. These are just the regular solutions listed in Eq. (12.6.14). The Neumann functions, on the other hand, are singular

$$n_l(\rho) \xrightarrow[\rho\to 0]{} -\frac{(2l-1)!!}{\rho^{l+1}} \tag{12.6.34}$$

and correspond to the irregular solutions listed in Eq. (12.6.14).

Free-particle solutions that are *regular in all space* are then

$$\psi_{Elm}(r, \theta, \phi)=j_l(kr)\,Y_l^m(\theta, \phi), \qquad E=\frac{\hbar^2k^2}{2\mu} \tag{12.6.35}$$

These satisfy

$$\iiint \psi^*_{Elm}\psi_{E'l'm'}\,r^2\,dr\,d\Omega=\frac{2}{\pi k^2}\,\delta(k-k')\delta_{ll'}\,\delta_{mm'} \tag{12.6.36}$$

We are using here the fact that

$$\int_0^\infty j_l(kr)j_l(k'r)r^2\,dr=\frac{\pi}{2k^2}\,\delta(k-k') \tag{12.6.37}$$

Exercise 12.6.6. (1)* Verify that Eqs. (12.6.21) and (12.6.22) are equivalent to Eq. (12.6.20)

(2) Verify Eq. (12.6.24).

Exercise 12.6.7. Verify that j_0 and j_1 have the limits given by Eq. (12.6.33).

*Exercise 12.6.8.** Find the energy levels of a particle in a spherical box of radius r_0 in the $l=0$ sector.

*Exercise 12.6.9.** Show that the quantization condition for $l=0$ bound states in a spherical well of depth $-V_0$ and radius r_0 is

$$k'/\kappa=-\tan k'r_0$$

where k' is the wave number inside the well and $i\kappa$ is the complex wave number for the exponential tail outside. Show that there are no bound states for $V_0<\pi^2\hbar^2/8\mu r_0^2$. (Recall Exercise 5.2.6.)

Connection with the Solution in Cartesian Coordinates

If we had attacked the free-particle problem in Cartesian coordinates, we would have readily obtained

$$\psi_E(x, y, z)=\frac{1}{(2\pi\hbar)^{3/2}}\,e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \qquad E=\frac{p^2}{2\mu}=\frac{\hbar^2k^2}{2\mu} \tag{12.6.38}$$

Consider now the case which corresponds to a particle moving along the z axis with momentum p. As

$$\mathbf{p}\cdot\mathbf{r}/\hbar=(pr\cos\theta)\hbar=kr\cos\theta$$

we get

$$\psi_E(r,\theta,\phi)=\frac{e^{ikr\cos\theta}}{(2\pi\hbar)^{3/2}},\qquad E=\frac{\hbar^2k^2}{2\mu}\tag{12.6.39}$$

It should be possible to express this solution, describing a particle moving in the z direction with energy $E=\hbar^2k^2/2\mu$, as a linear combination of the functions ψ_{Elm} which have the same energy, or equivalently, the same k:

$$e^{ikr\cos\theta}=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}C_l^m j_l(kr)Y_l^m(\theta,\phi)\tag{12.6.40}$$

Now, only terms with $m=0$ are relevant since the left-hand side is independent of ϕ. Physically this means that a particle moving along the z axis has no angular momentum in that direction. Since we have

$$Y_l^0(\theta)=\left(\frac{2l+1}{4\pi}\right)^{1/2}P_l(\cos\theta)$$

$$e^{ikr\cos\theta}=\sum_{l=0}^{\infty}C_lj_l(kr)P_l(\cos\theta),\qquad C_l=C_l^0\cdot\left(\frac{2l+1}{4\pi}\right)^{1/2}$$

It can be show that

$$C_l=i^l(2l+1)$$

so that

$$e^{ikr\cos\theta}=\sum_{l=0}^{\infty}i^l(2l+1)j_l(kr)P_l(\cos\theta)\tag{12.6.41}$$

This relation will come in handy when we study scattering. This concludes our study of the free particle.

Exercise 12.6.10. (Optional). Verify Eq. (12.6.41) given that

(1) $\displaystyle\int_{-1}^{1}P_l(\cos\theta)P_{l'}(\cos\theta)\,d(\cos\theta)=[2/(2l+1)]\delta_{ll'}$

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

(3) $\displaystyle\int_0^1(1-x^2)^m\,dx=\frac{(2m)!!}{(2m+1)!!}$

Hint: Consider the limit $kr\to 0$ after projecting out C_l.

We close this section on rotationally invariant problems with a brief study of the isotropic oscillator. The most celebrated member of this class, the hydrogen atom, will be discussed in detail in the next chapter.

The Isotropic Oscillator

The isotropic oscillator is described by the Hamiltonian

$$H=\frac{P_x^2+P_y^2+P_z^2}{2\mu}+\frac{1}{2}\mu\omega^2(X^2+Y^2+Z^2) \qquad (12.6.42)$$

If we write as usual

$$\psi_{Elm}=\frac{U_{El}(r)}{r}\,Y_l^m(\theta,\phi) \qquad (12.6.43)$$

we obtain the radial equation

$$\left\{\frac{d^2}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-\frac{1}{2}\mu\omega^2r^2-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]\right\}U_{El}=0 \qquad (12.6.44)$$

As $r\to\infty$, we find

$$U\sim e^{-y^2/2} \qquad (12.6.45)$$

where

$$y=\left(\frac{\mu\omega}{\hbar}\right)^{1/2}r \qquad (12.6.46)$$

is dimensionless. So we let

$$U(y)=e^{-y^2/2}v(y) \qquad (12.6.47)$$

and obtain the following equation for $v(y)$:

$$v''-2yv'+\left[2\lambda-1-\frac{l(l+1)}{y^2}\right]v=0, \qquad \lambda=\frac{E}{\hbar\omega} \qquad (12.6.48)$$

It is clear upon inspection that a two-term recursion relation will obtain if a power-series solution is plugged in. We set

$$v(y)=y^{l+1}\sum_{n=0}^{\infty}C_ny^n \qquad (12.6.49)$$

where we have incorporated the known behavior [Eq. (12.6.14)] near the origin.

By going through the usual steps (left as an exercise) we can arrive at the following quantization condition:

$$E=(2k+l+3/2)\hbar\omega, \qquad k=0, 1, 2, \ldots \tag{12.6.50}$$

If we define the principal quantum number (which controls the energy)

$$n=2k+l \tag{12.6.51}$$

we get

$$E=(n+3/2)\hbar\omega \tag{12.6.52}$$

At each n, the allowed l values are

$$l=n-2k=n, n-2, \ldots, 1 \text{ or } 0 \tag{12.6.53}$$

Here are the first few eigenstates:

$$\begin{array}{lll} n=0 & l=0 & m=0 \\ n=1 & l=1 & m=\pm 1, 0 \\ n=2 & l=0, 2 & m=0;\ \pm 2,\ \pm 1, 0 \\ n=3 & l=1, 3 & m=\pm 1, 0;\ \pm 3,\ \pm 2,\ \pm 1, 0 \\ \vdots & \vdots & \vdots \end{array}$$

Of particular interest to us is the fact that states of different l are degenerate. The degeneracy in m at each l we understand in terms of rotational invariance. The degeneracy of the different l states (which are not related by rotation operators or the generators) appears mysterious. For this reason it is occasionally termed *accidental degeneracy*. This is, however, a misnomer, for the degeneracy in l can be attributed to additional invariance properties of H. Exactly what these extra invariances or symmetries of H are, and how they explain the degeneracy in l, we will see in Chapter 15.

*Exercise 12.6.11.** (1) By combining Eqs. (12.6.48) and (12.6.49) derive the two-term recursion relation. Argue that $C_0 \neq 0$ if U is to have the right properties near $y=0$. Derive the quantizations condition, Eq. (12.6.50).

(2) Calculate the degeneracy and parity at each n and compare with Exercise 10.2.3, where the problem was solved in Cartesian coordinates.

(3) Construct the normalized eigenfunction ψ_{nlm} for $n=0$ and 1. Write them as linear combinations of the $n=0$ and $n=1$ eigenfunctions obtained in Cartesian coordinates.