

# Chapter 11

## Dirac Notation

We've reached a plateau. You now know how to solve problems in one, two, and three dimensions. Hopefully you have the basics under your belt. In this chapter, I present a somewhat more general way of specifying the state of a quantum system, based on a formalism developed by Dirac.<sup>1</sup>

### 11.1 Vector Spaces and Dirac Notation

Up to this point, I have focused on methods for obtaining the *eigenfunctions* associated with various Hamiltonians; moreover, the discussion has been limited mainly to the coordinate representation. The eigenfunctions form a complete set of functions, allowing you to expand any function as a linear superposition of the eigenfunctions. This is similar to, but not exactly identical to the situation with vectors. As you know you can expand a vector as

$$\mathbf{A} = A_x \mathbf{u}_x + A_y \mathbf{u}_y + A_z \mathbf{u}_z. \quad (11.1)$$

An *orthonormal basis set* ( $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z$ ) has been chosen for convenience. You can obtain any component of the vector by projection,

$$A_j = \mathbf{u}_j \cdot \mathbf{A}; \quad j = x, y, z. \quad (11.2)$$

In quantum mechanics, on the other hand, an arbitrary function  $\psi(\mathbf{r})$  can be expanded in the set of *basis functions* corresponding to the eigenfunctions  $\psi_f(\mathbf{r})$  of some Hermitian operator  $\hat{F}$ , namely

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<sup>1</sup>P. A. M. Dirac, *Principles of Quantum Mechanics, Fourth Edition* (Oxford University Press, Oxford, U.K., 1958).

$$\psi(\mathbf{r}) = \sum_f b_f \psi_f(\mathbf{r}), \quad (11.3)$$

where

$$b_f = (\psi_f, \psi) = \int d\mathbf{r} \psi_f^*(\mathbf{r}) \psi(\mathbf{r}); \quad (11.4)$$

the scalar product projection operation used for vectors is replaced by integration.

The analogy with vector spaces can be made exact if we deal with *eigenstates* and *state vectors* rather than eigenfunctions and wave functions. Dirac developed a powerful formalism for representing state vectors in quantum mechanics. Students leaving an introductory course in quantum mechanics often can *use* Dirac notation, but may not appreciate its significance.

### 11.1.1 Vector Spaces

It is probably easiest to think of Dirac notation in relation to a three-dimensional vector space. Any three dimensional vector can be written as

$$\mathbf{A} = A_x \mathbf{u}_x + A_y \mathbf{u}_y + A_z \mathbf{u}_z, \quad (11.5)$$

where  $A_x, A_y, A_z$  are the components of the vector in this  $x, y, z$  basis. I can represent the unit vectors as column vectors,

$$\mathbf{u}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; \quad \mathbf{u}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; \quad \mathbf{u}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (11.6)$$

such that the vector  $\mathbf{A}$  can be written as

$$\mathbf{A} = \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}. \quad (11.7)$$

Of course, the basis vectors  $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z$  are not unique; any set of three non-collinear unit vectors would do as well. Let's call one such set  $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ , such that

$$\mathbf{A} = A_1 \mathbf{u}_1 + A_2 \mathbf{u}_2 + A_3 \mathbf{u}_3. \quad (11.8)$$

The vector  $\mathbf{A}$  is *absolute* in the sense that it is basis-independent. For a given basis, the components of  $\mathbf{A}$  change in precisely the correct manner to insure that  $\mathbf{A}$  remains unchanged. The example in the problems should make this clear.

The scalar product of two vectors is defined in the usual fashion as the cosine of the angle between the vectors. Although not necessary, it is convenient to choose an *orthonormal basis*, one in which the scalar product of different basis vectors vanishes and the scalar product of a basis vector with itself is equal to unity. The basis vectors  $\mathbf{u}_x$ ,  $\mathbf{u}_y$ ,  $\mathbf{u}_z$  constitute an orthogonal basis since

$$\begin{aligned}\mathbf{u}_x \cdot \mathbf{u}_x &= \mathbf{u}_y \cdot \mathbf{u}_y = \mathbf{u}_z \cdot \mathbf{u}_z = 1; \\ \mathbf{u}_x \cdot \mathbf{u}_y &= \mathbf{u}_y \cdot \mathbf{u}_z = \mathbf{u}_x \cdot \mathbf{u}_z = 0.\end{aligned}\tag{11.9}$$

In addition to a geometric interpretation to the scalar product, I can give a definition based on matrix multiplication. Even though the vectors are real quantities, in preparation for quantum mechanics, I define the *adjoint* of a vector  $\mathbf{A}$  as

$$\mathbf{A}^\dagger = \left( A_x^* \ A_y^* \ A_z^* \right),\tag{11.10}$$

that is as a row matrix whose components are the complex conjugates of those of the column matrix  $\mathbf{A}$ . The scalar product of vectors  $\mathbf{A}$  and  $\mathbf{B}$  is then defined as

$$\mathbf{A} \cdot \mathbf{B} = \underline{\mathbf{A}}^\dagger \underline{\mathbf{B}} = \left( A_x^* \ A_y^* \ A_z^* \right) \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = A_x^* B_x + A_y^* B_y + A_z^* B_z,\tag{11.11}$$

such that

$$\mathbf{A} \cdot \mathbf{A} = \underline{\mathbf{A}}^\dagger \underline{\mathbf{A}} = \left( A_x^* \ A_y^* \ A_z^* \right) \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = |A_x|^2 + |A_y|^2 + |A_z|^2 = |\mathbf{A}|^2,\tag{11.12}$$

as desired. A line below a symbol indicates a matrix.

Expressed as matrices, the adjoints of the unit vectors given in Eq. (11.6) are

$$\underline{\mathbf{u}}_x^\dagger = (1 \ 0 \ 0); \quad \underline{\mathbf{u}}_y^\dagger = (0 \ 1 \ 0); \quad \underline{\mathbf{u}}_z^\dagger = (0 \ 0 \ 1).\tag{11.13}$$

You can verify that, consistent with Eq. (11.9),

$$\mathbf{u}_i \cdot \mathbf{u}_j = \underline{\mathbf{u}}_i^\dagger \underline{\mathbf{u}}_j = \delta_{ij}; \quad i, j = \{x, y, z\};\tag{11.14}$$

these unit vectors form an orthonormal basis. The  $j$ th component of a vector is then obtained by projection as

$$A_j = \mathbf{u}_j \cdot \mathbf{A} = \underline{\mathbf{u}}_j^\dagger \underline{\mathbf{A}}; \quad j = \{x, y, z\}.\tag{11.15}$$

Next, I define the action of an operator  $\hat{O}$  on a vector  $\mathbf{A}$  by the equation

$$\mathbf{A}' = \hat{O}\mathbf{A}; \quad (11.16)$$

that is, the operator  $\hat{O}$  acting on a vector  $\mathbf{A}$  produces a new vector  $\mathbf{A}'$ . For example, the operator  $\hat{O}$  may result in a translation or a rotation of the vector  $\mathbf{A}$ . It won't take you too much effort to realize that a translation doesn't change a vector, but a rotation mixes up its components in some specified manner. A *linear operator* is one that produces a new vector having components that are a linear combination of the initial components of the vector. In other words, a linear operator  $\hat{O}$  acting on a vector  $\mathbf{A}$  produces a new vector  $\mathbf{A}'$  having components

$$A'_x = O_{xx}A_x + O_{xy}A_y + O_{xz}A_z \quad (11.17a)$$

$$A'_y = O_{yx}A_x + O_{yy}A_y + O_{yz}A_z \quad (11.17b)$$

$$A'_z = O_{zx}A_x + O_{zy}A_y + O_{zz}A_z. \quad (11.17c)$$

Equation (11.16) corresponds to what is called an *active transformation*. The vector itself is operated on (e.g., the vector is rotated), but the basis vectors are left unchanged. Thus, the *new* vector is expressed in terms of the *original* basis as

$$\mathbf{A}' = A'_x\mathbf{u}_x + A'_y\mathbf{u}_y + A'_z\mathbf{u}_z. \quad (11.18)$$

It is possible to write Eq. (11.17) as a matrix equation if I define

$$\underline{O} = \begin{pmatrix} O_{xx} & O_{xy} & O_{xz} \\ O_{yx} & O_{yy} & O_{yz} \\ O_{zx} & O_{zy} & O_{zz} \end{pmatrix}; \quad (11.19)$$

that is, I represent a linear operator as a matrix, such that the transformation (11.16) can be written in matrix form as

$$\underline{A}' = \underline{O}\underline{A}. \quad (11.20)$$

This is an important result; *linear operators can be represented as matrices*. I can introduce a set of *basis matrices* of the form

$$\underline{m}_{xy} = \mathbf{u}_x\mathbf{u}_y^\dagger = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (0 \ 1 \ 0) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad (11.21)$$

that is, a one for the  $xy$  element and zeroes everywhere else. If I re-label  $x, y, z$  as  $1, 2, 3$ , then  $\underline{m}_{ij}$  has a one for the  $ij$  element and zeroes everywhere else, such that

$$\underline{O} = \sum_{i,j=1}^3 O_{ij} \underline{m}_{ij} \tag{11.22}$$

I also replace  $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z$  by  $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ . In that way, Eq. (11.22) remains valid in *any* orthonormal basis with

$$\underline{m}_{ij} = \underline{u}_i \underline{u}_j^\dagger; \quad i, j = \{1, 2, 3\}. \tag{11.23}$$

Of course, the matrix elements of the matrix  $\underline{O}$  depend on the basis. You are at liberty to represent the basis vectors as

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{11.24}$$

in any *one* orthonormal basis, but once you choose this basis, you must express all other unit vectors in terms of this specific basis. As with marriage, you make your choice and you live with it.

Note that, for orthonormal basis vectors,

$$\begin{aligned} \underline{u}_i^\dagger \underline{O} \underline{u}_j &= \sum_{i',j'=1}^3 \underline{u}_i^\dagger O_{i'j'} \underline{m}_{i'j'} \underline{u}_j = \sum_{i',j'=1}^3 O_{i'j'} \underline{u}_i^\dagger \underline{m}_{i'j'} \underline{u}_j \\ &= \sum_{i',j'=1}^3 O_{i'j'} \underline{u}_i^\dagger \underline{u}_{i'} \underline{u}_{j'}^\dagger \underline{u}_j = \sum_{i',j'=1}^3 O_{i'j'} \delta_{i,i'} \delta_{j,j'} = O_{ij}, \end{aligned} \tag{11.25}$$

which shows you how to get matrix elements by projection.

### 11.1.2 Hilbert Space

I can take these ideas over to quantum mechanics. Things will be a little vague and confusing at first, but I hope that they clear up as I proceed. I consider only time-independent operators and, for the moment, only time-independent state vectors. The analogue of the vector  $\mathbf{A}$  is the *state vector*  $|A\rangle$ , which is an abstract vector in a *Hilbert space* that can be finite or infinite-dimensional. Such a state vector is referred to as a *ket*. As in a normal vector space, I can introduce unit vectors or *basis kets*  $|n\rangle$ . Thus, the ket  $|n\rangle$  can be thought of as a column matrix having a 1 in the  $n^{\text{th}}$  place and a zero everywhere else. The state vector can be expanded as

$$|A\rangle = \sum_n A_n |n\rangle. \tag{11.26}$$

In other words, the state vector  $|A\rangle$  is a column matrix whose  $n$ th element is  $A_n$ . As in the vector case, the state vector  $|A\rangle$  has an absolute meaning. If I change the basis kets, I change the coordinates  $A_n$  but do not change  $|A\rangle$ . The adjoint of a ket is called a *bra* and can be represented by a row matrix. The adjoint of the basis ket  $|n\rangle$  is written as

$$\langle n| = (|n\rangle)^\dagger \quad (11.27)$$

If the basis kets are orthonormal, as is often the case, then

$$\langle n|m\rangle = \delta_{m,n}. \quad (11.28)$$

You can see the origin of the bra-ket (bracket) notation. Unless stated otherwise, I will assume that the basis kets are orthonormal. The adjoint of Eq.(11.26) is defined by

$$(|A\rangle)^\dagger = \langle A| = \sum_n A_n^* \langle n|, \quad (11.29)$$

such that, for any two state vectors  $|A\rangle$  and  $|B\rangle$  in the same Hilbert space,

$$\langle B|A\rangle = \sum_{n,n'} A_{n'} B_n^* \langle n|n'\rangle = \sum_n A_n B_n^* = \left( \sum_n A_n^* B_n \right)^* = \langle A|B\rangle^*. \quad (11.30)$$

I can use Eq.(11.28) to obtain the  $A_m$  appearing in Eq.(11.26) by multiplying that equation by  $\langle m|$  and using Eq.(11.28) to obtain

$$A_m = \langle m|A\rangle. \quad (11.31)$$

Furthermore,

$$|A\rangle = \sum_n A_n |n\rangle = \sum_n |n\rangle \langle n|A\rangle, \quad (11.32)$$

which implies that

$$\sum_n |n\rangle \langle n| = 1, \quad (11.33)$$

a statement of the completeness relation. For *continuous* kets such as  $|\mathbf{r}\rangle$ , the corresponding relationships are

$$\langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}'); \quad (11.34a)$$

$$\int d\mathbf{r} |\mathbf{r}\rangle \langle \mathbf{r}| = 1. \tag{11.34b}$$

Whereas the discrete kets are dimensionless, the continuous kets  $|\mathbf{r}\rangle$  have units of  $1/\sqrt{\text{volume}}$ .

I can also consider the effect of a linear operator  $\hat{O}$  acting on the state vector  $|A\rangle$ . It will produce a new state vector  $|A'\rangle$  that

$$|A'\rangle = \sum_n A'_n |n\rangle = \hat{O}|A\rangle = \hat{O} \sum_n A_n |n\rangle = \sum_n A_n \hat{O}|n\rangle. \tag{11.35}$$

If you multiply Eq. (11.35) on the left by  $\langle m|$  and use the orthonormal property of the bras and kets, you can obtain

$$A'_m = \sum_n A_n \langle m|\hat{O}|n\rangle = \sum_n O_{mn} A_n, \tag{11.36}$$

where

$$O_{mn} = \langle m|\hat{O}|n\rangle \tag{11.37}$$

is a matrix element of the operator  $\hat{O}$  in the  $|n\rangle$  basis. Linear operators can be represented as matrices, just as in three-dimensional vector space. It is convenient to define *unit matrices* by

$$\underline{m}_{nq} = |n\rangle \langle q|, \tag{11.38}$$

such that

$$\underline{O} = \sum_{ij} O_{ij} \underline{m}_{ij}. \tag{11.39}$$

Remember that  $|n\rangle \langle q|$  is a matrix with a one for the  $nq$  element and zeroes everywhere else. The matrix  $\underline{O}$  is Hermitian if  $O_{nm} = (O_{mn})^*$ .

I now come to the fundamental difference between a vector space and Hilbert space, as applied to quantum mechanics. In three-dimensional vector space, in general, one chooses the basis vectors without making any reference to the operators acting in the space. In quantum mechanics, a central feature is to choose a set of basis vectors that is *intimately connected* with operators acting in the Hilbert space. Moreover, it is assumed that the Hermitian operator associated with each physical observable has a matrix representation that is *diagonal* in its own basis.

That is, in a given basis  $|h\rangle$  associated with a Hermitian operator  $\hat{H}$ , it is assumed that  $\underline{H}$  is diagonal,

$$\langle h|\hat{H}|h'\rangle = h\delta_{h,h'}. \tag{11.40}$$

If I multiply this equation on the left by  $|h\rangle$  and sum over  $h$  using the completeness relation given in Eq. (11.33), I find

$$\hat{H} |h'\rangle = \sum_h h |h\rangle \delta_{h,h'} = h' |h'\rangle, \quad (11.41)$$

which is just an eigenvalue equation for  $\hat{H}$ ! Consequently, we can use all the results that were derived in connection with the eigenvalue problem (eigenkets exist, are complete, can be chosen to form an orthonormal basis, simultaneous eigenkets can always be chosen for commuting operators, etc.). The eigenvalues  $h$  are the only possible outcomes of a measurement of the physical observable associated with  $\hat{H}$  when made on a single quantum system.

I define the time-dependent state vector  $|\psi(t)\rangle$  to be the solution of the time-dependent Schrödinger equation,

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle. \quad (11.42)$$

It is a simple matter to show that the solution of this equation can be written in the form

$$|\psi(t)\rangle = \sum_E b_E e^{-iEt/\hbar} |E\rangle, \quad (11.43)$$

*provided*

$$\hat{H} |E\rangle = E |E\rangle. \quad (11.44)$$

Thus, if we solve Eq. (11.44), we have a complete solution to any problem for a Hamiltonian  $\hat{H}$ .

Since I have assumed that an operator is diagonal in its own basis, it follows that

$$\hat{H} |E\rangle = E |E\rangle; \quad (11.45a)$$

$$\hat{\mathbf{r}} |\mathbf{r}\rangle = \mathbf{r} |\mathbf{r}\rangle; \quad (11.45b)$$

$$\hat{\mathbf{p}} |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle. \quad (11.45c)$$

Furthermore, any operator corresponding to a classical variable that is a function only of  $\mathbf{r}$  has  $|\mathbf{r}\rangle$  as its eigenkets and any operator corresponding to a classical variable that is a function only of  $\mathbf{p}$  has  $|\mathbf{p}\rangle$  as its eigenkets; that is, for operators  $\hat{V}$  and  $\hat{p}^2$ , the matrices  $\underline{V}$  and  $\underline{p}^2$  associated with these operators are diagonal in the  $|\mathbf{r}\rangle$  and  $|\mathbf{p}\rangle$  bases, respectively,

$$\hat{V} |\mathbf{r}\rangle = V(\mathbf{r}) |\mathbf{r}\rangle; \quad (11.46a)$$

$$\hat{p}^2 |\mathbf{p}\rangle = p^2 |\mathbf{p}\rangle. \quad (11.46b)$$

All this is well and good, but what have I accomplished? Normally in quantum mechanics we want to find the eigenenergies of the Hamiltonian, now expressed as the matrix  $\underline{H}$ . In the  $|E\rangle$  basis,  $\underline{H}$  is simply a diagonal matrix whose elements *are* the eigenenergies, but we have no way of calculating them yet. In other words, if we don't know the eigenenergies, the equation  $\hat{H}|E\rangle = E|E\rangle$  doesn't help us to find them. It may be that we know the matrix elements of  $\underline{H}$  in some *other* basis, however. If that were the case, it turns out that if we diagonalize the matrix  $\underline{H}$ , we can find the eigenenergies of  $\hat{H}$ , as well as the eigenkets of  $\hat{H}$  in terms of the basis kets for which we know the matrix elements of  $\underline{H}$ .

Let me give you an example. Say that the Hamiltonian is that of a free particle,

$$\underline{H} = \frac{\mathbf{p}^2}{2m}. \quad (11.47)$$

Since  $\underline{H}$  is diagonal in the  $|\mathbf{p}\rangle$  basis, the  $|\mathbf{p}\rangle$  states *are* the eigenkets of  $\underline{H}$  and the corresponding eigenenergies are  $p^2/2m$ . But what if the Hamiltonian is of the form

$$\underline{H} = \frac{\mathbf{p}^2}{2m} + \underline{V}, \quad (11.48)$$

where  $\underline{V}$  is the matrix corresponding to the potential energy operator  $\hat{V}$ . I know the matrix elements of  $\hat{p}^2$  in the  $|\mathbf{p}\rangle$  basis and those of  $\hat{V}$  in the  $|\mathbf{r}\rangle$  basis, but not those of the *entire* Hamiltonian in any one basis.

To proceed further, I need to inject some quantum physics. Previously, one of the postulates I used was to assume that the wave functions in coordinate and momentum space were Fourier transforms of one another. This allowed me to calculate the momentum operator in coordinate space. I now replace this postulate by one in which the *Poisson bracket* of classical mechanics for two variables is replaced by the commutator of the matrices in quantum mechanics corresponding to those variables, multiplied by  $(i\hbar)^{-1}$ . The Poisson bracket of two arbitrary functions  $F$  and  $G$  with respect to canonical variables  $q$  and  $p$  is defined as

$$[F, G]_{q,p} = \frac{\partial F}{\partial q} \frac{\partial G}{\partial p} - \frac{\partial F}{\partial p} \frac{\partial G}{\partial q}. \quad (11.49)$$

As a consequence, the Poisson bracket of  $x$  and  $p_x$  is

$$[x, p_x]_{x,p_x} = \frac{\partial x}{\partial x} \frac{\partial p_x}{\partial p_x} - \frac{\partial x}{\partial p_x} \frac{\partial p_x}{\partial x} = 1. \quad (11.50)$$

To arrive at the analogous equation for quantum mechanics, I replace  $[x, p_x]_{x,p_x}$  by  $(i\hbar)^{-1} [\hat{x}, \hat{p}_x]$  to arrive at the commutator relation  $[\hat{x}, \hat{p}_x] = i\hbar$ . This will allow me to evaluate matrix elements of  $\hat{\mathbf{p}}$  in the  $|\mathbf{r}\rangle$  basis.

Armed with this commutator, I can try to evaluate matrix elements of

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \quad (11.51)$$

in the  $|\mathbf{r}\rangle$  basis. Matrix elements of the second term are easy to obtain since

$$\langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle = V(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'); \quad (11.52)$$

the potential energy matrix is diagonal in the  $|\mathbf{r}\rangle$  basis. But what about matrix elements of  $\hat{p}^2$  in the  $|\mathbf{r}\rangle$  basis? I start from the assumed form for the commutator,

$$[\hat{x}, \hat{p}_x] = i\hbar, \quad (11.53)$$

and evaluate

$$\begin{aligned} \langle x | [\hat{x}, \hat{p}_x] | x' \rangle &= i\hbar \langle x | x' \rangle = i\hbar \delta(x-x'); \\ \langle x | \hat{x}\hat{p}_x - \hat{p}_x\hat{x} | x' \rangle &= i\hbar \delta(x-x'). \end{aligned} \quad (11.54)$$

Since  $\hat{x}$  is a Hermitian operator and since  $\hat{x}|x'\rangle = x'|x'\rangle$ , it follows that

$$\langle x | \hat{x} = (\hat{x} | x \rangle)^\dagger = x \langle x |, \quad (11.55)$$

allowing me to rewrite Eq. (11.54) as

$$(x - x') \langle x | \hat{p}_x | x' \rangle = i\hbar \delta(x-x'). \quad (11.56)$$

Equation (11.56) is of the form  $xf(x) = a\delta(x)$ , which has as solution

$$f(x) = -a \frac{d}{dx} \delta(x). \quad (11.57)$$

To prove that this is a solution, I work backwards starting from

$$xf(x) = -ax \frac{d}{dx} \delta(x) = -a \frac{d}{dx} [x\delta(x)] + a\delta(x) = a\delta(x), \quad (11.58)$$

having used the relation  $x\delta(x) = 0$ . Thus,

$$\langle x | \hat{p}_x | x' \rangle = \frac{\hbar}{i} \frac{d}{dx} \delta(x-x'); \quad (11.59a)$$

$$\langle \mathbf{r} | \hat{p}_x | \mathbf{r}' \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \delta(\mathbf{r} - \mathbf{r}'); \quad (11.59b)$$

$$\langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle = \frac{\hbar}{i} \nabla_r \delta(\mathbf{r} - \mathbf{r}'). \quad (11.59c)$$

Similarly,

$$\langle \mathbf{p} | \hat{\mathbf{r}} | \mathbf{p}' \rangle = i\hbar \nabla_{\mathbf{p}} \delta(\mathbf{p} - \mathbf{p}'). \quad (11.60)$$

It is clear that  $\hat{p}_x$  is not diagonal in the  $|x\rangle$  basis since the derivative of a delta function is *not* proportional to  $\delta(x-x')$ ; that is, it is non-zero for values of  $x \neq x'$ . You can understand this easily. A delta function  $\delta(x)$  is like a narrow Gaussian centered at  $x = 0$  whose derivative vanishes at  $x = 0$ , has a sharp maximum for  $x < 0$ , and a sharp minimum for  $x > 0$ —it is non-zero for values of  $x \neq 0$ . Of course we knew beforehand that  $\hat{\mathbf{p}}$  could not be diagonal in the  $|\mathbf{r}\rangle$  basis since two operators can have simultaneous eigenkets if and only if the operators commute.

I have made some progress. Using the assumed commutation relation between  $\hat{x}$  and  $\hat{p}_x$ , I found a matrix representation of  $\hat{\mathbf{p}}$  in the  $|\mathbf{r}\rangle$  basis. The matrix is not diagonal, nor will the matrix  $\hat{\mathbf{p}}^2$  be diagonal. As a consequence, to get the eigenvalues of  $\hat{\mathbf{H}}$ , I must diagonalize  $\hat{\mathbf{H}}$ . In other words, I seek a linear combination of energy kets in the  $|\mathbf{r}\rangle$  basis,

$$|E\rangle = \int d\mathbf{r} \langle \mathbf{r} | E \rangle |\mathbf{r}\rangle \quad (11.61)$$

that diagonalizes  $\hat{\mathbf{H}}$ , that is, a basis for which

$$\hat{H} |E\rangle = E |E\rangle. \quad (11.62)$$

If I can find the expansion coefficients  $\langle \mathbf{r} | E \rangle$ , I will have accomplished this task. In other words, I will have found a basis in which  $\hat{H}$  is diagonal—the eigenenergies are simply the diagonal elements of the matrix  $\hat{\mathbf{H}}$  in the new basis.

To get the expansion components, I start from Eq. (11.62) and multiply on the left by  $\langle \mathbf{r} |$  to obtain

$$\langle \mathbf{r} | \left( \frac{\hat{p}^2}{2m} + \hat{V} \right) |E\rangle = E \langle \mathbf{r} | E \rangle. \quad (11.63)$$

I now use the completeness relation

$$\int d\mathbf{r} |\mathbf{r}\rangle \langle \mathbf{r}| = 1 \quad (11.64)$$

and insert complete sets at will. In fact, when dealing with Dirac notation and you are lost about what to do, you can always insert some complete sets and see what happens! Inserting Eq. (11.64) into Eq. (11.63), I find

$$\int d\mathbf{r}' \langle \mathbf{r} | \left( \frac{\hat{p}^2}{2m} + \hat{V} \right) | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle = E \langle \mathbf{r} | E \rangle, \quad (11.65a)$$

$$\int d\mathbf{r}' \left( \frac{\langle \mathbf{r} | \hat{p}^2 | \mathbf{r}' \rangle}{2m} + \langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle \right) \langle \mathbf{r}' | E \rangle = E \langle \mathbf{r} | E \rangle, \quad (11.65b)$$

$$\int d\mathbf{r}' \left( \frac{\langle \mathbf{r} | \hat{p}^2 | \mathbf{r}' \rangle}{2m} + V(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') \right) \langle \mathbf{r}' | E \rangle = E \langle \mathbf{r} | E \rangle, \quad (11.65c)$$

$$\int d\mathbf{r}' \frac{\langle \mathbf{r} | \hat{p}^2 | \mathbf{r}' \rangle}{2m} \langle \mathbf{r}' | E \rangle + V(\mathbf{r}) \langle \mathbf{r} | E \rangle = E \langle \mathbf{r} | E \rangle, \quad (11.65d)$$

and the problem reduces to evaluating

$$\begin{aligned} \int d\mathbf{r}' \langle \mathbf{r} | \hat{p}^2 | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle &= \int d\mathbf{r}'' \int d\mathbf{r}' \langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}'' \rangle \cdot \langle \mathbf{r}'' | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle \\ &= \int d\mathbf{r}'' \int d\mathbf{r}' \frac{\hbar}{i} \nabla_r \delta(\mathbf{r} - \mathbf{r}'') \cdot \langle \mathbf{r}'' | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle. \end{aligned} \quad (11.66)$$

Since  $\nabla_r$  acts only on  $\mathbf{r}$ , I can take it out of the integral and obtain

$$\begin{aligned} &\int d\mathbf{r}' \langle \mathbf{r} | \hat{p}^2 | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle \\ &= \frac{\hbar}{i} \nabla_r \int d\mathbf{r}'' \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}'') \cdot \langle \mathbf{r}'' | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle \\ &= \frac{\hbar}{i} \nabla_r \cdot \int d\mathbf{r}' \langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | E \rangle = \frac{\hbar}{i} \nabla_r \cdot \int d\mathbf{r}' \frac{\hbar}{i} \nabla_r \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | E \rangle \\ &= -\hbar^2 \nabla_r \cdot \nabla_r \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | E \rangle = -\hbar^2 \nabla_r^2 \langle \mathbf{r} | E \rangle \end{aligned} \quad (11.67)$$

or

$$-\frac{\hbar^2}{2m} \nabla_r^2 \langle \mathbf{r} | E \rangle + V(\mathbf{r}) \langle \mathbf{r} | E \rangle = E \langle \mathbf{r} | E \rangle. \quad (11.68)$$

But this is nothing more (or less) than Schrödinger's equation if I identify

$$\langle \mathbf{r} | E \rangle = \psi_E(\mathbf{r}). \quad (11.69)$$

*Diagonalizing  $\underline{H}$  in the  $|\mathbf{r}\rangle$  basis is equivalent to solving the Schrödinger equation!* I now have the connection between Dirac notation and the wave function. In general, the bra-ket notation doesn't simplify the problem, since we still have to solve the Schrödinger equation. Nevertheless Dirac notation provides a powerful formalism that lets us express results in a basis-independent fashion.

Often, I will need to calculate the matrix elements of an operator  $\hat{A}$  in the energy basis, namely  $\langle E | \hat{A} | E' \rangle$ . Suppose that the operator  $\hat{A}$  corresponds to a physical variable  $A(\mathbf{r})$  that is a function of coordinates only— $\hat{A}$  is diagonal in the  $|\mathbf{r}\rangle$  basis.

Then

$$\begin{aligned}
 \langle E | \hat{A} | E' \rangle &= \int d\mathbf{r} d\mathbf{r}' \langle E | \mathbf{r} \rangle \langle \mathbf{r} | \hat{A} | \mathbf{r}' \rangle \langle \mathbf{r}' | E' \rangle \\
 &= \int d\mathbf{r} d\mathbf{r}' \psi_E^*(\mathbf{r}) A(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \psi_{E'}(\mathbf{r}') \\
 &= \int d\mathbf{r} \psi_E^*(\mathbf{r}) \hat{A}(\mathbf{r}) \psi_{E'}(\mathbf{r})
 \end{aligned} \tag{11.70}$$

is the way in which matrix elements are most often evaluated.

### 11.1.3 Schrödinger's Equation in Momentum Space

As an example of the use of Dirac notation, I derive the time-independent Schrödinger's equation in momentum space. As in coordinate space, I expand

$$|E\rangle = \int d\mathbf{p} \langle \mathbf{p} | E \rangle | \mathbf{p} \rangle \tag{11.71}$$

and try to find the expansion coefficients  $\langle \mathbf{p} | E \rangle$ . I start from  $\hat{H} | E \rangle = E | E \rangle$  and multiply on the left by  $\langle \mathbf{p} |$  to get

$$\langle \mathbf{p} | \left( \frac{\hat{p}^2}{2m} + \hat{V} \right) | E \rangle = E \langle \mathbf{p} | E \rangle. \tag{11.72}$$

I proceed as before and obtain

$$\begin{aligned}
 &\int d\mathbf{p}' \langle \mathbf{p} | \left( \frac{\hat{p}^2}{2m} + \hat{V} \right) | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle = E \langle \mathbf{p} | E \rangle; \\
 &\int d\mathbf{p}' \left( \frac{p'^2}{2m} \delta(\mathbf{p} - \mathbf{p}') + \langle \mathbf{p} | \hat{V} | \mathbf{p}' \rangle \right) \langle \mathbf{p}' | E \rangle = E \langle \mathbf{p} | E \rangle; \\
 &\frac{p^2}{2m} \langle \mathbf{p} | E \rangle + \int d\mathbf{p}' \langle \mathbf{p} | \hat{V} | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle = E \langle \mathbf{p} | E \rangle.
 \end{aligned} \tag{11.73}$$

However, I do not know matrix elements of  $\hat{V}$  in the  $|\mathbf{p}\rangle$  basis, but do know them in the  $|\mathbf{r}\rangle$  basis. So I add some more completeness relations:

$$\begin{aligned}
 &\int d\mathbf{p}' \langle \mathbf{p} | \hat{V} | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle \\
 &= \int d\mathbf{r}' \int d\mathbf{r} \int d\mathbf{p}'' \langle \mathbf{p} | \mathbf{r} \rangle \langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle \langle \mathbf{r}' | \mathbf{p}'' \rangle \langle \mathbf{p}'' | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle
 \end{aligned}$$

$$\begin{aligned}
&= \int d\mathbf{r}' \int d\mathbf{r} \int d\mathbf{p}' \langle \mathbf{p} | \mathbf{r} \rangle V(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle \\
&= \int d\mathbf{r} V(\mathbf{r}) \int d\mathbf{p}' \langle \mathbf{p} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle.
\end{aligned} \tag{11.74}$$

To evaluate this I need to know the value of  $\langle \mathbf{p} | \mathbf{r} \rangle = \langle \mathbf{r} | \mathbf{p} \rangle^*$ .

To evaluate  $\langle \mathbf{r} | \mathbf{p} \rangle$ , I start from the eigenvalue equation

$$\hat{\mathbf{p}} |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle; \tag{11.75}$$

$$\langle \mathbf{r} | \hat{\mathbf{p}} |\mathbf{p}\rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle; \tag{11.76}$$

$$\int d\mathbf{r}' \langle \mathbf{r} | \hat{\mathbf{p}} |\mathbf{r}'\rangle \langle \mathbf{r}' | \mathbf{p} \rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle; \tag{11.77}$$

$$\frac{\hbar}{i} \int d\mathbf{r}' \nabla_r \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | \mathbf{p} \rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle; \tag{11.78}$$

$$\frac{\hbar}{i} \nabla_r \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | \mathbf{p} \rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle; \tag{11.79}$$

$$\frac{\hbar}{i} \nabla_r \langle \mathbf{r} | \mathbf{p} \rangle = \mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle; \tag{11.80}$$

$$\langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} = \langle \mathbf{p} | \mathbf{r} \rangle^*, \tag{11.81}$$

where a normalization factor has been included to ensure that

$$\langle \mathbf{r} | \mathbf{r}' \rangle = \int d\mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}' \rangle = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{p} e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')/\hbar} = \delta(\mathbf{r} - \mathbf{r}'). \tag{11.82}$$

Substituting Eq. (11.81) into Eq. (11.74) I obtain

$$\begin{aligned}
\int d\mathbf{p}' \langle \mathbf{p} | \hat{V} | \mathbf{p}' \rangle \langle \mathbf{p}' | E \rangle &= (2\pi\hbar)^{-3} \int d\mathbf{p}' \int d\mathbf{r} V(\mathbf{r}) e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} \langle \mathbf{p}' | E \rangle \\
&= (2\pi\hbar)^{-3/2} \int d\mathbf{p}' \tilde{V}(\mathbf{p} - \mathbf{p}') \langle \mathbf{p}' | E \rangle,
\end{aligned} \tag{11.83}$$

where

$$\tilde{V}(\mathbf{q}) = (2\pi\hbar)^{-3/2} \int d\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}/\hbar} \tag{11.84}$$

is the Fourier transform of  $V(\mathbf{r})$ . Combining Eqs. (11.73), (11.74), and (11.83), I arrive at

$$\frac{p^2}{2m} \Phi_E(\mathbf{p}) + \frac{1}{(2\pi\hbar)^{3/2}} \int d\mathbf{p}' \tilde{V}(\mathbf{p} - \mathbf{p}') \Phi_E(\mathbf{p}') = E \Phi_E(\mathbf{p}), \quad (11.85)$$

which is Schrödinger's equation in momentum space for the wave function

$$\Phi_E(\mathbf{p}) = \langle \mathbf{p} | E \rangle. \quad (11.86)$$

In momentum space, Schrödinger's equation is an integral equation.

Also, given the fact that

$$|\mathbf{r}\rangle = \int d\mathbf{p} \langle \mathbf{p} | \mathbf{r} \rangle |\mathbf{p}\rangle, \quad (11.87)$$

I can multiply on the left by  $\langle E |$  and use Eq. (11.81) to obtain

$$\langle E | \mathbf{r} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d\mathbf{p} \langle E | \mathbf{p} \rangle e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (11.88)$$

Taking the complex conjugate of this equation and using Eqs. (11.69) and (11.86), I find

$$\psi_E(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d\mathbf{p} \Phi_E(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (11.89)$$

The energy eigenfunctions in coordinate and momentum space are Fourier transforms of one another. Earlier I postulated this result and was able to derive the commutation relations for the position and momentum operators. Here I postulated the commutation relations and was led to the result that  $\psi_E(\mathbf{r})$  and  $\Phi_E(\mathbf{p})$  are Fourier transforms of one another.

Although I have shown that diagonalizing the Hamiltonian in the coordinate representation is equivalent to solving the Schrödinger equation, there are some cases where it is possible to get the eigenvalues and eigenfunctions working directly from the Dirac notation formalism. I now turn my attention to two such cases, the simple harmonic oscillator and the angular momentum operator.

## 11.2 Simple Harmonic Oscillator

Let us reconsider the SHO in 1-D which has a Hamiltonian in units of  $\hbar\omega$  given by

$$\hat{H}' = \frac{\hat{H}}{\hbar\omega} = \frac{1}{2} (\hat{\eta}^2 + \hat{\xi}^2), \quad (11.90)$$

where

$$\hat{\xi} = \sqrt{\frac{m\omega}{\hbar}} \hat{x}; \quad (11.91a)$$

$$\hat{\eta} = \sqrt{\frac{1}{\hbar m\omega}} \hat{p} = \frac{1}{i} \frac{\partial}{\partial \xi}. \quad (11.91b)$$

It will prove convenient to introduce operators  $a$  and  $a^\dagger$  (I don't put hats on them even though they are operators) that are defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} + i \frac{\hat{p}}{m\omega} \right) = \frac{\hat{\xi} + i\hat{\eta}}{\sqrt{2}}; \quad (11.92a)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} - i \frac{\hat{p}}{m\omega} \right) = \frac{\hat{\xi} - i\hat{\eta}}{\sqrt{2}}. \quad (11.92b)$$

In terms of these operators,

$$\hat{H}' = a^\dagger a + \frac{1}{2} = \hat{n} + \frac{1}{2}, \quad (11.93)$$

where

$$\hat{n} = a^\dagger a. \quad (11.94)$$

The operators  $a$  and  $a^\dagger$  satisfy the commutation relations

$$[a, a^\dagger] = -[a^\dagger, a] = 1; \quad [a, a] = [a^\dagger, a^\dagger] = 0. \quad (11.95)$$

It turns out, by being a bit clever, you can find the eigenenergies and eigenfunctions of the SHO without solving the Schrödinger equation. For reasons that will become obvious, the operators  $a$  and  $a^\dagger$  are often referred to as *ladder operators* and  $\hat{n}$  as the *number operator*.

To start, I label the eigenkets of  $\hat{n}$  by  $|n\rangle$  without any restriction on  $n$  (it need not be an integer) such that

$$\hat{H}' |n\rangle = \left( \hat{n} + \frac{1}{2} \right) |n\rangle = \epsilon_n |n\rangle \quad (11.96)$$

where

$$\epsilon_n = E_n/\hbar\omega = (n + 1/2). \quad (11.97)$$

and the energy  $E_n$  is given by

$$E_n = (n + 1/2)\hbar\omega. \quad (11.98)$$

This is perfectly arbitrary since there is no restriction on  $n$ .

The operator  $a$  is a *lowering* or *destruction* operator, which can be proved as follows: First I note that

$$\hat{H}'(a|n\rangle) = \hat{H}'a|n\rangle = \left( [\hat{H}', a] + a\hat{H}' \right) |n\rangle. \quad (11.99)$$

But

$$[\hat{H}', a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a] a = -a, \quad (11.100)$$

implying that

$$\begin{aligned} \hat{H}'(a|n\rangle) &= (-a + a\hat{H}')|n\rangle = [-a + a(n + 1/2)]|n\rangle \\ &= [(n - 1) + 1/2](a|n\rangle). \end{aligned} \quad (11.101)$$

In other words,  $(a|n\rangle)$  is an eigenket of  $\hat{H}'$  having eigenvalue  $n - 1$ .

By successively applying the operator  $a$ , I keep lowering the eigenvalue by one. However, the expectation value of the number operator is always positive or zero, since

$$\langle n | \hat{n} | n \rangle = \langle n | a^\dagger a | n \rangle = (a|n\rangle)^\dagger (a|n\rangle) \geq 0. \quad (11.102)$$

Thus as I keep applying the operator  $a$ , I must come to a lowest state  $|n_{\min}\rangle$  for which  $a|n_{\min}\rangle = 0$ . As a consequence,

$$a^\dagger(a|n_{\min}\rangle) = 0 = \hat{n}|n_{\min}\rangle = n_{\min}|n_{\min}\rangle, \quad (11.103)$$

which requires that  $n_{\min} = 0$ . The value of  $n_{\min} = 0$  was reached by continually lowering  $n$  by one; therefore,  $n$  must be a positive integer or zero and the (dimensionless) eigenenergies are

$$\epsilon_n = (n + 1/2); \quad n = 0, 1, 2, 3, \dots \quad (11.104)$$

I have obtained the eigenenergies without having solved Schrödinger's equation.

Since  $(a|n\rangle)$  is an eigenket of  $\hat{H}$  having eigenvalue  $n - 1$ , I can write

$$a|n\rangle = c_n|n - 1\rangle, \quad (11.105)$$

where  $c_n$  is a constant. Thus

$$\begin{aligned} n &= \langle n | a^\dagger a | n \rangle = (a|n\rangle)^\dagger (a|n\rangle) = (c_n|n - 1\rangle)^\dagger (c_n|n - 1\rangle) \\ &= |c_n|^2 \langle n - 1 | n - 1 \rangle = |c_n|^2. \end{aligned} \quad (11.106)$$

If I choose the phase of  $c_n$  equal to zero, then  $c_n = \sqrt{n}$  and

$$a|n\rangle = \sqrt{n}|n-1\rangle. \quad (11.107)$$

In a similar manner I can show that  $a^\dagger$  is a *raising* or *creation* operator and that

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad (11.108)$$

such that the number operator leaves the ket unchanged,

$$\hat{n}|n\rangle = a^\dagger a|n\rangle = n|n\rangle, \quad (11.109)$$

as required since the Hamiltonian is diagonal in the  $|n\rangle$  basis.

From Eq. (11.108), it follows that

$$|1\rangle = \frac{a^\dagger}{\sqrt{1!}}|0\rangle; \quad |2\rangle = \frac{a^\dagger}{\sqrt{1!}}|1\rangle = \frac{(a^\dagger)^2}{\sqrt{2!}}|0\rangle, \quad (11.110)$$

and so forth, leading to

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (11.111)$$

The (dimensionless) wave function in terms of dimensionless variables is given by

$$\psi_n(\xi) = \langle \xi | n \rangle. \quad (11.112)$$

Using ladder operators I have obtained the eigenenergies and expressions for all the eigenkets in terms of the eigenket  $|0\rangle$ , but have not yet found explicit expressions for the wave functions.

To do so, I look at the equation

$$a|0\rangle = 0, \quad (11.113)$$

put in a complete set via

$$\int_{-\infty}^{\infty} d\xi' a|\xi'\rangle \langle \xi' | 0 \rangle = 0, \quad (11.114)$$

and multiply on the left by  $\langle \xi |$ ,

$$\int_{-\infty}^{\infty} d\xi' \langle \xi | a |\xi'\rangle \psi_0(\xi') = 0; \quad (11.115a)$$

$$\int_{-\infty}^{\infty} d\xi' \langle \xi | \left( \hat{\xi} + i\hat{\eta} \right) |\xi'\rangle \psi_0(\xi') = 0; \quad (11.115b)$$

$$\int_{-\infty}^{\infty} d\xi' \left[ \xi \delta(\xi - \xi') + \frac{d\delta(\xi - \xi')}{d\xi} \right] \psi_0(\xi') = 0; \quad (11.115c)$$

$$\xi \psi_0(\xi) + \frac{d}{d\xi} \int_{-\infty}^{\infty} d\xi' \delta(\xi - \xi') \psi_0(\xi') = 0, \quad (11.115d)$$

which leads to

$$\xi \psi_0(\xi) + \frac{d\psi_0(\xi)}{d\xi} = 0. \quad (11.116)$$

The solution of this equation is

$$\psi_0(\xi) = N \exp(-\xi^2/2) \quad (11.117)$$

where  $N = \pi^{-1/4}$  is a normalization factor. Thus I have found the ground state wave function. Higher order wave functions can be calculated using the recursion relations that are given in Chap. 7. In fact I could derive the needed recursion relation by starting from Eq. (11.108) and multiplying on the left by  $\langle \xi |$ ; that is,

$$\langle \xi | a^\dagger | n \rangle = \sqrt{n+1} \langle \xi | n+1 \rangle = \sqrt{n+1} \psi_{n+1}(\xi) = \langle \xi | (\hat{\xi} - i\hat{\eta}) | n \rangle / \sqrt{2}. \quad (11.118)$$

Following the same procedure that led to Eq. (11.116), I find

$$\sqrt{2(n+1)} \psi_{n+1}(\xi) = \xi \psi_n(\xi) - \frac{d\psi_n(\xi)}{d\xi}, \quad (11.119)$$

which is Eq. (7.47c) and allows you to calculate all the wave functions if you know  $\psi_0(\xi)$ . The ladder operators  $a$  and  $a^\dagger$  are particularly useful for obtaining matrix elements of operators of the form  $\xi^m$  for the harmonic oscillator. I will use them in applications of perturbation theory.

### 11.2.1 Coherent State

I want to return to the coherent state that I have already introduced in my discussion of the harmonic oscillator in Chap. 7, where I found that, for an initial wave function

$$\psi_{\text{coh}}(\xi, 0) = \frac{1}{\pi^{1/4}} e^{-(\xi - \xi_0)^2/2} = \sum_{n=0}^{\infty} \frac{(\xi_0/\sqrt{2})^n e^{-(\xi_0/\sqrt{2})^2/2}}{\sqrt{n!}} \psi_n(\xi), \quad (11.120)$$

the wave packet envelope does not change its shape as a function of time. In terms of Dirac notation this state is

$$|\psi(0)\rangle_{\text{coh}} = \sum_{n=0}^{\infty} \frac{\left(\xi_0/\sqrt{2}\right)^n e^{-(\xi_0/\sqrt{2})^2/2}}{\sqrt{n!}} |n\rangle, \quad (11.121)$$

such that

$$\begin{aligned} |\psi(t)\rangle_{\text{coh}} &= e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{\left(\xi_0/\sqrt{2}\right)^n e^{-(\xi_0/\sqrt{2})^2/2} e^{-in\omega t}}{\sqrt{n!}} |n\rangle \\ &= e^{-i\omega t/2} |\psi_{\text{coh}}(t)\rangle, \end{aligned} \quad (11.122)$$

where

$$|\psi_{\text{coh}}(t)\rangle = \sum_{n=0}^{\infty} \frac{\left(\xi_0/\sqrt{2}\right)^n e^{-(\xi_0/\sqrt{2})^2/2} e^{-in\omega t}}{\sqrt{n!}} |n\rangle. \quad (11.123)$$

is the conventional form for a coherent state vector. In taking expectation values of operators, it makes no difference whether I use  $|\psi(t)\rangle_{\text{coh}}$  or  $|\psi_{\text{coh}}(t)\rangle$ .

It is now a relatively simple matter to calculate

$$\langle \hat{\xi} \rangle_{\text{coh}} = \frac{1}{\sqrt{2}} \langle \psi_{\text{coh}}(t) | (a + a^\dagger) | \psi_{\text{coh}}(t) \rangle \quad (11.124)$$

and

$$\begin{aligned} \langle \hat{\xi}^2 \rangle_{\text{coh}} &= \frac{1}{2} \langle \psi_{\text{coh}}(t) | (a + a^\dagger)^2 | \psi_{\text{coh}}(t) \rangle \\ &= \frac{1}{2} \langle \psi_{\text{coh}}(t) | (a^2 + a^{\dagger 2} + 2a^\dagger a + 1) | \psi_{\text{coh}}(t) \rangle \end{aligned} \quad (11.125)$$

and show they are consistent with a wave packet that oscillates in the potential without changing its shape.

Instead, I adopt somewhat different method that is useful in oscillator problems and in quantum optics. I define

$$\xi(t) = \xi_0 e^{-i\omega t} / \sqrt{2} \quad (11.126)$$

and operate with the destruction operator on  $|\psi_{\text{coh}}(t)\rangle$ ,

$$a |\psi_{\text{coh}}(t)\rangle = \sum_{n=0}^{\infty} \frac{[\xi(t)]^n e^{-|\xi(t)|^2/2}}{\sqrt{n!}} \sqrt{n} |n-1\rangle$$

$$\begin{aligned}
&= \xi(t) \sum_{n=1}^{\infty} \frac{[\xi(t)]^{n-1} e^{-|\xi(t)|^2/2}}{\sqrt{(n-1)!}} |n-1\rangle \\
&= \xi(t) \sum_{n=0}^{\infty} \frac{[\xi(t)]^n e^{-|\xi(t)|^2/2}}{\sqrt{n!}} |n\rangle \\
&= \xi(t) |\psi_{\text{coh}}(t)\rangle. \tag{11.127}
\end{aligned}$$

Thus, the coherent state at time  $t$  is an eigenstate of the destruction operator with eigenvalue  $\xi(t)$ .<sup>2</sup> I change the notation by writing

$$|\xi(t)\rangle_{\text{coh}} \equiv |\psi_{\text{coh}}(t)\rangle = \sum_{n=0}^{\infty} \frac{[\xi(t)]^n e^{-|\xi(t)|^2/2}}{\sqrt{n!}} |n\rangle, \tag{11.128a}$$

such that

$$a |\xi(t)\rangle_{\text{coh}} = \xi(t) |\xi(t)\rangle_{\text{coh}}. \tag{11.128b}$$

Somewhat more generally, the coherent state of an oscillator,  $|\alpha\rangle$ , can be defined by

$$a |\alpha\rangle = \alpha |\alpha\rangle \tag{11.129}$$

with

$$\begin{aligned}
|\alpha\rangle &= \sum_n \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2} |n\rangle \\
&= \sum_n \frac{(\alpha a^\dagger)^n}{n!} e^{-|\alpha|^2/2} |0\rangle = e^{\alpha a^\dagger} e^{-|\alpha|^2/2} |0\rangle. \tag{11.130}
\end{aligned}$$

Equation (11.129) is an alternative definition of a coherent state. Thus for the coherent state  $|\psi_{\text{coh}}(t)\rangle$  having

$$\alpha(t) = \left( \xi_0 e^{-i\omega t} / \sqrt{2} \right), \tag{11.131}$$

with  $\xi_0$  real,

$$\langle \xi \rangle_{\text{coh}} = \frac{1}{\sqrt{2}} \langle \alpha(t) | (a + a^\dagger) | \alpha(t) \rangle = \frac{\alpha(t) + \alpha^*(t)}{\sqrt{2}} = \xi_0 \cos(\omega t) \tag{11.132}$$

<sup>2</sup>Since  $\hat{a}$  is not a Hermitian operator, there is no guarantee that it possesses an orthonormal set of eigenkets (in fact, the eigenkets are *not* orthogonal). If you try to follow a procedure similar to the one that led to Eq. (11.127) to arrive at an eigenvalue equation for  $\hat{a}^\dagger$ , you will find that it is not possible—a set of normalizable eigenkets does not exist for the operator  $\hat{a}^\dagger$ .

and

$$\begin{aligned}
 \langle \xi^2 \rangle_{\text{coh}} &= \frac{1}{2} \langle \alpha(t) | \frac{(a^2 + a^{\dagger 2} + 2a^\dagger a + 1)}{2} | \alpha(t) \rangle \\
 &= \frac{1}{2} \left[ \alpha^2(t) + [\alpha^*(t)]^2 + 2|\alpha(t)|^2 + 1 \right] \\
 &= \left( \frac{\xi_0}{\sqrt{2}} \right)^2 \frac{e^{2i\omega t} + e^{-2i\omega t} + 2}{2} + \frac{1}{2} \\
 &= \xi_0^2 \cos^2(\omega t) + 1/2.
 \end{aligned} \tag{11.133}$$

From Eqs. (11.132) and (11.133), I find that the variance

$$\Delta \xi^2 = \langle \xi^2 \rangle - \langle \xi \rangle^2 = \frac{1}{2} \tag{11.134}$$

is constant in time—the wave packet does not spread.<sup>3</sup> The coherent state with  $\xi_0 = 0$  is the *vacuum state* of the oscillator and is simply the ground state of the oscillator. For  $\xi_0 \neq 0$ , the wave packet corresponds to the ground state eigenfunction displaced by an amount  $\xi_0$  and oscillates in the potential without changing its shape.

### 11.3 Angular Momentum Operator

Angular momentum can also be analyzed using ladder operators. I designate the simultaneous eigenkets of  $\hat{L}^2$  and  $\hat{L}_z$  by  $|\gamma\beta\rangle$ ; that is,

$$\hat{L}^2 |\gamma\beta\rangle = \hbar^2 \gamma |\gamma\beta\rangle \tag{11.135a}$$

$$\hat{L}_z |\gamma\beta\rangle = \hbar \beta |\gamma\beta\rangle. \tag{11.135b}$$

At this point,  $\gamma$  and  $\beta$  are totally arbitrary. Given that  $\hat{L}$  is Hermitian,  $\hat{L}^2 = \hat{L}^\dagger \cdot \hat{L}$  must have non-negative eigenvalues;  $\gamma \geq 0$ . Moreover, since the expectation value of  $\hat{L}_x^2 + \hat{L}_y^2$  in any state must also be non-negative, it follows that

$$\langle \gamma\beta | (\hat{L}^2 - \hat{L}_z^2) | \gamma\beta \rangle = \langle \gamma\beta | (\hat{L}_x^2 + \hat{L}_y^2) | \gamma\beta \rangle = \hbar^2 (\gamma - \beta^2) \geq 0, \tag{11.136}$$

<sup>3</sup> I have proved only that the variance is constant, not that the absolute square of the wave function does not change its shape. That result was proved in Chap. 7. However, you can prove that all moments of the coordinate for the oscillator are constant, which is equivalent to proving the wave packet does not change its shape.

or

$$\gamma \geq \beta^2. \quad (11.137)$$

This is not a surprising result—we expect the  $z$ -component of angular momentum to be less than or equal to the magnitude of the angular momentum.

I now form ladder operators

$$\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y. \quad (11.138)$$

The fact that these are ladder operators follows from the commutation relations

$$[\hat{L}_z, \hat{L}_{\pm}] = [\hat{L}_z, \hat{L}_x \pm i\hat{L}_y] = i\hbar (\hat{L}_y \mp i\hat{L}_x) = \pm\hbar\hat{L}_{\pm}. \quad (11.139)$$

Using these commutation relations, I find

$$\hat{L}_{\pm}\hat{L}_z|\gamma\beta\rangle = \hbar\beta\hat{L}_{\pm}|\gamma\beta\rangle = (\mp\hbar\hat{L}_{\pm} + \hat{L}_z\hat{L}_{\pm})|\gamma\beta\rangle, \quad (11.140)$$

or

$$\hat{L}_z[\hat{L}_{\pm}|\gamma\beta\rangle] = \hbar(\beta \pm 1)[\hat{L}_{\pm}|\gamma\beta\rangle]. \quad (11.141)$$

In other words,  $\hat{L}_{\pm}|\gamma\beta\rangle$  is an eigenket of  $\hat{L}_z$  having eigenvalue  $\hbar(\beta \pm 1)$ , namely

$$\hat{L}_{\pm}|\gamma\beta\rangle = \hbar C_{\pm}(\gamma, \beta)|\gamma, \beta \pm 1\rangle, \quad (11.142)$$

where  $C_{\pm}(\gamma, \beta)$  is a constant.

Thus, by applying  $\hat{L}_{\pm}$  to  $|\gamma\beta\rangle$  successively, I keep raising or lowering the eigenvalues by one unit of  $\hbar$ . This cannot go on forever, however, since I know that  $\gamma \geq \beta^2$ . Thus there must be a maximum value  $\beta_{\max}$  and a minimum value  $\beta_{\min}$  for which

$$\hat{L}_+|\gamma, \beta_{\max}\rangle = 0; \quad (11.143a)$$

$$\hat{L}_-|\gamma, \beta_{\min}\rangle = 0, \quad (11.143b)$$

implying that

$$(\beta_{\max} - \beta_{\min}) = \text{positive integer or zero.} \quad (11.144)$$

I now calculate

$$\langle\gamma, \beta_{\max}|\hat{L}_-\hat{L}_+|\gamma\beta_{\max}\rangle = 0; \quad (11.145)$$

$$\langle\gamma, \beta_{\max}|\left(\hat{L}_x - i\hat{L}_y\right)\left(\hat{L}_x + i\hat{L}_y\right)|\gamma\beta_{\max}\rangle = 0; \quad (11.146)$$

$$\langle \gamma, \beta_{\max} | \hat{L}_x^2 + \hat{L}_y^2 - i [\hat{L}_y, \hat{L}_x] | \gamma \beta_{\max} \rangle = 0; \quad (11.147)$$

$$\langle \gamma, \beta_{\max} | \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z | \gamma \beta_{\max} \rangle = 0; \quad (11.148)$$

$$\gamma - \beta_{\max}^2 - \beta_{\max} = 0; \quad (11.149)$$

$$\gamma = \beta_{\max} (\beta_{\max} + 1). \quad (11.150)$$

Similarly by considering  $\langle \gamma, \beta_{\min} | \hat{L}_+ \hat{L}_- | \gamma \beta_{\min} \rangle = 0$ , I find

$$\gamma = \beta_{\min} (\beta_{\min} - 1), \quad (11.151)$$

from which it follows that  $\beta_{\min} = -\beta_{\max}$  and, using Eq. (11.144), that

$$2\beta_{\max} = \text{positive integer or zero.} \quad (11.152)$$

From Eqs. (11.150) and (11.144) you see that  $\gamma = \ell(\ell + 1)$ , where  $\ell = \beta_{\max}$  is a positive half-integer, integer, or zero, and  $\beta$ , which I now denote by  $m$ , can take on values from  $-\ell$  to  $\ell$  in integer steps. Thus, as for the SHO, I obtained the eigenvalues of the operators  $\hat{L}^2$  and  $\hat{L}_z$  without solving a differential equation.

To obtain the values of  $C_+(\ell, m)$  appearing in Eq. (11.142), I evaluate

$$\begin{aligned} \langle \ell, m | \hat{L}_- \hat{L}_+ | \ell, m \rangle &= \left( \hat{L}_+ | \ell, m \rangle \right)^\dagger \hat{L}_+ | \ell, m \rangle \\ &= \hbar^2 |C_+(\ell, m)|^2 \langle \ell, m+1 | \ell, m+1 \rangle = \hbar^2 |C_+(\ell, m)|^2 \\ &= \langle \ell, m | \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z | \ell, m \rangle = \hbar^2 [\ell(\ell + 1) - m^2 - m], \end{aligned} \quad (11.153)$$

having used the identity  $\hat{L}_- \hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z$ . Consequently,

$$C_+(\ell, m) = \sqrt{\ell(\ell + 1) - m^2 - m} \quad (11.154)$$

and

$$\begin{aligned} \hat{L}_+ | \ell, m \rangle &= \hbar C_+(\ell, m) | \ell, m+1 \rangle = \hbar \sqrt{\ell(\ell + 1) - m^2 - m} | \ell, m+1 \rangle \\ &= \hbar \sqrt{(\ell - m)(\ell + m + 1)} | \ell, m+1 \rangle. \end{aligned} \quad (11.155)$$

Similarly, you can show that

$$C_-(\ell, m) = \sqrt{\ell(\ell + 1) - m^2 + m} \quad (11.156)$$

and

$$\begin{aligned} \hat{L}_- | \ell, m \rangle &= \hbar C_-(\ell, m) | \ell, m-1 \rangle = \hbar \sqrt{\ell(\ell + 1) - m^2 + m} | \ell, m-1 \rangle \\ &= \hbar \sqrt{(\ell + m)(\ell - m + 1)} | \ell, m-1 \rangle. \end{aligned} \quad (11.157)$$

These are equations that will prove useful in later chapters.

Finally, I need to say something about the half-integral values of  $\ell$  and  $m$ , which are not ruled out by this discussion. Half-integral values of angular momentum *are* possible when electron spin is included. However, without spin I can expand the  $|\ell m\rangle$  kets in terms of the kets in coordinate space as

$$|\ell m\rangle = \int d\mathbf{r} \langle \mathbf{r} | \ell m \rangle |\mathbf{r}\rangle. \quad (11.158)$$

In Appendix B, I obtain matrix elements of  $\hat{\mathbf{L}}$  in the  $|\mathbf{r}\rangle$  basis and, starting from

$$\hat{L}_z |\ell m\rangle = m\hbar |\ell m\rangle; \quad (11.159a)$$

$$\hat{L}^2 |\ell m\rangle = \hbar^2 \ell(\ell + 1) |\ell m\rangle, \quad (11.159b)$$

I prove that the expansion coefficients  $\langle \mathbf{r} | \ell m \rangle$  are solutions of the differential equation for the spherical harmonics. I have already shown that the only physically acceptable solutions for the spherical harmonics that are regular at both  $\theta = 0, \pi$  and are unchanged when  $\phi \rightarrow \phi + 2\pi$  correspond to integral values of  $\ell$  and  $m$  with  $\ell \geq |m|$ . As a consequence, the half-integral values of  $\ell$  and  $m$  must be rejected.

The expansion coefficient  $\langle \mathbf{r} | \ell m \rangle$  is proportional to, but not equal to  $Y_\ell^m(\theta, \phi)$  (it has the wrong units). To identify the spherical harmonic with an inner product in Dirac notation, I write the ket  $|\mathbf{r}\rangle$  as

$$|\mathbf{r}\rangle = \frac{|r\rangle |\mathbf{u}_r\rangle}{r}, \quad (11.160)$$

where  $|\mathbf{u}_r\rangle$  satisfies the orthogonality condition

$$\langle \mathbf{u}_r | \mathbf{u}'_r \rangle = \delta(\cos \theta - \cos \theta') \delta(\phi - \phi') \quad (11.161)$$

and can be interpreted as a solid-angle ket since the unit vector  $\mathbf{u}_r$  depends only on the spherical angles  $\theta$  and  $\phi$ . Equations (11.160) and (11.161) are consistent with the fact that

$$\langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') = \frac{\delta(r - r') \delta(\cos \theta - \cos \theta') \delta(\phi - \phi')}{r^2}. \quad (11.162)$$

In terms of these solid angle kets (see Appendix B)

$$\langle \mathbf{u}_r | \ell m \rangle = Y_\ell^m(\theta, \phi), \quad (11.163)$$

which relates the spherical harmonics to inner products in Dirac notation.

## 11.4 Solving Problems Using Dirac Notation

Things have been a bit formal in discussing Dirac notation, so let me summarize where and when you use it in practical situations relative to the Schrödinger equation. In general, you can often solve problems involving a discrete subspace using Dirac notation, but need the Schrödinger equation to solve problems involving an infinite number of levels. I give a few examples below to help illustrate these points.

### 11.4.1 Hydrogen Atom

I have already solved Schrödinger's equation for the hydrogen atom potential and found that, if  $E < 0$ , there is an infinite number of bound states. I also obtained the wave functions associated with these bound states. For  $E > 0$ , there is an infinite number of continuum states along with their associated eigenfunctions.

If you try to solve this problem using Dirac notation, you start from

$$\hat{H} |E\rangle = E |E\rangle, \quad (11.164)$$

but this is useless for obtaining the eigenvalues since you don't already know them! To proceed, you expand

$$|E\rangle = \int d\mathbf{r} \langle \mathbf{r} | E \rangle |\mathbf{r}\rangle \quad (11.165)$$

and try to find the expansion coefficients  $\langle \mathbf{r} | E \rangle$ . I have already shown that these expansion coefficients satisfy the Schrödinger equation, so there is no advantage in using Dirac notation to obtain the eigenvalues and eigenfunctions of the hydrogen atom. On the other hand, you can label the eigenkets of the hydrogen atom by the eigenvalues of the commuting operators  $\hat{H}, \hat{L}^2, \hat{L}_z$ , namely  $|n, \ell, m\rangle$ , where  $n, \ell, m$  are the quantum numbers corresponding to these physical quantities.

### 11.4.2 Harmonic Oscillator

This is a mixed case. You can solve for the eigenfunctions and eigenvalues using the Schrödinger equation without much trouble. However, as we have seen, it is also possible to introduce ladder operators and solve for the eigenvalues and eigenfunctions without having ever solved the Schrödinger equation directly. Calculation of matrix elements is easiest using the ladder operators. Although not so obvious, it is also possible to solve for the eigenvalues of the hydrogen atom

without solving the Schrödinger equation based on the group  $O(4)$  and the fact that both angular momentum and the Lenz vector are conserved.<sup>4</sup>

### 11.4.3 Angular Momentum

I will discuss formal aspects of angular momentum in Chaps. 19–20. Dirac notation is the preferred notation for dealing with angular momentum since you can label the simultaneous eigenkets of  $\hat{L}^2$  and  $\hat{L}_z$  by  $|\ell m_\ell\rangle$  and write matrices for both  $L^2$  and  $\hat{L}_z$ . For a given integral value of  $\ell$ , each of these diagonal matrices has dimension  $(2\ell + 1) \times (2\ell + 1)$ .

To illustrate the power of Dirac notation, I would like to discuss the eigenkets of  $\hat{L}^2$  and either  $\hat{L}_x$  and  $\hat{L}_z$ . I represent the eigenkets of  $\hat{L}^2$  and  $\hat{L}_x$  by  $|\ell, \ell_x\rangle$  and those of  $\hat{L}^2$  and  $\hat{L}_z$  by  $|\ell, \ell_z\rangle$ . Clearly the *eigenvalues* must be identical, since there is nothing *physically* that can distinguish  $\hat{L}_x$  from  $\hat{L}_z$ . I can take the basis kets (a column vector with a 1 in one place and zeroes everywhere else) to be those of  $\hat{L}_x$  or  $\hat{L}_z$ , but *not both*. For example, let me take the basis kets to be  $|\ell, \ell_z\rangle$  and take  $\ell = 1$ . In this  $\ell = 1$  subspace

$$\underline{L}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar, \quad (11.166)$$

where the order is  $\ell_z = 1, 0, -1$ . Moreover, using ladder operators, it is easy to calculate

$$\underline{L}_x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{\hbar}{\sqrt{2}}. \quad (11.167)$$

By diagonalizing  $\underline{L}_x$  I find the eigenvalues  $\ell_x = 1, 0, -1$  as expected. The eigenkets (with the  $\ell = 1$  label suppressed) are given by

$$\begin{aligned} |\ell_x = 1\rangle &= \frac{1}{2} (|\ell_z = 1\rangle + \sqrt{2} |\ell_z = 0\rangle + |\ell_z = -1\rangle); \\ |\ell_x = 0\rangle &= \frac{1}{\sqrt{2}} (|\ell_z = 1\rangle - |\ell_z = -1\rangle); \\ |\ell_x = -1\rangle &= \frac{1}{2} (|\ell_z = 1\rangle - \sqrt{2} |\ell_z = 0\rangle + |\ell_z = -1\rangle). \end{aligned} \quad (11.168)$$

<sup>4</sup>For a concise, excellent discussion, see Chap. 7 in *Quantum Mechanics*, Third Edition (McGraw Hill, New York, 1968) by L. Schiff.

The difference between  $\hat{L}_x$  and  $\hat{L}_z$  becomes apparent when I consider the eigenfunctions rather than the eigenkets. The reason for this is that the spherical coordinate system is one in which the polar angle is measured from the  $z$  axis, making the eigenfunctions of  $\hat{L}_z$  simpler than those of  $\hat{L}_x$ . If I take the inner product of Eqs. (11.168) with  $\langle \mathbf{u}_r |$  and use the fact that  $\langle \mathbf{u}_r | \ell, \ell_z \rangle \equiv \langle \mathbf{u}_r | \ell m \rangle = Y_\ell^m(\theta, \phi)$ , I find

$$\begin{aligned}\Phi_1^1(\theta, \phi) &= \frac{1}{2} \left[ Y_1^1(\theta, \phi) + \sqrt{2}Y_1^0(\theta, \phi) + Y_1^{-1}(\theta, \phi) \right] \\ \Phi_1^0(\theta, \phi) &= \frac{1}{\sqrt{2}} \left[ Y_1^1(\theta, \phi) - Y_1^{-1}(\theta, \phi) \right] \\ \Phi_1^{-1}(\theta, \phi) &= \frac{1}{2} \left[ Y_1^1(\theta, \phi) - \sqrt{2}Y_1^0(\theta, \phi) + Y_1^{-1}(\theta, \phi) \right]\end{aligned}\quad (11.169)$$

are the eigenfunctions of  $\hat{L}_x$ . You see that, although the eigenkets are essentially identical, the eigenfunctions are most simply expressed if you use  $\hat{L}_z$  rather than  $\hat{L}_x$ . To solve for the eigenfunctions of  $\hat{L}_x$  directly using  $\hat{L}_x \Phi_1^m(\theta, \phi) = m\hbar \Phi_1^m(\theta, \phi)$  with  $\hat{L}_x$  given by Eq. (9.31a) would be more difficult.

#### 11.4.4 Limited Subspaces

Sometimes an atom–field interaction is limited to a discrete subspace. Examples are an atom interacting with a field that is resonant with its ground to first excited state transition frequency or a magnetic field acting on an atom in its ground state, including spin. Whenever there are just a few levels in the problem, Dirac notation is usually the method of choice for attacking the problem.

### 11.5 Connection with Linear Algebra

Suppose you have a Hamiltonian matrix of the form

$$\underline{H} = \begin{pmatrix} 1 & 0.5 & 2 \\ 0.5 & 5 & 1 \\ 2 & 1 & 8 \end{pmatrix}. \quad (11.170)$$

You know this is not the Hamiltonian in the energy basis since it would be *diagonal* in that basis. Let us imagine that Eq. (11.170) represents the Hamiltonian in the  $u$  basis with

$$\underline{u}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; \quad \underline{u}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; \quad \underline{u}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (11.171)$$

How can I get the eigenvalues of  $\underline{H}$  and its eigenvectors expressed in the  $u$  basis? To do so I expand

$$|E\rangle = \sum_{n=1}^3 \langle u_n | E \rangle |u_n\rangle \quad (11.172)$$

and show that obtaining the  $\langle u_n | E \rangle$  is equivalent to diagonalizing the  $\underline{H}$  matrix. I start from

$$\underline{H} |E\rangle = \sum_{n=1}^3 \underline{H} |u_n\rangle \langle u_n | E \rangle = E |E\rangle \quad (11.173)$$

and multiply by  $\langle u_m |$  to obtain

$$\sum_{n=1}^3 \langle u_m | \underline{H} |u_n\rangle \langle u_n | E \rangle = E \langle u_m | E \rangle. \quad (11.174)$$

This is just the equation that you encountered in linear algebra to diagonalize a matrix and find its eigenvectors, that is

$$(\underline{H}_{11} - E) \langle u_1 | E \rangle + \underline{H}_{21} \langle u_2 | E \rangle + \underline{H}_{31} \langle u_3 | E \rangle = 0; \quad (11.175a)$$

$$\underline{H}_{21} \langle u_1 | E \rangle + (\underline{H}_{22} - E) \langle u_2 | E \rangle + \underline{H}_{23} \langle u_3 | E \rangle = 0; \quad (11.175b)$$

$$\underline{H}_{31} \langle u_1 | E \rangle + \underline{H}_{32} \langle u_2 | E \rangle + (\underline{H}_{33} - E) \langle u_3 | E \rangle = 0. \quad (11.175c)$$

The equation has a non-trivial solution only if the determinant of the coefficients vanishes. By setting the determinant of the coefficients equal to zero, I can use this result to obtain the three energy eigenvalues  $E_n \{n = 1, 2, 3\}$ . For each eigenenergy  $E_m$ , Eqs. (11.175) are solved for the  $\langle u_n | E_m \rangle \{n = 1, 2, 3\}$ , allowing me to obtain the eigenkets as

$$|E_m\rangle = \sum_{n=1}^3 \langle u_n | E_m \rangle |u_n\rangle = \sum_{n=1}^3 a_n^{(m)} |u_n\rangle, \quad (11.176)$$

where

$$a_n^{(m)} = \langle u_n | E_m \rangle. \quad (11.177)$$

In matrix form,

$$|E_1\rangle = \begin{pmatrix} \langle u_1 | E_1 \rangle \\ \langle u_2 | E_1 \rangle \\ \langle u_3 | E_1 \rangle \end{pmatrix}; \quad |E_2\rangle = \begin{pmatrix} \langle u_1 | E_2 \rangle \\ \langle u_2 | E_2 \rangle \\ \langle u_3 | E_2 \rangle \end{pmatrix}; \quad |E_3\rangle = \begin{pmatrix} \langle u_1 | E_3 \rangle \\ \langle u_2 | E_3 \rangle \\ \langle u_3 | E_3 \rangle \end{pmatrix}. \quad (11.178)$$

Thus, finding the expansion coefficients of  $|E\rangle$  in the  $u$  basis is equivalent to diagonalizing the Hamiltonian.

I form a matrix  $\underline{S}^\dagger$  by placing the eigenvectors in *columns*, such that

$$\underline{S}^\dagger = \begin{pmatrix} \langle u_1 | E_1 \rangle & \langle u_1 | E_2 \rangle & \langle u_1 | E_3 \rangle \\ \langle u_2 | E_1 \rangle & \langle u_2 | E_2 \rangle & \langle u_2 | E_3 \rangle \\ \langle u_3 | E_1 \rangle & \langle u_3 | E_2 \rangle & \langle u_3 | E_3 \rangle \end{pmatrix}. \quad (11.179)$$

The eigenvectors are then given by

$$\begin{pmatrix} |E_1\rangle \\ |E_2\rangle \\ |E_3\rangle \end{pmatrix} = (\underline{S}^\dagger)^T \begin{pmatrix} |u_1\rangle \\ |u_2\rangle \\ |u_3\rangle \end{pmatrix} = \underline{S}^* \begin{pmatrix} |u_1\rangle \\ |u_2\rangle \\ |u_3\rangle \end{pmatrix} \quad (11.180)$$

For *normalized* eigenkets,  $\underline{S}^\dagger$  is a unitary matrix, having inverse of  $(\underline{S}^\dagger)^{-1} = \underline{S}$  and

$$\underline{S}\underline{H}\underline{S}^\dagger = \underline{E} \quad (11.181)$$

where  $\underline{E}$  is a diagonal matrix whose elements are the eigenvalues of  $\underline{H}$ . To get the matrix  $\underline{S}^\dagger$  in Mathematica, use `Transpose[Orthogonalize[Eigenvectors[H]]]`, where  $\underline{H} = \{\{h_{11}, h_{12}, h_{13}\}, \{h_{21}, h_{22}, h_{23}\}, \{h_{31}, h_{32}, h_{33}\}\}$ . To get the eigenvalues, use `Eigenvalues[H]`.

It is easy to show that  $\underline{S}\underline{H}\underline{S}^\dagger = \underline{E}$ , in general; that is, for matrices having arbitrary dimension. Since  $\underline{H}|E_m\rangle = E_m |E_m\rangle$ , it follows that

$$\langle E_n | H | E_m \rangle = E_n \delta_{n,m}; \quad (11.182)$$

$$\sum_{p,q} \langle E_n | u_p \rangle \langle u_p | H | u_q \rangle \langle u_q | E_m \rangle = E_n \delta_{n,m}; \quad (11.183)$$

$$\sum_{p,q} (a_p^{(n)})^* H_{pq} a_q^{(m)} = E_n \delta_{n,m}; \quad (11.184)$$

$$\sum_{p,q} (S^\dagger)_{pn}^* H_{pq} (S^\dagger)_{qm} = \sum_{p,q} S_{np} H_{pq} (S^\dagger)_{qm} = E_n \delta_{n,m}; \quad (11.185)$$

$$(\underline{S}\underline{H}\underline{S}^\dagger)_{nm} = E_n \delta_{n,m}. \quad (11.186)$$

As an example, consider

$$\underline{H} = \begin{pmatrix} 2 & -2i \\ 2i & 5 \end{pmatrix} \quad (11.187)$$

in the  $|1\rangle, |2\rangle$  basis in some arbitrary units. To diagonalize  $\underline{H}$ , I set

$$|\underline{H}| = \begin{vmatrix} 2-E & -2i \\ 2i & 5-E \end{vmatrix} = 0 \quad (11.188)$$

and evaluate the determinant to obtain

$$E^2 - 7E + 6 = 0; \quad E = 6, 1. \quad (11.189)$$

For  $E = 6$

$$\begin{aligned} -4a_1^{(1)} - 2ia_2^{(1)} &= 0; \\ a_2^{(1)} &= 2ia_1^{(1)} \end{aligned} \quad (11.190)$$

Therefore

$$|E_1\rangle = a_1^{(1)} (|1\rangle + 2i|2\rangle). \quad (11.191)$$

I normalize by taking

$$\begin{aligned} |a_1^{(1)}|^2 (1 + 4) &= 1; \\ a_1^{(1)} &= \frac{1}{\sqrt{5}}, \end{aligned} \quad (11.192)$$

such that

$$|E_1\rangle = \frac{1}{\sqrt{5}} (|1\rangle + 2i|2\rangle). \quad (11.193)$$

Similarly, for  $E = 1$

$$\begin{aligned} a_1^{(2)} - 2ia_2^{(2)} &= 0; \\ a_1^{(2)} &= 2ia_2^{(2)} \end{aligned} \quad (11.194)$$

and

$$|E_2\rangle = a_2^{(2)} (2i|1\rangle + |2\rangle) = \frac{1}{\sqrt{5}} (2i|1\rangle + |2\rangle). \quad (11.195)$$

Therefore

$$\underline{\mathbb{S}}^\dagger = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix}; \quad \underline{\mathbb{S}} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & -2i \\ -2i & 1 \end{pmatrix}, \quad (11.196)$$

$$\begin{pmatrix} |E_1\rangle \\ |E_2\rangle \end{pmatrix} = \underline{\mathbb{S}}^* \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix} \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix}, \quad (11.197)$$

and

$$\underline{S}\underline{H}\underline{S}^\dagger = \begin{pmatrix} 6 & 0 \\ 0 & 1 \end{pmatrix}. \quad (11.198)$$

Note that for any matrix that is  $3 \times 3$  or larger, you need to diagonalize numerically rather than analytically since the characteristic equation to find the eigenvalues will be cubic or higher. In Mathematica, simply put a decimal point in one of the entries. Thus for

$$\underline{H} = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 5 & 3 \\ 2 & 3 & 8 \end{pmatrix}, \quad (11.199)$$

you can write

$$h = \{\{1., 1, 2\}, \{1, 5, 3\}, \{2, 3, 8\}\} \quad (11.200)$$

and Mathematica gives eigenvalues

$$\{10.383, 3.1598, 0.457203\}$$

and eigenvectors  $\{\{0.231057, 0.50604, 0.830985\}, \{0.0690456, -0.860472, 0.504798\}, \{0.970487, -0.0592615, -0.233758\}\}$ , corresponding to

$$|E_1\rangle = 0.231057 |1\rangle + 0.50604 |2\rangle + 0.830985 |3\rangle; \quad (11.201a)$$

$$|E_2\rangle = 0.0690456 |1\rangle - 0.860472 |2\rangle + 0.504798 |3\rangle; \quad (11.201b)$$

$$|E_3\rangle = 0.970487 |1\rangle - 0.0592615 |2\rangle - 0.233758 |3\rangle, \quad (11.201c)$$

with energies from highest to lowest.

### 11.5.1 Time Dependence

The time-dependent Schrödinger equation is solved in the same manner used in the wave function approach, once the eigenvectors and eigenkets are determined. The only tricky problem is that the initial conditions are often given in terms of the *original* basis rather than the eigenket basis. A simple example illustrates this point. Consider the matrix

$$\underline{H} = \hbar\omega \begin{pmatrix} 2 & -2i \\ 2i & 5 \end{pmatrix} \quad (11.202)$$

in the  $|1\rangle, |2\rangle$  basis; the variable  $\omega$  has units of frequency. Suppose at  $t = 0$  the system is in state  $|1\rangle$ . What is  $|\psi(t)\rangle$ ? I have already calculated the eigenenergies and eigenkets of this Hamiltonian in the previous section. Using Eq. (11.43), I expand  $|\psi(t)\rangle$  as

$$|\psi(t)\rangle = b_1 e^{-iE_1 t/\hbar} |E_1\rangle + b_2 e^{-iE_2 t/\hbar} |E_2\rangle. \quad (11.203)$$

The initial condition is

$$|\psi(0)\rangle = |1\rangle = b_1 |E_1\rangle + b_2 |E_2\rangle. \quad (11.204)$$

Taking inner products with the eigenkets and using Eqs. (11.193) and (11.195), I find the expansion coefficients

$$b_1 = \langle E_1 | \psi(0)\rangle = \langle E_1 | 1\rangle = \frac{1}{\sqrt{5}} (\langle 1 | - 2i \langle 2 |) 1\rangle = \frac{1}{\sqrt{5}}; \quad (11.205a)$$

$$b_2 = \langle E_2 | \psi(0)\rangle = \langle E_2 | 1\rangle = \frac{1}{\sqrt{5}} (-2i \langle 1 | + \langle 2 |) 1\rangle = \frac{-2i}{\sqrt{5}}, \quad (11.205b)$$

and then use Eq. (11.203) to obtain the state vector

$$|\psi(t)\rangle = \frac{1}{\sqrt{5}} (e^{-6i\omega t} |E_1\rangle - 2ie^{-i\omega t} |E_2\rangle). \quad (11.206)$$

The state vector can be re-expressed in terms of the *original* basis as

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{5}} \left( \frac{e^{-6i\omega t}}{\sqrt{5}} (|1\rangle + 2i|2\rangle) - \frac{2i}{\sqrt{5}} e^{-i\omega t} (2i|1\rangle + |2\rangle) \right) \\ &= \frac{1}{5} [(e^{-6i\omega t} + 4e^{-i\omega t}) |1\rangle + 2i(e^{-6i\omega t} - e^{-i\omega t}) |2\rangle]. \end{aligned} \quad (11.207)$$

As a consequence the state probabilities in terms of the original basis states are

$$P_1(t) = \frac{1}{25} [17 + 8 \cos(5\omega t)]; \quad (11.208a)$$

$$P_2(t) = \frac{8}{25} [1 - \cos(5\omega t)], \quad (11.208b)$$

and both these probabilities oscillate in time.

In general, for an arbitrary system, the state vector is

$$|\psi(t)\rangle = \sum_n b_n e^{-iE_n t/\hbar} |E_n\rangle = \sum_n \langle n | \psi(0)\rangle e^{-iE_n t/\hbar} |E_n\rangle, \quad (11.209)$$

where the eigenkets  $|E_n\rangle$  are the eigenkets of a Hamiltonian  $\underline{H}$  having eigenenergies  $E_n$ . Suppose, however, that we know matrix elements of the Hamiltonian only in some other basis denoted by  $|n\rangle$  and that, although  $\underline{H}$  is not diagonal in this basis, the initial state vector  $|\psi(0)\rangle$  can be expressed in this basis as

$$|\psi(0)\rangle = \sum_n a_n |n\rangle. \quad (11.210)$$

You can then calculate the state vector at any time using Eq. (11.209) to be

$$|\psi(t)\rangle = \sum_{m,n} a_n \langle E_m | n \rangle e^{-iE_m t/\hbar} |E_m\rangle. \quad (11.211)$$

However, from Eq. (11.180), you know that

$$|E_m\rangle = \sum_{n'} (S^*)_{mn'} |n'\rangle. \quad (11.212)$$

The adjoint of this equation is

$$\langle E_m | = \sum_{m'} (S)_{mm'} \langle m' | \quad (11.213)$$

(note the use of different dummy variables). Substituting these expressions into Eq. (11.211), I find

$$\begin{aligned} |\psi(t)\rangle &= \sum_{n,n',m,m'} a_n (S)_{mm'} \langle m' | n \rangle e^{-iE_m t/\hbar} (S^*)_{mn'} |n'\rangle \\ &= \sum_{n,n',m} a_n (S)_{mn} e^{-iE_m t/\hbar} (S^*)_{mn'} |n'\rangle \\ &= \sum_{n,n',m} a_n (S^\dagger)_{n'm} (S)_{mn} e^{-iE_m t/\hbar} |n'\rangle, \end{aligned} \quad (11.214)$$

which is the desired result.

In our previous example,  $a_1 = 1$ ,  $a_2 = 0$ , and

$$\underline{S}^\dagger = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix}; \quad \underline{S} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & -2i \\ -2i & 1 \end{pmatrix}, \quad (11.215)$$

such that

$$\begin{aligned}
 |\psi(t)\rangle &= \sum_{n,m} (S^\dagger)_{nm} (S)_{m1} e^{-iE_m t/\hbar} |n\rangle \\
 &= \left[ (S^\dagger)_{11} (S)_{11} e^{-iE_1 t/\hbar} + (S^\dagger)_{12} (S)_{21} e^{-iE_2 t/\hbar} \right] |1\rangle \\
 &\quad + \left[ (S^\dagger)_{21} (S)_{11} e^{-iE_1 t/\hbar} + (S^\dagger)_{22} (S)_{21} e^{-iE_2 t/\hbar} \right] |2\rangle \\
 &= \frac{1}{5} \left[ (e^{-6i\omega t} + 4e^{-i\omega t}) |1\rangle + 2i (e^{-6i\omega t} - e^{-i\omega t}) |2\rangle \right], \quad (11.216)
 \end{aligned}$$

in agreement with Eq. (11.207).

## 11.6 Summary

I have shown that Dirac notation is a powerful method for dealing with problems in quantum mechanics. Rather than specify a given representation, you can write state vectors in a basis-independent manner. Connection with specific representations such as the coordinate or momentum representation can then be obtained by taking inner products. In Dirac notation, operators are represented by matrices. As such Dirac notation is closely related to Heisenberg's matrix formulation of quantum mechanics.

## 11.7 Appendix A: Matrix Properties

In this Appendix, I list some matrix properties. I simply use standard type for all matrices, rather than underlined quantities. The *identity matrix*  $I$  has  $I_{ij} = \delta_{ij}$ , that is, ones along the diagonal and zeroes everywhere else. The *inverse*  $A^{-1}$  of a matrix  $A$  satisfies

$$A^{-1}A = AA^{-1} = 1. \quad (11.217)$$

The *transpose*  $A^T$  of a matrix  $A$  is defined by

$$(A^T)_{ij} = A_{ji}. \quad (11.218)$$

The Hermitian adjoint  $A^\dagger$  of a matrix  $A$  is defined by

$$(A^\dagger)_{ij} = A_{ji}^* \text{ or } A^\dagger = (A^T)^* \quad (11.219)$$

and

$$(AB)^{-1} = B^{-1}A^{-1}; \quad (11.220a)$$

$$(AB)^T = B^T A^T; \quad (11.220b)$$

$$(AB)^\dagger = B^\dagger A^\dagger. \quad (11.220c)$$

A matrix  $U$  is *unitary* if

$$U^\dagger U = U U^\dagger = 1 \quad (11.221)$$

and a matrix  $O$  is *orthogonal* if

$$O^T O = O O^T = 1. \quad (11.222)$$

For a unitary matrix  $U^{-1} = U^\dagger$  and the determinant of  $U$  is a complex number having unit magnitude. For an orthogonal matrix  $O^{-1} = O^T$  and the determinant of  $O$  is unity.

A matrix  $H$  is Hermitian if

$$H^\dagger = H. \quad (11.223)$$

For any Hermitian matrix it is always possible to find a unitary matrix  $U$  such that

$$U H U^\dagger = E \quad (11.224)$$

where  $E$  is a diagonal matrix. The columns of  $U^\dagger$  are the eigenvectors and the diagonal elements of  $E$  are the eigenvalues. If  $H$  is real, then  $U$  is also real so it is an orthogonal matrix.

## 11.8 Appendix B: Spherical Harmonics in Dirac Notation

To express the spherical harmonics in Dirac notation, I first obtain matrix elements of  $\hat{\mathbf{L}}$  in the  $|\mathbf{r}\rangle$  basis. To do so, I write  $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$  and use Eq. (11.59c) to arrive at

$$\langle \mathbf{r} | \hat{L}_x | \mathbf{r}' \rangle = \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \delta(\mathbf{r} - \mathbf{r}'), \quad (11.225)$$

along with its cyclical permutations. I next use the the relationships  $r = \sqrt{x^2 + y^2 + z^2}$ ,  $\theta = \cos^{-1}(z/r)$ ,  $\phi = \tan^{-1}(y/x)$ ,  $x = r \sin \theta \cos \phi$ , and  $y = r \sin \theta \sin \phi$  to express the partial derivatives in spherical coordinates as

$$\begin{aligned}\frac{\partial}{\partial x} &= \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} \\ &= \frac{x}{r} \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi};\end{aligned}\quad (11.226a)$$

$$\frac{\partial}{\partial y} = \frac{y}{r} \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi}; \quad (11.226b)$$

$$\frac{\partial}{\partial z} = \frac{z}{r} \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta}. \quad (11.226c)$$

It then follows that

$$\langle \mathbf{r} | \hat{L}_x | \mathbf{r}' \rangle = -\frac{\hbar}{i} \left( \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) \delta(\mathbf{r} - \mathbf{r}'); \quad (11.227a)$$

$$\langle \mathbf{r} | \hat{L}_y | \mathbf{r}' \rangle = \frac{\hbar}{i} \left( \cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right) \delta(\mathbf{r} - \mathbf{r}'); \quad (11.227b)$$

$$\langle \mathbf{r} | \hat{L}_z | \mathbf{r}' \rangle = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \delta(\mathbf{r} - \mathbf{r}') \quad (11.227c)$$

and

$$\begin{aligned}\langle \mathbf{r} | \hat{L}^2 | \mathbf{r}' \rangle &= \int d\mathbf{r}'' \langle \mathbf{r} | \hat{L}_x | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{L}_x | \mathbf{r}' \rangle \\ &+ \int d\mathbf{r}'' \langle \mathbf{r} | \hat{L}_y | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{L}_y | \mathbf{r}' \rangle \\ &+ \int d\mathbf{r}'' \langle \mathbf{r} | \hat{L}_z | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{L}_z | \mathbf{r}' \rangle \\ &= -\hbar^2 \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \delta(\mathbf{r} - \mathbf{r}').\end{aligned}\quad (11.228)$$

Using the eigenvalue equation

$$\hat{L}_z |\ell m\rangle = m\hbar |\ell m\rangle, \quad (11.229)$$

I insert a complete set and multiply on the left by  $\langle \mathbf{r} |$  to transform this equation into

$$\int d\mathbf{r}' \langle \mathbf{r} | \hat{L}_z | \mathbf{r}' \rangle \langle \mathbf{r}' | \ell m \rangle = m\hbar \langle \mathbf{r} | \ell m \rangle \quad (11.230)$$

and then use Eq. (11.227c) to obtain

$$\int d\mathbf{r}' \frac{\partial}{\partial \phi} \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r}' | \ell m \rangle = im \langle \mathbf{r} | \ell m \rangle ;$$

$$\frac{\partial}{\partial \phi} \langle \mathbf{r} | \ell m \rangle = im \langle \mathbf{r} | \ell m \rangle . \quad (11.231)$$

Similarly, starting from

$$\hat{L}^2 | \ell m \rangle = \hbar^2 \ell (\ell + 1) | \ell m \rangle , \quad (11.232)$$

and using Eq. (11.228), I find

$$-\left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \langle \mathbf{r} | \ell m \rangle = \ell (\ell + 1) \langle \mathbf{r} | \ell m \rangle . \quad (11.233)$$

To relate the  $\langle \mathbf{r} | \ell m \rangle$  to the spherical harmonics I write the ket  $|\mathbf{r}\rangle$  as

$$|\mathbf{r}\rangle = \frac{|r\rangle |\mathbf{u}_r\rangle}{r} , \quad (11.234)$$

multiply Eqs. (11.231) and (11.233) by  $r^2 |r\rangle$ , integrate over  $r$ , and use the completeness relation

$$\int_0^\infty dr r^2 |r\rangle \langle r| = 1 \quad (11.235)$$

to arrive at

$$\frac{\partial}{\partial \phi} \langle \mathbf{u}_r | \ell m \rangle = im \langle \mathbf{u}_r | \ell m \rangle ; \quad (11.236a)$$

$$-\left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \langle \mathbf{u}_r | \ell m \rangle = \ell (\ell + 1) \langle \mathbf{u}_r | \ell m \rangle , \quad (11.236b)$$

implying that

$$\langle \mathbf{u}_r | \ell m \rangle = Y_\ell^m (\theta, \phi) . \quad (11.237)$$

Note that Eq. (11.237) has the correct normalization, since

$$\begin{aligned} \langle \ell' m' | \ell m \rangle &= \int d\Omega \langle \ell' m' | \mathbf{u}_r \rangle \langle \mathbf{u}_r | \ell m \rangle \\ &= \int d\Omega \left[ Y_{\ell'}^{m'} (\theta, \phi) \right]^* Y_\ell^m (\theta, \phi) = \delta_{\ell, \ell'} \delta_{m, m'} . \end{aligned} \quad (11.238)$$

## 11.9 Problems

1. In Dirac notation, how are Hermitian operators represented? What does it mean to say that the matrix elements of an operator depend on the basis? Give an example by considering the matrix elements of the operator  $\hat{x}$  in the coordinate and momentum bases. Is it diagonal in the coordinate basis? in the momentum basis? Why is the diagonalization of the Hamiltonian in the coordinate basis equivalent to solving the Schrödinger equation?
2. Consider the two-dimensional vector  $\mathbf{A} = \mathbf{u}_x + 2\mathbf{u}_y$ . Suppose you want to use different orthonormal basis vectors defined by

$$\mathbf{u}_{1,2} = \frac{\mathbf{u}_x \pm \mathbf{u}_y}{\sqrt{2}}.$$

Express the unit vectors  $\mathbf{u}_x$  and  $\mathbf{u}_y$  as column vectors in this basis and find the coordinates of  $\mathbf{A}$  in this basis. Show explicitly that  $A_1\mathbf{u}_1 + A_2\mathbf{u}_2 = A_x\mathbf{u}_x + A_y\mathbf{u}_y$ .

3. The adjoint or Hermitian conjugate  $A^\dagger$  of a matrix  $A$  is defined by  $(A^\dagger)_{mn} = (A_{nm})^*$ . Show that for two matrices  $A$  and  $B$  for which matrix multiplication can be defined,  $(AB)^\dagger = B^\dagger A^\dagger$ . As a consequence prove that  $\hat{A}\hat{B}$  is Hermitian only if  $[\hat{A}, \hat{B}] = 0$ .
4. Using Dirac notation, prove that the eigenvalues of a Hermitian operator are real and the eigenkets having nondegenerate eigenvalues are orthogonal.
5. Using Dirac notation prove that two Hermitian operators can possess simultaneous eigenkets if, and only if, the operators commute.
6. Suppose that in the  $|g\rangle$  basis, a Hamiltonian has the form

$$H = \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix}.$$

Find the eigenvalues and (normalized) eigenvectors (express the eigenvectors in the  $|g\rangle$  basis). Do the calculation yourself and then check the result on a computer using, for example, the Eigenvalues and Eigenvectors operations in Mathematica (e.g., `Orthogonalize[Eigenvectors[{{3.,1},{1,2}}]]`)—putting the decimal point in will give you numerical values).

7. In Problem 11.6, find a matrix  $\underline{S}$  such that  $\underline{S}\underline{H}\underline{S}^\dagger$  is a diagonal matrix having diagonal elements equal to the eigenvalues of  $\underline{H}$ . Check your answer using a computer program.
8. In Problem 11.6, suppose that at  $t = 0$  a particle is in the state  $|1\rangle$  in the  $|g\rangle$  basis. Find the wave function as a function of time in terms of the  $|g\rangle$  basis. Show that the probability to be in state  $|1\rangle$  in the  $|g\rangle$  basis oscillates as a function of time.

9. The time-dependent Schrödinger equation in Dirac notation can be written as

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle.$$

For an operator  $\hat{A}$  that has no explicit time dependence, prove

$$d\langle\psi(t)|\hat{A}|\psi(t)\rangle/dt = \frac{1}{i\hbar}\langle\psi(t)|[\hat{A}, \hat{H}]|\psi(t)\rangle.$$

What can you conclude about operators that commute with the Hamiltonian?

10. Using ladder operators, evaluate matrix elements  $\langle n|\hat{x}|q\rangle$  and  $\langle n|\hat{x}^2|q\rangle$  for the 1-D harmonic oscillator. What is the general structure of the matrices  $\underline{H}$ ,  $\underline{x}$ , and  $\underline{x}^2$  in the  $|n\rangle$  basis? That is, are these matrices diagonal or, if not, which elements are non-vanishing?

11. Using ladder operators, evaluate matrix elements  $\langle n|\hat{p}_x|m\rangle$  and  $\langle n|\hat{p}_x^2|m\rangle$  for the 1-D harmonic oscillator. Moreover, prove that

$$\left(\frac{\langle n|\hat{p}_x^2|q\rangle}{2m} + \frac{m\omega^2\langle n|\hat{x}^2|q\rangle}{2}\right) = \hbar\omega\left(n + \frac{1}{2}\right)\delta_{n,q} = E_n\delta_{n,q}.$$

12. Using ladder operators, evaluate matrix elements,

$$\langle n|\hat{p}_x\hat{x}|q\rangle \text{ and } \langle n|\hat{x}\hat{p}_x|q\rangle,$$

for the 1-D harmonic oscillator and show explicitly that

$$\langle n|\hat{x}\hat{p}_x|q\rangle - \langle n|\hat{p}_x\hat{x}|q\rangle = i\hbar\delta_{n,q}.$$

13. At  $t = 0$ , a particle having mass  $m$  moving in a one-dimensional oscillator potential having associated frequency  $\omega$  is in the state

$$|\psi(0)\rangle = N(|0\rangle + 2|1\rangle),$$

where  $N$  is a normalization constant. Find the expectation value of the position operator as a function of time.

14–15. Consider the one-dimensional harmonic oscillator in dimensionless coordinates for which

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{\eta}^2 + \xi^2) = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

Suppose that the normalized state vector at time  $t$  is given by

$$|\psi(t)\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} a_n e^{-in\omega t} |n\rangle,$$

where  $|n\rangle$  are the eigenkets of  $\hat{H}$ .

- (a) Using this state vector, evaluate  $\langle \hat{\xi}^2 \rangle = \langle \psi(t) | \hat{\xi}^2 | \psi(t) \rangle$  and show that it has a time-independent component and a component that oscillates with frequency  $2\omega$ . How does this dependence compare with that of  $x(t)^2$  for a classical oscillator?
- (b) Evaluate  $\langle \hat{H} \rangle$ .
- (c) Obtain a differential equation for  $d^2 \langle \hat{\xi}^2 \rangle / dt^2$  that could be solved in terms of the initial conditions and the value of  $\langle \hat{H} \rangle$ . [Hint: First obtain an equation for  $d \langle \hat{\xi}^2 \rangle / dt$  that will involve some product of operators. Then obtain an equation of motion for this product of operators and use the fact that  $\langle \hat{H} \rangle = \frac{\hbar\omega}{2} \langle \hat{\eta}^2 + \hat{\xi}^2 \rangle$  to eliminate  $\langle \hat{\eta}^2 \rangle$ .]
- (d) Show that the solution of the differential equation of part (c) has the correct form found in part (a).

Note: The answers to parts (a) and (b) will be in the form of sums.

16–17. Starting from the coherent state

$$|\psi(t)\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{(\xi_0/\sqrt{2})^n e^{-(\xi_0/\sqrt{2})^2/2} e^{-in\omega t}}{\sqrt{n!}} |n\rangle,$$

use Eqs. (11.107) and (11.108) to calculate

$$\langle \xi \rangle = \langle \psi(t) | (a + a^\dagger) | \psi(t) \rangle / \sqrt{2}$$

and

$$\langle \hat{\xi}^2 \rangle = \langle \psi(t) | (a + a^\dagger)^2 | \psi(t) \rangle / 2.$$

Show that the results agree with Eqs. (11.132) and (11.133).

18. (a) Using your knowledge of Dirac notation, evaluate

$$\int d\Omega \left[ Y_{\ell'}^{m'}(\theta, \phi) \right]^* \hat{L}_x Y_{\ell}^m(\theta, \phi),$$

where the integral is over solid angle.

(b) Given an *arbitrary* operator  $\hat{A}$  that commutes with  $\hat{L}^2$ . Prove that

$$\langle \ell' m' | \hat{A} | \ell m \rangle = 0$$

unless  $\ell = \ell'$ .

19. Evaluate  $\langle \ell m | \hat{L}_y | \ell' m' \rangle$  using ladder operators and find explicit expressions for the eigenkets of  $\hat{L}_y$  for  $\ell = 1$ , in terms of the  $|\ell m\rangle$  basis.

20–21. Show that for a spherically symmetric potential, the momentum space eigenfunctions in spherical (momentum) coordinates can be written as

$$\Phi_E(\mathbf{p}) = P_{E\ell}(p) Y_\ell^m(\theta_p, \phi_p),$$

where the “radial” wave function  $P_{E\ell}(p)$  is a solution of

$$(p^2 - 2mE) P_{E\ell}(p) = -\frac{2m}{(2\pi\hbar)^{3/2}} \int_0^\infty p'^2 dp' \tilde{V}_\ell(p, p') P_{E\ell}(p'),$$

and

$$\tilde{V}_\ell(p, p') = \frac{(4\pi)^2}{(2\pi\hbar)^{3/2}} \int_0^\infty r^2 dr V(r) j_\ell(pr/\hbar) j_\ell(p'r/\hbar).$$

Find  $P_{E\ell}(p)$  for a free particle.

To solve this problem you will need to use the expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr) [Y_\ell^m(\theta, \phi)]^* Y_\ell^m(\theta_k, \phi_k),$$

in which  $j_\ell(kr)$  is a spherical Bessel function.