Appendix DD

The Angular Momentum Operators

GENERALIZATION OF THE QUANTUM RULES

The quantum rules given in Chapter 3 may be generalized to three dimensions. The position of a particle in three dimensions can be represented by a vector **r**, which extends from the origin to the particle, while the momentum of a particle moving in three-dimensional space is represented by a vector **p**, which points in the direction of the particle's motion.

For a particle moving in three dimensions, the operator associated with the momentum, which we denote by $\hat{\mathbf{p}}$, is defined to be

$$\hat{\mathbf{p}} = -i\hbar\nabla, \tag{DD.1}$$

where ∇ is the gradient operator discussed in Appendix AA. The gradient of a function is a vector that points in the direction in which the function changes most rapidly and has a magnitude equal to the rate of change of the function in that direction. It is the natural generalization of the concept of the derivative to three dimensions.

The expression for the energy in three dimensions is

$$E = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{r}), \tag{DD.2}$$

where **p** and **r** are the momentum and radius vectors. Substituting the momentum operator (DD.1) into Eq. (DD.2) for the energy leads to the following Hamiltonian operator

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}), \tag{DD.3}$$

where ∇^2 is the Laplacian operator discussed in Appendix F.

Once one has constructed an operator O corresponding to a variable of a microscopic system, the wave function of the system and the possible values that can be obtained by measuring the variable are determined by forming the eigenvalue equation

$$O\psi(\mathbf{r}) = \lambda\psi(\mathbf{r}). \tag{DD.4}$$

As for the eigenvalue problems considered in Chapter 3, the values of λ, for which there is a solution of Eq. (DD.4) satisfying the boundary conditions, are the possible values that can be obtained in a measurement of the variable. The wave function $\psi(\mathbf{r})$ describes the system when it is in a state corresponding to the eigenvalue λ.

COMMUTION RELATIONS

The operators used in quantum mechanics to represent physical variables satisfy certain algebraic relations. Recall that the commutator of two operators, A and B, was defined in Section 3.2 by the equation

$$[A, B] = AB - BA. \tag{DD.5}$$

In this appendix, we shall discard the carrot symbol (ˆ) associated with operators denoting the operator corresponding to a variable with the same symbol used to denote the variable itself. The operator corresponding to the x-component of the momentum, for instance, will be denote simply as p_x. With this notation the commutation relation between x and p_x, which is given in Section 3.2, is written

$$[x, p_x] = i\hbar. \tag{DD.6}$$

Other commutation relations can be obtained from this relation by making the cyclic replacements, $x \to y$, $y \to z$, $z \to x$. This leads to the additional commutation relations

$$[y, p_y] = i\hbar, \quad [z, p_z] = i\hbar. \tag{DD.7}$$

We recall that the commutators that can be formed with one component of the position vector **r** and another component of the momentum operator **p** are equal to zero. For instance, we have

$$[x, p_y] = 0. \tag{DD.8}$$

The commutators formed from two components of the position vector or two components of the momentum are also zero.

As discussed in Appendix AA, the operator corresponding to the orbital angular momentum can be obtained by replacing the momentum **p** in the defining equation for the angular momentum,

$$\mathbf{l} = \mathbf{r} \times \mathbf{p}, \tag{DD.9}$$

with the operator (DD.1) to obtain

$$\mathbf{l} = -i\hbar\, \mathbf{r} \times \nabla. \tag{DD.10}$$

We shall now derive commutation relations for the angular momentum operators. These commutation relations will then be used to derive the spectra of eigenvalues of the angular momentum. To make it easier for us to evaluate the commutators of the angular momentum operators, we first derive a few general properties of the commutation relations of operators, which we denote by A, B, and C. Using the definition of the commutator (DD.5), we may write

$$\begin{aligned} [A, (B + C)] &= A(B + C) - (B + C)A = AB + AC - BA - CA \\ &= (AB - BA) + (AC - CA). \end{aligned} \tag{DD.11}$$

The two terms appearing within parentheses on the right may be identified as the commutators, $[A, B]$ and $[A, C]$. We thus have

$$[A, (B + C)] = [A, B] + [A, C]. \tag{DD.12}$$

One may prove in a similar fashion that

$$[(A + B), C] = [A, C] + [B, C]. \tag{DD.13}$$

The commutation relations can thus be said to be linear.

We next consider the commutation $[A, BC]$. Again, we use the definition of the commutator (DD.5) to obtain

$$[A, BC] = ABC - BCA. \tag{DD.14}$$

Subtracting and adding the term BAC after the first term on the right, we have

$$\begin{aligned} [A, BC] &= ABC - BAC + BAC - BCA \\ &= (AB - BA)C + B(AC - CA). \end{aligned} \tag{DD.15}$$

Again, identifying the two terms within parentheses on the right as the commutators, $[A, B]$ and $[A, C]$, we have

$$[A, BC] = [A, B]C + B[A, C]. \tag{DD.16}$$

Similarly, one may prove that

$$[AB, C] = A[B, C] + [A, C]B. \tag{DD.17}$$

These last two commutation relations can be described in simple terms. The commutator of a single operator with the product of two operators can be written as a sum of two terms involving the commutator of the single operator with each of the operators of the product. For each of these terms, the operator not appearing in the commutator is pulled to the front or the back to preserve the order of the operators within the product. In the first term on the right-hand side of Eq. (DD.16), the operator C is pulled to the back, while in the second term on the right, the operator B is pulled to the front. In the two terms of the resulting equation, B appears before C. Similarly, in the first term on the right-hand side of Eq. (DD.17), the operator

A is pulled to the front so that it appears before B, while in the second term, B is pulled to the back so that it appears after A.

We now evaluate the commutator $[l_x, l_y]$ involving the x- and y-components of the angular momentum operator $\mathbf{l}$. Using the definition of the orbital angular momentum given by Eq. (DD.9), the x-component of the angular momentum operator can be seen to be $l_x = yp_z - zp_y$ and the y-component may be seen to be $l_y = zp_x - xp_z$. We may thus use Eq. (DD.12) to obtain

$$\begin{aligned}[l_x, l_y] &= [l_x, zp_x - xp_z] = [l_x, zp_x] - [l_x, xp_z] \\ &= [(yp_z - zp_y), zp_x] - [(yp_z - zp_y), xp_z].\end{aligned} \tag{DD.18}$$

Using Eq. (DD.13), this becomes

$$[l_x, l_y] = [yp_z, zp_x] - [zp_y, zp_x] - [yp_z, xp_z] + [zp_y, xp_z]. \tag{DD.19}$$

We now note that of the commutators that can be formed from the operators on the right-hand side of the above equation, the commutators, $[x, p_x]$, $[y, p_y]$, and $[z, p_z]$, are each equal to $\mathrm{i}\hbar$. All other commutators are equal to zero. Omitting the second and third terms on the right-hand side of Eq. (DD.19), which do not contain operators having a nonzero commutator, the equation becomes

$$[l_x, l_y] = [yp_z, zp_x] + [zp_y, xp_z]. \tag{DD.20}$$

The commutators on the right-hand side of this equation may be evaluated as we have described following Eqs. (DD.16) and (DD.17). For the first term on the right-hand side, we pull y to the front and p_x to the back giving $y[p_z, z]p_x$. Similarly, for the second term on the right, we pull x toward the front and p_y toward the back giving $x[z, p_z]p_y$. Equation (DD.20) then becomes

$$[l_x, l_y] = y[p_z, z]p_x + x[z, p_z]p_y. \tag{DD.21}$$

Like the commutator $[x, p_x]$, the commutator $[z, p_z]$ is equal to $\mathrm{i}\hbar$. The commutator $[p_z, z]$, for which the operators p_z and z are interchanged, is equal to $-i\hbar$. We thus obtain

$$[l_x, l_y] = \mathrm{i}\hbar(xp_y - yp_x). \tag{DD.22}$$

The term within parentheses on the right may be identified as l_z and hence the equation may be written

$$[l_x, l_y] = \mathrm{i}\hbar l_z. \tag{DD.23}$$

The commutation relations (DD.23) assume a more simple form if the angular momentum is measured in units of $\hbar$. Commutation relations for the new angular momentum operators can be obtained by dividing Eq. (DD.23) by $\hbar^2$ to obtain

$$[(l_x/\hbar), (l_y/\hbar)] = \mathrm{i}(l_z/\hbar). \tag{DD.24}$$

If the orbital angular momentum is measured in units of $\hbar$, the angular momentum operators thus satisfy the commutation relations

$$[l_x, l_y] = \mathrm{i}l_z. \tag{DD.25}$$

The orbital angular momentum is then represented by the operator $\hbar\mathbf{l}$. Other commutation relations can be obtained from Eq. (DD.25) by making the cyclic replacements, $x \to y$, $y \to z$, and $z \to x$.

We consider now the commutation relation involving l_z and the operator,

$$\mathbf{l}^2 = l_x l_x + l_y l_y + l_z l_z. \tag{DD.26}$$

Using Eqs. (DD.12), we may write

$$[l_z, \mathbf{l}^2] = [l_z, l_x l_x + l_y l_y + l_z l_z] = [l_z, l_x l_x] + [l_z, l_y l_y] + [l_z, l_z l_z]. \tag{DD.27}$$

We now use Eq. (DD.16) and take advantage of the fact that l_z commutes with itself to write

$$[l_z, \mathbf{l}^2] = l_x[l_z, l_x] + [l_z, l_x]l_x + l_y[l_z, l_y] + [l_z, l_y]l_y. \tag{DD.28}$$

We now note that the commutators in the first and second terms are in cyclic order, while the commutators in the third and fourth terms are not in cyclic order. The above equation thus becomes

$$[l_z, \mathbf{l}^2] = \mathrm{i}[l_x l_y + l_y l_x - l_y l_x - l_x l_y = 0. \tag{DD.29}$$

We thus find that the operators $\mathbf{l}^2$ and l_z commute with each other. In quantum theory, commuting operators corresponding to variables that can be accurately measured simultaneously. It is generally possible to find simultaneous eigenfunctions for such variables. The common eigenfunctions represent states of the system in which the variables corresponding to the operators have definite values. It is easy to find physical examples of these results. For the hydrogen atom, the states of the electron are described by the quantum numbers, l and m_l, corresponding to well-defined values of both $\mathbf{l}^2$ and l_z. In a magnetic field the magnetic moment and the angular momentum of an electron precess about the direction of the magnetic field with the magnitude of the angular momentum and the projection of the angular momentum upon the direction of the magnetic field having constant values.

The definition of the angular momentum by Eq. (DD.9) does not apply to the spin. We shall require, though, that the components of the spin angular momentum satisfy commutation relations analogous to Eq. (DD.25). We have

$$[s_x, s_y] = \mathrm{i}s_z. \tag{DD.30}$$

It is thus convenient to regard the commutation relations between the components of the angular momentum operators as the definition the angular momentum. Analogous commutations relations apply to the components of the orbital and spin angular momentum and to the components of the total angular momentum.

SPECTRUM OF EIGENVALUES

We conclude this appendix by showing that the commutation relations of the angular momentum operators determine the spectrum of eigenvalues of these operators. Our arguments will be very general applying to any angular momentum operator. Using the symbol $\mathbf{j}$ to denote an angular momentum operator, the commutation relations satisfied by the components of the angular momentum operators may be obtained by writing j in place of l in Eq. (DD.25) or j in place of s in Eq. (DD.30) giving

$$[j_x, j_y] = \mathrm{i}j_z. \tag{DD.31}$$

The symbol $\mathbf{j}$ denotes the angular momentum operator in units of $\hbar$. As for the orbital angular momentum operators considered previously, the operator j_z commutes with the operator

$$\mathbf{j}^2 = j_x j_x + j_y j_y + j_z j_z. \tag{DD.32}$$

We have

$$[j_z, \mathbf{j}^2] = 0. \tag{DD.33}$$

Eq. (DD.33) can be derived as before from the commutation relation (DD.31) and the other commutation relations obtained from this basic equation by making the cyclic replacements, $j_x \rightarrow j_y, j_y \rightarrow j_z$, and $j_z \rightarrow j_x$.

Since the operators, $\mathbf{j}^2$ and j_z, commute, they have a common set of eigenfuctions. Denoting a typical eigenvalue of $\mathbf{j}^2$ by μ and an eigenvalue of j_z by μ_z, we denote the simultaneous eigenfunctions of $\mathbf{j}^2$ and j_z by $\psi(\mu, \mu_z)$. These functions satisfy the eigenvalue equations,

$$\mathbf{j}^2\, \psi(\mu, \mu_z) = \mu\psi(\mu, \mu_z) \tag{DD.34}$$

and

$$j_z\, \psi(\mu, \mu_z) = \mu_z\psi(\mu, \mu_z). \tag{DD.35}$$

In order to study the properties of the angular momentum eigenfunctions, we introduce new operators by the equations

$$j_+ = j_x + i\,j_y \tag{DD.36}$$

and

$$j_- = j_x - i\,j_y \tag{DD.37}$$

Since j_+ and j_- are linear combinations of j_x and j_y, and since j_x and j_y commute with $\mathbf{j}^2$, j_+ and j_- must also commute with $\mathbf{j}^2$. One may easily confirm this result using the defining Eqs. (DD.36) and (DD.37) together with Eq. (DD.13).

In order to evaluate the commutation relation of j_z with j_+, we first use Eqs. (DD.36) and (DD.12) to write the commutator as follows

$$\begin{aligned} [j_z\,, j_+] &= [j_z, (j_x + ij_y)] \\ &= [j_z, j_x] + i[j_z, j_y] \end{aligned} \tag{DD.38}$$

The commutation relation satisfied by the components of the angular momentum may then be used to obtain

$$[j_z\,,j_+] = ij_y + j_x. \tag{DD.39}$$

The above equality can be written

$$[j_z,j_+] = j_+. \tag{DD.40}$$

The commutator of j_z with j_- may be evaluated in a similar way. We obtain

$$[j_z\,,j_-] = -j_-. \tag{DD.41}$$

In order to evaluate the operator product j_+j_-, we first use the definitions, (DD.37) and (DD.36), to write

$$\begin{aligned} j_-j_+ &= (j_x - ij_y)(j_x + ij_y) \\ &= j_x^2 + j_y^2 + i[j_x,j_y] \\ &= \mathbf{j}^2 - j_z^2 + i[j_x,j_y]. \end{aligned} \tag{DD.42}$$

We then use the commutation relations (DD.31) to obtain

$$j_-j_+ = \mathbf{j}^2 - j_z^2 - j_z. \tag{DD.43}$$

Similarly, the product j_+j_- may be evaluated giving

$$j_+j_- = \mathbf{j}^2 - j_z^2 + j_z. \tag{DD.44}$$

Operating now on the eigenvalue equation (DD.34) with j_+ and using the fact that j_+ and $\mathbf{j}^2$ commute, we obtain

$$\mathbf{j}^2 j_+\psi(\mu,\mu_z) = \mu j_+\psi(\mu,\mu_z). \tag{DD.45}$$

The function $j_+\psi(\mu,\mu_z)$ is thus also an eigenfunction of $\mathbf{j}^2$ corresponding to the eigenvalue μ. Similarly, multiplying the eigenvalue equation (DD.35) by the operator j_+ gives

$$j_+j_z\psi(\mu,\mu_z) = \mu_z j_+\psi(\mu,\mu_z). \tag{DD.46}$$

We may now use the definition of the commutator of two operators and Eq. (DD.40) to write

$$j_+j_z = j_zj_+ - [j_z,j_+] = j_zj_+ - j_+. \tag{DD.47}$$

Substituting this expression for j_+j_z into Eq. (DD.46) and bringing the term with j_+ over to the right-hand side of the equation, we then obtain

$$j_zj_+\psi(\mu,\mu_z) = (\mu_z + 1)j_+\psi(\mu,\mu_z). \tag{DD.48}$$

The function $j_+\psi(\mu,\mu_z)$ is thus an eigenfunction of j_z corresponding to the eigenvalue $\mu_z + 1$. So, operating on the function $\psi(\mu,\mu_z)$ with j_+ gives a new eigenfunction belonging to the same eigenvalue of $\mathbf{j}^2$ but to the eigenvalue $(\mu_z + 1)$ of j_z. By repeatedly operating with j_+ on $\psi(\mu,\mu_z)$, we can generate a whole series of eigenfunctions of j_z belonging to the eigenvalues $\mu_z, \mu_z + 1, \mu_z + 2, \ldots$ and all belonging to the eigenvalue μ of $\mathbf{j}^2$. For this reason, j_+ is called a *step-up* operator.

Equations similar to Eqs. (DD.45) and (DD.48) may be derived by multiplying the eigenvalue equations (DD.34) and (DD.35) by j_-. We have

$$\mathbf{j}^2 j_-\psi(\mu,\mu_z) = \mu j_-\psi(\mu,\mu_z), \tag{DD.49}$$

$$j_zj_-\psi(\mu,\mu_z) = (\mu_z - 1)j_-\psi(\mu,\mu_z). \tag{DD.50}$$

The function $j_-\psi(\mu,\mu_z)$ is an eigenfunction of $\mathbf{j}^2$ corresponding to the eigenvalue μ and an eigenfunction of the operator j_z corresponding to the eigenvalue $(\mu_z - 1)$. The operator j_- may thus be thought of as a *step-down* operator.

We now determine the possible values of μ and μ_z. For a definite value of μ, there must be a limit to how large or how small μ_z can become. The eigenvalue μ gives the square of the length of the vector $\mathbf{j}$, while μ_z is the projection of the vector $\mathbf{j}$ upon the z-axis. The projection of a vector upon the z-axis cannot be larger than the length of the vector itself. We denote the maximum eigenvalue of j_z by j and the eigenfunction corresponding to the maximum eigenvalue by $\psi(\mu,j)$. Multiplying the function $\psi(\mu,j)$ by j_+ must give zero

$$j_+\psi(\mu,j) = 0. \tag{DD.51}$$

For, otherwise, $j_+\psi(\mu,j)$ would be an eigenfunction of j_z corresponding to the eigenvalue $j+1$. We note that setting $j_+\,\psi(\mu,j)$ equal to zero gives a solution to Eqs. (DD.45) and (DD.48). Substituting the value of j_- in Eq. (DD.51) gives

$$j_-j_+\psi(\mu,j) = 0. \tag{DD.52}$$

Using Eq. (DD.43), the above equation can be written

$$(\mu - j^2 - j)\psi(\mu,j) = 0. \tag{DD.53}$$

Since the function $\psi(\mu,j)$ cannot vanish at all points, it follows that

$$\mu = j(j+1). \tag{DD.54}$$

Similarly, let $(j-r)$ be the least eigenvalue of j_z. Then it follows that

$$j_-\psi(\mu,j-r) = 0. \tag{DD.55}$$

and

$$j_+j_-\psi(\mu,j-r) = 0. \tag{DD.56}$$

Using Eq. (DD.44), then leads to the equation

$$[\mu - (j-r)^2 + (j-r)]\psi(\mu,j-r) = 0, \tag{DD.57}$$

and we must have

$$\mu - (j-r)^2 + (j-r) = 0. \tag{DD.58}$$

Substituting the value of μ given by Eq. (DD.54) into this last equation leads to the quadratic equation

$$r^2 - r(2j-1) - 2j = 0. \tag{DD.59}$$

which has only one positive root, $r = 2j$. Thus, the least eigenvalue of j_z is equal to $j - r = -j$. This means that for a particular eigenvalue $\mu = j(j+1)$ of $\mathbf{j}^2$, there are $2j+1$ eigenfunctions $\psi(\mu,m)$ of j_z corresponding to the eigenvalues

$$m = j, j-1, \ldots, -j+1, -j. \tag{DD.60}$$

It is also clear from the above argument that $2j$ must be an integer, which means that the quantum number j of the angular momentum *must be an integer or a half-integer*.

Using commutation relations of the angular momentum operators, we have thus shown that the eigenvalues of $\mathbf{j}^2$ are $j(j+1)$ where j may an integer or half-integer. For a particular value of j, the eigenvalues of j_z are $m = j, j-1, \ldots, -j$. Denoting the simultaneous eigenfunctions of $\mathbf{j}^2$ and j_z by the quantum numbers, j and m, the eigenvalue equations become

$$\mathbf{j}^2\psi(jm) = j(j+1)\psi(jm), \tag{DD.61}$$

$$j_z\psi(jm) = m\psi(jm). \tag{DD.62}$$

The operators $\mathbf{j}^2$ and j_z give the square of the angular momentum operator and the z-component of the angular momentum in units of $\hbar$. The operators, $(\hbar\mathbf{j})^2$ and $\hbar j_z$, which represent the angular momentum in an absolute sense, have eigenvalues $j(j+1)\hbar^2$ and $m\hbar$.

The general results we have obtained for the angular momentum can be applied to the orbital and spin angular momenta. The operator corresponding to the square of the orbital angular momentum, which we have denoted previously by $\mathbf{l}^2$, has eigenvalues $l(l+1)\hbar^2$. For a given value of l, the z-component of the orbital angular momentum, which we denote by l_z, has the values $m_l\hbar$, where $m_l = -1, -l+1, \ldots, l$. The spin quantum number of the electron has the value $s = 1/2$ with the eigenvalues of the spin operator $\mathbf{s}^2$ being $(1/2)\cdot(3/2)\hbar^2$ and the spin operator s_z has eigenvalues $\pm(1/2)\hbar$.