14

The Angular Momentum Eigenvalue Problem (Revisited)

A Simultaneous Eigenvectors of Commuting Hermitian Operators

So far, we have solved the angular momentum eigenvalue problem very specifically in the coordinate representation for the case of the orbital angular momentum eigenfunctions, the well-known spherical harmonics. Let us look at this problem once more from a much more general point of view, which can be taken over for *any* angular momentum problem, or even more generally for any problem involving three hermitian operators with the same commutation relations as the L_x, L_y, and L_z. We want to solve the problem of finding the simultaneous eigenvalues and eigenvectors of the two (commuting) operators $\vec{L} \cdot \vec{L}$, and L_z. We will now write the eigenequations in the new language

$$\begin{aligned}(\vec{L} \cdot \vec{L})|\lambda m\rangle &= \lambda|\lambda m\rangle \\ L_z|\lambda m\rangle &= m|\lambda m\rangle,\end{aligned} \tag{1}$$

where we have purposely used the Dirac notation for the eigenvectors, so no implication is made as to a choice of representation.

The problem of finding the simultaneous eigenvectors of a pair (or more generally a number) of commuting hermitian operators is a very general one, because the complete specification of a base vector for an n-degree of freedom problem will in general involve n quantum numbers, associated with the eigenvalues of n commuting, hermitian operators. Let us first look at the case with $n = 2$. Let us first prove a theorem as follows.

Theorem: Two hermitian operators A and B have the same set of eigenvectors if and only if they commute.

First, assume the set of vectors $|\alpha\rangle$ are eigenvectors of both A and B:

$$\begin{aligned} A|\alpha\rangle &= a_\alpha|\alpha\rangle, \\ B|\alpha\rangle &= b_\alpha|\alpha\rangle. \end{aligned} \tag{2}$$

Now, let $[A, B] = (AB - BA)$ act on an arbitrary state vector $|\psi\rangle$ of our vector space. We shall assume the states $|\alpha\rangle$ form a complete set, and also note that a particular $|\alpha\rangle$ may require more than one label for a complete specification, so α may be a shorthand for two labels. Then, with

$$\sum_\alpha |\alpha\rangle\langle\alpha| = 1 \tag{3}$$

in the subspace in which A, and B act, we can project an arbitrary state vector $|\psi\rangle$ onto the $|\alpha\rangle$ basis to get

$$(AB - BA)|\psi\rangle = \sum_\alpha (AB - BA)|\alpha\rangle\langle\alpha|\psi\rangle = \sum_\alpha (a_\alpha b_\alpha - b_\alpha a_\alpha)|\alpha\rangle\langle\alpha|\psi\rangle = 0, \tag{4}$$

because the a_α and b_α are ordinary real numbers.

Conversely, if the $|\alpha\rangle$ are eigenvectors of the operator A, and if $[A, B] = 0$,

$$\begin{aligned} (AB - BA)|\psi\rangle &= 0 \\ &= (AB - BA)\sum_\alpha |\alpha\rangle\langle\alpha|\psi\rangle \\ &= \sum_\alpha (A - a_\alpha)B|\alpha\rangle\langle\alpha|\psi\rangle \\ &= \sum_{\alpha,\alpha'} (A - a_\alpha)|\alpha'\rangle\langle\alpha'|B|\alpha\rangle\langle\alpha|\psi\rangle \\ &= \sum_{\alpha,\alpha'} (a_{\alpha'} - a_\alpha)\langle\alpha'|B|\alpha\rangle\langle\alpha|\psi\rangle. \end{aligned} \tag{5}$$

Because $|\psi\rangle$ is an arbitrary vector and the $|\alpha\rangle$ are assumed to form a basis for the subspace of our vector space, we must have, for each pair of basis states $|\alpha\rangle$, $|\alpha'\rangle$,

$$(a_{\alpha'} - a_\alpha)\langle\alpha'|B|\alpha\rangle = 0. \tag{6}$$

Hence,

$$\langle\alpha'|B|\alpha\rangle = 0, \qquad \text{if} \qquad a_{\alpha'} \neq a_\alpha. \tag{7}$$

If the eigenvalues a_α have no degeneracies, i.e., if but a single eigenvector associated with each a_α exists, the matrix of B is diagonal in the $|\alpha\rangle$ basis, and $\langle\alpha'|B|\alpha\rangle = \delta_{\alpha,\alpha'} b_\alpha$. The more common situation, however, is one in which degeneracies associated with the eigenvalues of A exist. For example, if $A = \vec{L}^2$, $(2l + 1)$ eigenvectors associated with each eigenvalue of A exist. Then, with

$$A|\alpha^{(i)}\rangle = a_\alpha|\alpha^{(i)}\rangle, \qquad \text{with} \quad i = 1, 2, \dots g_{a_\alpha}, \tag{8}$$

$$\langle\alpha'^{(j)}|B|\alpha^{(i)}\rangle = \delta_{\alpha,\alpha'}\langle\alpha^{(j)}|B|\alpha^{(i)}\rangle. \tag{9}$$

In this case, it is still possible to take a linear combination of the $|\alpha^{(i)}\rangle$, with the same eigenvalue, a_α of the operator A, to make the matrix of the operator B diagonal in this g_{a_α}- dimensional subspace. To specify the basis completely, we then need the simultaneous eigenvalues of both operators A and B.

B The Angular Momentum Algebra

With this introduction, let us look at the eigenvalue problem of eq. (1) for the operators L_z, and $\vec{L}^2$, built from the three (dimensionless) operators, L_x, L_y, L_z, where these satisfy the commutation relations

$$[L_x, L_y] = iL_z, \quad \text{and cyclically,} \quad \text{or} \quad [L_j, L_k] = i\epsilon_{jk\nu}L_\nu. \tag{10}$$

Our results will depend only on these commutation relations. Hence, other operators with these same commutation relations will also be interesting. The other angular momentum example involves the three components of the spin operator, S_x, S_y, S_z. In the case of the orbital angular momentum operator, we were able to write the operators in terms of functions of θ, ϕ, $\frac{\partial}{\partial\theta}$, and $\frac{\partial}{\partial\phi}$, i.e., in terms of explicit functions of the orbital coordinates. In the case of the electron, and other fundamental particles, we know nothing about the intrinsic or internal coordinates of such particles. In 1924, G. E. Uhlenbeck and S. Goudsmit had a picture in their mind of an electron that was like a little rotating sphere, but to the best of our ability to measure anything today to many significant figures, the electron is still a point particle (with no observable internal structure). Hence, we cannot relate the spin operators to internal "angles." In the case of a rotating molecule, we can write the rotational, internal angular momentum in terms of three Euler angles and their partial derivatives (as we shall see). Even though we know nothing about the internal structure of an electron, however, it will be reasonable to assume the three components of $\vec{S}$ obey the same commutation relations as the three components of $\vec{L}$:

$$[S_j, S_k] = i\epsilon_{jk\nu}S_\nu. \tag{11}$$

In addition, because the spin-degree of freedom will involve only internal or intrinsic degrees of freedom of the electron, it will be natural to assume all components of $\vec{S}$ commute with all components of $\vec{L}$. With this additional relation, the three components of $\vec{J}$, the total angular momentum, with

$$\vec{J} = \vec{L} + \vec{S}, \tag{12}$$

will also have the basic commutation relations of angular momentum

$$[J_j, J_k] = i\epsilon_{jk\nu}J_\nu. \tag{13}$$

Still other operators exist, which may not be at all the three components of an angular momentum, but have the same commutation relations. For example, the three operators

$$M_1 = \frac{1}{4}\left[(p_x^2 + x^2) - (p_y^2 + y^2)\right],$$
$$M_2 = \frac{1}{2}\left(p_x p_y + xy\right),$$
$$M_3 = \frac{1}{2}\left(xp_y - yp_x\right), \tag{14}$$

where x and p_x are dimensionless coordinate and momenta, with x and y measured in appropriate length units, such that $[p_j, x_k] = -i\delta_{jk}$. From these commutation relations, it follows that

$$[M_j, M_k] = i\epsilon_{jk\nu} M_\nu. \tag{15}$$

Because we shall prove the eigenvalues of M_3 (like those of S_z, or J_z) can only be either integers or $\frac{1}{2}$-integers, and because $M_3 = \frac{1}{2}L_z$, we now have the proof that the orbital angular momentum quantum number m must be an integer. (It cannot be a $\frac{1}{2}$-integer, as the corresponding m quantum number of an arbitrary "spin.") The operators M_j of eq. (14), which are single-particle operators, can be generalized to operators for a many-body system by summing over N particle indices, e.g.,

$$M_3 = \frac{1}{2}\sum_{n=1}^{n=N}\left(x_n p_{y_n} - y_n p_{x_n}\right). \tag{16}$$

Thus, the result can be generalized to the m quantum number of an N-body system.

C General Angular Momenta

Let us consider the generic operators J_x, J_y, J_z. Again, we define

$$J_\pm = (J_x \pm iJ_y), \qquad J_0 = J_z. \tag{17}$$

The commutation relations translate to

$$[J_0, J_+] = +J_+, \qquad [J_0, J_-] = -J_-, \qquad [J_+, J_-] = 2J_0. \tag{18}$$

It will be useful to rewrite $\vec{J}^2$ in various ways

$$\begin{aligned}\vec{J}^2 &= \frac{1}{2}(J_x + iJ_y)(J_x - iJ_y) + \frac{1}{2}(J_x - iJ_y)(J_x + iJ_y) + J_z^2 \\ &= \frac{1}{2}(J_+J_- + J_-J_+) + J_0^2 \\ &= J_-J_+ + J_0^2 + J_0 \\ &= J_+J_- + J_0^2 - J_0,\end{aligned} \tag{19}$$

where we have used $[J_+, J_-] = 2J_0$ to write the operator in two basic forms. Now, let us assume $|\lambda m\rangle$ is simultaneously an eigenvector of $\vec{J}^2$ and J_0, with eigenvalues λ and m, respectively, where these are (so far) arbitrary real numbers:

$$\vec{J}^2|\lambda m\rangle = \lambda|\lambda m\rangle,$$

$$J_0|\lambda m\rangle = m|\lambda m\rangle. \tag{20}$$

Acting on these two equations from the left with the operator J_+ and using the commutation relations, $[J_+, \vec{J}^2] = 0$ and $[J_+, J_0] = -J_+$, we get

$$\begin{aligned} \vec{J}^2\Big(J_+|\lambda m\rangle\Big) &= \lambda\Big(J_+|\lambda m\rangle\Big), \\ J_0\Big(J_+|\lambda m\rangle\Big) &= (m+1)\Big(J_+|\lambda m\rangle\Big). \end{aligned} \tag{21}$$

Similarly, acting on both equations from the left with J_-, we get

$$\begin{aligned} \vec{J}^2\Big(J_-|\lambda m\rangle\Big) &= \lambda\Big(J_-|\lambda m\rangle\Big), \\ J_0\Big(J_-|\lambda m\rangle\Big) &= (m-1)\Big(J_-|\lambda m\rangle\Big). \end{aligned} \tag{22}$$

Thus, if $|\lambda m\rangle$ is an eigenvector of $\vec{J}^2$ and J_0 with eigenvalues λ and m, two possibilities exist. Either $(J_+|\lambda m\rangle)$ is an eigenvector of $\vec{J}^2$ and J_0, with eigenvalues λ and $(m+1)$, or $J_+|\lambda m\rangle = 0$. Similarly, either $(J_-|\lambda m\rangle)$ is an eigenvector of $\vec{J}^2$ and J_0, with eigenvalues λ and $(m-1)$, or $J_-|\lambda m\rangle = 0$.

Let us assume the first possibility for the operator J_+. Using eq. (19), let us evaluate the diagonal matrix element of J_-J_+ for the eigenstate $|\lambda m\rangle$

$$\begin{aligned} \langle\lambda m|J_-J_+|\lambda m\rangle &= \langle\lambda m|(\vec{J}^2 - J_0^2 - J_0)|\lambda m\rangle = [\lambda - m(m+1)]\langle\lambda m|\lambda m\rangle \\ &= \sum_{\lambda',m'}\langle\lambda m|J_-|\lambda'm'\rangle\langle\lambda'm'|J_+|\lambda m\rangle \\ &= \sum_{\lambda',m'}\langle\lambda'm'|J_-^\dagger|\lambda m\rangle^*\langle\lambda'm'|J_+|\lambda m\rangle = \sum_{\lambda',m'}|\langle\lambda'm'|J_+|\lambda m\rangle|^2 \\ &= [\lambda - m(m+1)]. \end{aligned} \tag{23}$$

The state $J_+|\lambda m\rangle$ can exist if $\lambda > m(m+1)$. In that case, we could act with J_+ to make the new state with $(m+1)$ and calculate the diagonal matrix element in the state $|\lambda(m+1)\rangle$. Moreover, we could repeat this process to ladder our way up to a state with $(m+n)$, but the same λ, so

$$\sum_{\lambda',m'}|\langle\lambda'm'|J_+|\lambda(m+n)\rangle|^2 = [\lambda - (m+n)(m+n+1)]. \tag{24}$$

An integer n will then be large enough that the negative quantity $-(m+n)(m+n+1)$ will overwhelm the positive λ, and we will have a patently positive quantity on the left-hand side of the equation equal to a negative quantity on the right. Therefore, the assumption that $\langle\lambda m|\lambda m\rangle = 1$ for the starting value of m must have been wrong. If the starting value of m is such that the laddering process has an upper bound, however, we must come to a maximum value of m, such that $(m+n) = m_{\max}$, with

$$J_+|\lambda m_{\max}\rangle = 0, \tag{25}$$

and, hence,

$$\lambda = m_{\max}(m_{\max}+1). \tag{26}$$

Similarly, using the last form of eq. (19), $J_+J_- = (\vec{J}^2 - J_0^2 + J_0)$, we arrive in the same way at the result

$$\langle\lambda m|J_+J_-|\lambda m\rangle = \sum_{\lambda''m''}|\langle\lambda''m''|J_-|\lambda m\rangle|^2 = [\lambda - m(m-1)]. \tag{27}$$

Now, we can repeat the step-down process and step-down m until it would become such a large negative number, so the negative quantity $-m(m-1) = -|m|(|m|+1)$ would overwhelm the positive λ. Thus, again the step-down ladder must quit at a value $m = m_{\text{min}}$ for which

$$J_-|\lambda m_{\text{min}}\rangle = 0, \tag{28}$$

and

$$\lambda = m_{\text{min}}(m_{\text{min}} - 1). \tag{29}$$

Hence,

$$\lambda = m_{\text{max}}(m_{\text{max}} + 1) = m_{\text{min}}(m_{\text{min}} - 1), \tag{30}$$

leading to $m_{\text{min.}} = +\frac{1}{2} \pm \sqrt{(m_{\text{max.}} + \frac{1}{2})^2}$, so $m_{\text{min.}} = -m_{\text{max}}$. The other root, $m_{\text{min.}} = (m_{\text{max.}} + 1)$, is of course meaningless. Let us now name $m_{\text{max.}} = j$. Because now $(m_{\text{max.}} - m_{\text{min.}}) = 2m_{\text{max.}} = 2j =$ integer, the quantum number j can only be an integer or a $\frac{1}{2}$-integer; with

$$\lambda = j(j+1), \qquad \text{where} \qquad m = +j, (j-1), \ldots, -j. \tag{31}$$

In addition, because the operators $J_\pm$ do not change the eigenvalue λ, the sums over λ' or λ'' in eqs. (24) and (27) collapse to the single value λ. Also, if the eigenvectors are such that the state $|\lambda m_{\text{max.}}\rangle$ is nondegenerate, the state $(J_-|\lambda m_{\text{max.}}\rangle)$ will also be nondegenerate; similarly for states with even lower m values. Then, the sum over m' in eq. (23) and m'' in eq. (27) collapses to a single value. Thus, replacing the label λ with the quantum number j,

$$|\langle j(m+1)|J_+|jm\rangle|^2 = [j(j+1) - m(m+1)], \tag{32}$$

$$|\langle j(m-1)|J_-|jm\rangle|^2 = [j(j+1) - m(m-1)]. \tag{33}$$

Choosing the matrix elements themselves to be real, we get

$$\langle j(m+1)|J_+|jm\rangle = \sqrt{(j-m)(j+m+1)}, \tag{34}$$

$$\langle j(m-1)|J_-|jm\rangle = \sqrt{(j+m)(j-m+1)}, \tag{35}$$

and, with $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{i}{2}(J_- - J_+)$,

$$\begin{aligned}
&\langle jm'|J_x|jm\rangle = \\
&\tfrac{1}{2}\Big(\delta_{m'(m+1)}\sqrt{(j-m)(j+m+1)} + \delta_{m'(m-1)}\sqrt{(j+m)(j-m+1)}\Big), \\
&\langle jm'|J_y|jm\rangle = \\
&\tfrac{1}{2}\Big(-i\delta_{m'(m+1)}\sqrt{(j-m)(j+m+1)} + i\delta_{m'(m-1)}\sqrt{(j+m)(j-m+1)}\Big), \\
&\langle jm|J_z|jm\rangle = m.
\end{aligned} \tag{36}$$

For $j = \frac{1}{2}$, these matrices are very simple 2×2 matrices with rows and columns labeled by $m = +\frac{1}{2}, m = -\frac{1}{2}$, in that order. It is convenient to factor out the factor $\frac{1}{2}$, and to define the operator $\vec{\sigma}$, via

$$\vec{J} = \frac{1}{2}\vec{\sigma}, \tag{37}$$

where the matrices have the simple form

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{38}$$

These equations are the famous Pauli spin-matrices. They satisfy

$$\sigma_j \sigma_k = i\epsilon_{jk\alpha}\sigma_\alpha + \delta_{jk}. \tag{39}$$

As a final small exercise, let us calculate ΔJ_x for an angular momentum system is in a definite angular momentum eigenstate $|jm\rangle$. We note

$$\langle jm|J_x|jm\rangle = 0, \tag{40}$$

so the expectation value of this perpendicular component of $\vec{J}$ is zero in the eigenstate with definite value of J_z. Also,

$$\begin{aligned} \langle jm|J_x^2|jm\rangle &= \sum_{m'=(m\pm 1)} \langle jm|J_x|jm'\rangle\langle jm'|J_x|jm\rangle \\ &= \sum_{m'=(m\pm 1)} |\langle jm'|J_x|jm\rangle|^2 \\ &= \frac{1}{4}\big([j(j+1) - m(m+1)] + [j(j+1) - m(m-1)]\big) \\ &= \frac{1}{2}[j(j+1) - m^2]. \end{aligned} \tag{41}$$

Furthermore, the diagonal matrix elements of J_y and J_y^2 have the same values as those for the x component. Thus, converting now to physical components with angular momentum in units of $\hbar$,

$$\Delta J_x = \Delta J_y = \hbar\sqrt{\frac{j(j+1) - m^2}{2}}, \tag{42}$$

in the state $|jm\rangle$ for which J_z has the precise value $\hbar m$, so $\Delta J_z = 0$. This is illustrated with the semiclassical vector model in which the vector $\vec{J}$, now of length $\hbar\sqrt{j(j+1)}$, is pictured to precess about its z-component with precise value $\hbar m$, which is less than $\hbar\sqrt{j(j+1)}$ even in the state with $m = j$. Also, for $j = \frac{1}{2}, m = \pm\frac{1}{2}$, we have $\Delta J_x = \Delta J_y = \frac{1}{2}\hbar$, the minimum quantum-mechanical uncertainty.

Final Remark: With our choice of phase for eqs. (34) and (35), we have made the matrix elements of J_y pure imaginary, and the matrix elements for J_x real. This is the standard angular momentum phase convention. All three components, however, are of course equivalent. We could, e.g., have used a basis in which J_x is diagonal, J_y real and off-diagonal, and J_z pure imaginary and off-diagonal.