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Angular momentum

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1 Rotations and angular momentum

Rotations R in space are implemented on QM systems by unitary transformations,

$$U(R) = e^{-i\theta^i J_i/\hbar}, \tag{1}$$

where J_i are the hermitian generators of rotation. The J_i are also the angular momentum operators, and are conserved if the Hamiltonian is invariant under rotations. The rotation group structure implies the commutation relations,

$$[J_i, J_j] = i\hbar\epsilon^{ijk}J_k. \tag{2}$$

Special cases of these are the orbital angular momentum of a single particle, spin of a single particle, or the total spin and orbital angular momentum of a collection of particles.

2 Irreducible representations of the rotation group

Since $[J_z, J^2] = 0$,[1] we can simultaneously diagonalize J_z and J^2. Call the (normalized) eigenstates $|jm\rangle$, where

$$J_z|jm\rangle = m|jm\rangle, \qquad J^2|jm\rangle = j(j+1)|jm\rangle, \tag{3}$$

[1]This means that the scalar J^2 is invariant under infinitesimal rotations about the z axis.

with $\hbar = 1$ from now on. It can be shown that the commutation relations (2) and hermiticity of J_i imply that the possible values of j and m are

$$j = 0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ 2, \ldots, \qquad m = j,\ j-1,\ j-2,\ \ldots, -j. \tag{4}$$

Although $|jm\rangle$ is not an eigenstate of J_x and J_y, the vectors $J_x|jm\rangle$ and $J_y|jm\rangle$ are linear combinations of the form $a|j, m+1\rangle + b|j, m-1\rangle$. The relation is neatly expressed using $J_\pm := J_x \pm iJ_y$. Namely:

$$J_\pm|jm\rangle = \sqrt{j(j+1) - m(m\pm 1)}\,|j, m\pm 1\rangle. \tag{5}$$

If any rotation is applied to the state $|jm\rangle$, it therefore mixes with the other states $|jm'\rangle$ with the same value of j. That is, the space spanned by the set of states $\{|jm\rangle\}$ for a fixed j is closed under rotations. One says that it carries a unitary representation of the rotation group. Moreover, no linear subspace of that space is closed under rotations,[2] and for this reason it's called an "irreducible" representation. The representation with a given j is called the "spin-j" representation, or "multiplet", and it is $2j+1$ dimensional. Note that the representation is an abstract structure, which can be realized by many different physical or mathematical systems.

3 Addition of angular momenta

The tensor product $j_1 \otimes j_2$ of any two representations is spanned by the product basis, $\{|j_1 m_1\rangle|j_2 m_2\rangle\}$. This decomposes into irreducible representations (irreps). To enumerate these, start with the "top" J_z state, $|j_1 j_1\rangle|j_2 j_2\rangle$, i.e. the state with the largest possible value of $J_z (= J_{1z} + J_{2z})$, which is $j_1 + j_2$, and work down to lower values of J_z by applying the lowering operator $J_- (= J_{1-} + J_{2-})$. At each step the result will be a linear combination of all the product states with $m_1 + m_2$ equal to a given value of the total J_z. When this process lands on the lowest possible J_z value, here $-(j_1 + j_2)$, it has filled out a spin-$(j_1 + j_2)$ representation. Next, construct the spin-$(j_1 + j_2 - 1)$ representation. The "top" state is the linear combination of the two states with $J_z = j_1 + j_2 - 1$ that is orthogonal to the state used already in building the spin-$(j_1 + j_2)$ representation; the other states are obtained by successively applying J_-. Repeating this process until all the states are used up, one obtains the decomposition

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus |j_1 - j_2|. \tag{6}$$

One can check that the total dimension $(2j_1 + 1)(2j_2 + 1)$ of $j_1 \otimes j_2$ is equal to the sum of $2j + 1$ over the j values stepping by integers from $j_1 + j_2$ down to $|j_1 - j_2|$.

[2] Although I don't now see a way to make that fact obvious, it seems intuitively reasonable, given that $J_\pm$ move the states up and down the ladder, filling out the whole multiplet. This itself is not (as far as I can see) a demonstration of irreducibility, since $J_\pm$ are not, by themselves, rotations. However, a general rotation has the form $\exp(zJ_+ - \bar{z}J_- + i\theta J_z)$, where the real number θ and the complex number z are arbitrary. It seems clear that, when z and θ vary arbitrarily, there can be no invariant linear subspace.

3.1 Examples

- The simplest example is the addition of two spin-1/2 systems:

$$\tfrac{1}{2} \otimes \tfrac{1}{2} = 1 \oplus 0 \longleftrightarrow \quad 2 \times 2 = 3 + 1 \tag{7}$$

  This is the decomposition into the spin triplet states and the spin singlet.

- For a second example, consider the p-wave electron states in an alkalai atom, with orbital angular momentum $\ell = 1$. These transform under the spin-1 representation, while the spin of the electron transforms under the spin-1/2 representation. The Hilbert space for these orbital and spin degrees of freedom is the tensor product of the two, $1 \otimes \frac{1}{2}$, which decomposes into the sum of two irreps,

$$1 \otimes \tfrac{1}{2} = \tfrac{3}{2} \oplus \tfrac{1}{2} \longleftrightarrow \quad 3 \times 2 = 4 + 2 \tag{8}$$

- For a third example, consider the two $2p$ electrons in carbon. Hund's first and second rules imply that in the ground state, the total spin of these is $S = 1$, and the total orbital angular momentum is $L = 1$. The total angular momentum of the pair is the sum of their orbital and spin angular momenta, so the relevant addition is

$$1 \otimes 1 = 2 \oplus 1 \oplus 0 \longleftrightarrow \quad 3 \times 3 = 5 + 3 + 1. \tag{9}$$

  Hund's third rule tells us that in this case, the joint state has $J = 0$, i.e. it lies in the singlet subspace on the right hand side.

4 Clebsch-Gordan coefficients

The identity operator on the product $j_1 \otimes j_2$ can be expanded in $\{|j_1 m_1\rangle |j_2 m_2\rangle\}$ states, or in $|jm\rangle$ states:

$$I_{j_1 \otimes j_2} = \sum_{m1,\, m2} |m_1 m_2\rangle\langle m_1 m_2| = \sum_{j\, m} |jm\rangle\langle jm|. \tag{10}$$

Here I use the notational abbreviation $|m_1 m_2\rangle := |j_1 m_1\rangle|j_2 m_2\rangle$, suppressing the j_1 and j_2 labels since they are the same for all the states. Applying the identity in the form of the first of these sums yields

$$|jm\rangle = \sum_{m_1+m_2=m} |m_1 m_2\rangle\langle m_1 m_2|jm\rangle. \tag{11}$$

Similarly, applying the identity in the form of the second sum in (10) yields

$$|m_1 m_2\rangle = \sum_j |jm\rangle\langle jm|m_1 m_2\rangle, \tag{12}$$

with $m = m_1 + m_2$ (since otherwise the inner product vanishes). The inner products that serve as the expansion coefficients are called *Clebsch-Gordan (CG) coefficients.*

The decomposition into the irreps discussed above introduces only algebraic functions involving the square root coefficients appearing in (5). Therefore the CG coefficients can always be taken to be real, and we have (restoring the explicit $j_1 j_2$ dependence)

$$\langle j_1 m_1 j_2 m_2 | jm \rangle = \langle jm | j_1 m_1 j_2 m_2 \rangle^* = \langle jm | j_1 m_1 j_2 m_2 \rangle. \tag{13}$$

There remains a sign ambiguity, which is typically fixed by requiring that the coefficient of $|m_1 = j_1\rangle |m_2 = j - j_1\rangle$ in the the expansion of the top state $|jj\rangle$ of the spin-j representation is positive, i.e. $\langle j_1, j - j_1 | jj \rangle > 0$.

The CG coefficients are displayed in printed tables, and they can be called in Mathematica: ClebschGordan[$\{j_1, m_1\}, \{j_2, m_2\}, \{j, m\}$]. Fundamentally, they are obtained using the what we know about the action of the operators J_z and $J_\pm$, (3) and (5), orthogonality of the eigenvectors of hermitian operators, and normalization of the states. In particular cases one can sometimes conveniently find them from scratch this way. There are recursion relations for them, a projection operator method, and, amazingly enough, a *closed form* formula found by Wigner. The formula was given in a more symmetrical form by Racah, but it's too complicated to be usable. See (106.14) of Landau & Lifshitz, QM. ,

4.1 Example: $1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$

Let's think of the first factor as the orbital angular momentum and the second factor as the spin. The states $|1 m_l\rangle$, for $m_l = 1, 0, -1$, form a basis for the first factor, and the states $|\frac{1}{2} m_s\rangle$, for $m_s = \frac{1}{2}, -\frac{1}{2}$ form a basis for the second factor. The six states $|1 m_l\rangle |\frac{1}{2} m_s\rangle$ form a basis for the tensor product $1 \otimes \frac{1}{2}$. These basis vectors are eigenvectors of L^2, L_z, S^2, and S_z. They are also eigenvectors of $J_z := L_z + S_z$, with eigenvalues $(m_l + m_s)\hbar$, but they are *not* eigenvectors of $J^2 = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S})$.

We can also find a basis of eigenvectors of J^2 and J_z. The eigenvalues of J^2 have the form $j(j+1)\hbar^2$, where $j\hbar$ is the maximum J_z value. The possible values of j in the present case are $j = \frac{3}{2}, \frac{1}{2}$, so the full space is spanned by a basis composed of the four vectors $|\frac{3}{2} m_j\rangle$ (with $m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$) and the two vectors $|\frac{1}{2} m_j\rangle$ (with $m_j = \frac{1}{2}, -\frac{1}{2}$).

Any vector from one of these bases can be expanded as a linear combination of vectors from the other basis. For example,

$$|\tfrac{3}{2}\tfrac{1}{2}\rangle = \sum_{m_l, m_s} C_{m_l, m_s} |1 m_l\rangle |\tfrac{1}{2} m_s\rangle. \tag{14}$$

Conversely,

$$|10\rangle |\tfrac{1}{2}\tfrac{1}{2}\rangle = \sum_{j,m} D_{j,m} |j, m\rangle. \tag{15}$$

The coefficients C_{m_l, m_s} and $D_{j,m}$ are examples of Clebsch-Gordan coefficients. They are equal to the inner products $C_{m_l, m_s} = \langle 1 m_l | \langle \frac{1}{2} m_s | \frac{3}{2} \frac{1}{2} \rangle \equiv \langle 1 m_l \frac{1}{2} m_s | \frac{3}{2} \frac{1}{2} \rangle$, and $D_{jm} = \langle jm || 10 \rangle | \frac{1}{2} \frac{1}{2} \rangle \equiv \langle jm | 10 \frac{1}{2} \frac{1}{2} \rangle$.[3] The CG coefficient table is constructed using

[3] The expressions after $\equiv$ are just a notational change, which combines the labels of the factors into one "ket".

the what we know about the action of the operators J_z and $J_\pm$, (3) and (5), and orthogonality of the eigenvectors of hermitian operators. Instead of using the table, we can sometimes conveniently evaluate the coefficients directly, using these properties. For example, the left hand side of (15) is an eigenstate of $J_z = L_z + S_z$ with eigenvalue $(0+\frac{1}{2})\hbar$, so the right hand side must be as well. This implies that D_{jm} must vanish unless $m = \frac{1}{2}$. Instead of having a sum of six terms, therefore, only two terms actually contribute:

$$|10\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle = \alpha|\tfrac{3}{2}\tfrac{1}{2}\rangle + \beta|\tfrac{1}{2}\tfrac{1}{2}\rangle \tag{16}$$

Our task thus reduces to finding just the two coefficients α and β. (If we only need their absolute values, one of these will be enough, since we can find the other by imposing the normalization condition $\langle\frac{3}{2}\frac{1}{2}|\frac{3}{2}\frac{1}{2}\rangle = 1$.) Let's now apply $J_+ = L_+ + S_+$ to both sides of (16). On the left, $L_+|10\rangle = \sqrt{2}|11\rangle$, and $S_+|\frac{1}{2}\frac{1}{2}\rangle = 0$, since the latter is the top state. So J_+ on the left hand side yields $\sqrt{2}|11\rangle|\frac{1}{2}\frac{1}{2}\rangle$. On the right hand side, $J_+|\frac{3}{2}\frac{1}{2}\rangle = \sqrt{3}|\frac{3}{2}\frac{3}{2}\rangle$, and $J_+|\frac{1}{2}\frac{1}{2}\rangle = 0$, since the latter is the top state. Thus the action of J_+ on (16) yields

$$\sqrt{2}|11\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle = \alpha\sqrt{3}|\tfrac{3}{2}\tfrac{3}{2}\rangle. \tag{17}$$

The ket product on the lhs is equal to the ket on the rhs, so we can solve for $\alpha = \sqrt{2/3}$.

5 Why a filled shell has zero angular momentum

The concept of a filled shell refers to fermionic (antisymmetric) composite states in which a complete set of states in a given spin-j representation are filled. If a rotation operator is applied to such a state, the result remains antisymmetric. Since there is only one such "totally filled" state, it is evidently therefore invariant under rotations. The angular momentum components are the infinitesimal generators of rotations, so the fact that the state is rotationally invariant implies that $\vec{J}$ annihilates it.

To illustrate this with the smallest example, consider a composite of two spin-$\frac{1}{2}$ systems. The unique antisymmetric state we can form using the two basis vectors $|\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ is $(|\frac{1}{2}\rangle|-\frac{1}{2}\rangle - |-\frac{1}{2}\rangle|+\frac{1}{2}\rangle)/\sqrt{2}$. One cannot form other antisymmetric states using different basis vectors: the antisymmetric state constructed from a new basis $\{\alpha|\frac{1}{2}\rangle + \beta|-\frac{1}{2}\rangle, \alpha'|\frac{1}{2}\rangle + \beta'|-\frac{1}{2}\rangle\}$ is $(\alpha\beta' - \alpha'\beta)(|\frac{1}{2}\rangle|-\frac{1}{2}\rangle - |-\frac{1}{2}\rangle|-\frac{1}{2}\rangle)/\sqrt{2}$, which is proportional to the previous state.

To see why this works in general, consider the totally antisymmetric combination of products of the $2j+1$ states of a spin-j representation (i.e. the Slater determinant of these states). Now act with any rotation on this state. Each of the states in the product will be acted on by the same rotation operator, and the resulting state will still be totally antisymmetric. But there is only one totally antisymmetric tensor product of n vectors in an n-dimensional vector space, so after the rotation the state is the same, up to a possible scalar multiple. In fact the scalar multiple is nothing but the determinant of the 1-particle rotation matrix, which is 1. This means the antisymmetric state is invariant under all rotations. Another way to see that in addition to J_z, both J_x and J_y annihilate the totally antisymmetric state, is to act with $J_\pm = J_x \pm iJ_y$ on the state. Every term either vanishes because $m = j$ cant be raised, or because $m = -j$ cant be lowered, or because the result of the action is to make two m values the same, which yields zero because of the antisymmetry of the state.

In atomic physics, when an ℓ-orbital shell is filled with $2\ell + 1$ electrons, all with the same spin state, the total L vanishes, but of course $S \neq 0$. If on the other hand the shell is filled with $2(2\ell + 1)$ electrons, then L, S, and J all vanish. I suppose the easiest way to see this is to note first that L_z and S_z vanish by inspection, and that the action of the ladder oprators $L_\pm$ and $S_\pm$ do as well, for the same reason as just explained for $J_\pm$.