Lecture 20 (Nov. 20, 2017)

20.1 Matrix Elements of Angular Momentum Operators

Assume that we have normalized $|j,m\rangle$. By definition, since these are eigenstates of $\boldsymbol{J}^2$ and J_z, these operators are diagonal, with

$$\begin{aligned}\langle j',m'|\boldsymbol{J}^2|j,m\rangle &= j(j+1)\hbar^2\delta_{jj'}\delta_{mm'}\,,\\ \langle j',m'|J_z|j,m\rangle &= m\hbar\delta_{jj'}\delta_{mm'}\,.\end{aligned} \tag{20.1}$$

Now we only need to compute the matrix elements of J_x and J_y. We will make use of the identity

$$\langle j,m|J_+J_-|j,m\rangle = \langle j,m|\boldsymbol{J}^2 - J_z^2 - \hbar J_z|jm\rangle = \hbar^2\big(j(j+1) - m^2 - m\big)\,. \tag{20.2}$$

We also know that

$$J_+|j,m\rangle = c_{j,m}^{(+)}|j,m+1\rangle\,. \tag{20.3}$$

We still need to determine the coefficient $c_{j,m}^{(+)}$. Using (20.2) and $J_- = J_+^\dagger$, we see that

$$\left|c_{j,m}^{(+)}\right|^2 = \hbar^2(j(j+1) - m(m+1)) = \hbar^2(j-m)(j+m+1)\,. \tag{20.4}$$

We will choose (by convention) for $c_{j,m}^{(+)}$ to be real and positive, which then gives us

$$J_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle\,. \tag{20.5}$$

A similar argument gives us

$$J_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle\,. \tag{20.6}$$

Packaging these results together, we have

$$\langle j',m'|J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\delta_{jj'}\delta_{m',m\pm1}\,. \tag{20.7}$$

We see that when $m=+j$, the state is annihilated by J_+, and when $m=-j$, the state is annihilated by J_-, exactly as required.

We can now easily calculate the matrix elements of J_x and J_y, as they are linear combinations of $J_\pm$. This allows us to explicitly write matrix representations of $\boldsymbol{J}$ for fixed j. As an example, consider $j=1$. In this case,

$$J_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}, \tag{20.8}$$

where the basis is ordered as $m=+1,0,-1$. Using the matrix elements for $J_\pm$, we can write down

$$\begin{aligned}J_x &= \frac{J_+ + J_-}{2} = \frac{\hbar}{2}\begin{pmatrix}0 & \sqrt{2} & 0\\ \sqrt{2} & 0 & \sqrt{2}\\ 0 & \sqrt{2} & 0\end{pmatrix},\\ J_y &= \frac{J_x - J_y}{2i} = \frac{\hbar}{2}\begin{pmatrix}0 & -\sqrt{2}i & 0\\ \sqrt{2}i & 0 & -\sqrt{2}i\\ 0 & \sqrt{2}i & 0\end{pmatrix}.\end{aligned} \tag{20.9}$$

For any fixed j, we can now also construct matrix elements of the finite rotation operator $\mathcal{D}(R)$. For a fixed j, the angular momentum operators are $(2j+1)\times(2j+1)$ Hermitian matrices, and so the rotation matrix $\mathcal{D}(R)$ will be $(2j+1)\times(2j+1)$ unitary matrices. Consider a rotation by angle θ about the axis $\hat{\boldsymbol{n}}$. First, we construct an infinitesimal rotation by $\delta\theta$ about the axis $\hat{\boldsymbol{n}}$:

$$\mathcal{D}(R_{\delta\theta}) = 1 - \frac{i}{\hbar}(\boldsymbol{J}\cdot\hat{\boldsymbol{n}})\delta\theta + O\big(\delta\theta^2\big)\,. \tag{20.10}$$

We can then build up a finite rotation by multiplying infinitesimal rotations N times and taking $N\to\infty$,

$$\begin{aligned}\mathcal{D}(R(\theta,\hat{\boldsymbol{n}})) &= \lim_{N\to\infty}(\mathcal{D}(\theta/N,\hat{\boldsymbol{n}}))^N \\ &= \lim_{N\to\infty}\left(1 - \frac{i}{\hbar}(\boldsymbol{J}\cdot\hat{\boldsymbol{n}})\frac{\theta}{N} + O\big((\theta/N)^2\big)\right)^N \\ &= e^{-i\theta\boldsymbol{J}\cdot\hat{\boldsymbol{n}}/\hbar}\,.\end{aligned} \tag{20.11}$$

20.2 Rotation Groups

In general, symmetry operations form a mathematical structure called a *group*.

Definition 1. A set $\{g_i\} := G$ forms a group if there exists a multiplication operation $\cdot$ such that:

- for all $g_1, g_2 \in G$, $g_1\cdot g_2 \in G$;
- multiplication is associative: for all $g_1, g_2, g_3 \in G$,

$$(g_1\cdot g_2)\cdot g_3 = g_1\cdot(g_2\cdot g_3)\,; \tag{20.12}$$

- there exists $1\in G$ such that

$$1\cdot g = g\cdot 1 = g\,; \tag{20.13}$$

- for every $g\in G$, there exists $g^{-1}\in G$ such that

$$g\cdot g^{-1} = g^{-1}\cdot g = 1\,. \tag{20.14}$$

For example, the set of 3×3 orthogonal matrices forms a group under the operation of matrix multiplication. This group is known as the *orthogonal group* O(3). If we restrict our attention to rotations with $\det R = +1$, then we get a subgroup (a subset that is itself also a group under matrix multiplication) called the *special orthogonal group* SO(3).

There is another pertinent group to the discussion of rotations, which is the group of 2×2 unitary matrices satisfying $\det U = 1$. Any matrix of this kind can be written in the form

$$U(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{20.15}$$

with $|a|^2+|b|^2 = 1$. Such matrices form a group under matrix multiplication, known as the *special unitary group* SU(2).

In quantum mechanics, rotations are represented by unitary operators $\mathcal{D}(R)$. These unitary operators must themselves form a group, because the product of two of these operators must give another, the composition is associative, there is an identity operation, and $\mathcal{D}\big(R^{-1}\big)$ is the inverse of $\mathcal{D}(R)$. In particular, we can see that the $\mathcal{D}(R)$ must satisfy the same group identities as the group of rotations R.

The matrix elements of $\mathcal{D}(R)$ are

$$\mathcal{D}^{(j)}_{m',m}(R) = \langle j, m'|e^{-i\theta \boldsymbol{J}\cdot\hat{\boldsymbol{n}}/\hbar}|j, m\rangle\,. \tag{20.16}$$

Note that we have chosen the same j for both the bra and ket; this is because $\mathcal{D}(R)$ commutes with $\boldsymbol{J}^2$, so a rotation cannot change the value of $\boldsymbol{J}^2$. As a result, in the full ket space, the (infinite-dimensional) matrix for $\mathcal{D}(R)$ is block diagonal in the (j, m) basis, where each block corresponds to one value of j. The block corresponding to j will be a $(2j + 1) \times (2j + 1)$ submatrix.

An explicit set of matrices that satisfies the same group identities as a group is called a *(linear) group representation.* Thus, the $\mathcal{D}(R)$ form a representation of SO(3). In particular, this representation is called a *completely reducible* representation, because it can be written in block diagonal form. Each block on the diagonal of $\mathcal{D}(R)$, taken as a standalone matrix $\mathcal{D}^{(j)}_{m',m}$ for fixed j, is an *irreducible* representation (sometimes referred to as an *irrep*), as it has no invariant subspaces.

Consider $j = 1/2$. In this case, m and m' take on the values $\pm\frac{1}{2}$. The rotation operator matrix elements are

$$\mathcal{D}^{(1/2)}_{m',m}(\theta, \hat{\boldsymbol{n}}) = \langle m'|e^{-i\theta\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}/2}|m\rangle\,. \tag{20.17}$$

That is, the rotation operators are

$$\begin{aligned}\mathcal{D}^{(1/2)}(\theta, \hat{\boldsymbol{n}}) &= e^{-i\theta\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}/2}\\ &= \cos\frac{\theta}{2} - i(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}})\sin\frac{\theta}{2}\,.\end{aligned} \tag{20.18}$$

Explicitly,

$$\mathcal{D}^{(1/2)}(\theta, \hat{\boldsymbol{n}}) = \begin{pmatrix} \cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2} & (-in_x - n_y)\sin\frac{\theta}{2} \\ (-in_x + n_y)\sin\frac{\theta}{2} & \cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2}\end{pmatrix}. \tag{20.19}$$

This may seem unusual, because this is an SU(2) matrix. The operators $\mathcal{D}^{(1/2)}(\theta, \hat{\boldsymbol{n}})$ form a representation of SU(2), even though we originally set out to find a representation of SO(3).

Rotations of 3D space can be characterized either by an SO(3) matrix R (a three-dimensional irrep) or by an SU(2) matrix U (a two-dimensional irrep). But SO(3) and SU(2) are not in one-to-one correspondence. Suppose we consider a rotation by $\theta = 2\pi$ along some axis $\hat{\boldsymbol{n}}$. For SO(3),

$$R(2\pi, \hat{\boldsymbol{n}}) = \mathbb{1}_3\,, \tag{20.20}$$

while for SU(2),

$$\mathcal{D}^{(1/2)}(2\pi, \hat{\boldsymbol{n}}) = e^{-i\pi\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}} = -\mathbb{1}_2\,. \tag{20.21}$$

The result is that for any spin-$\frac{1}{2}$ system, the phase of the wavefunction is rotated by π under a physical 2π rotation.