The rotation group and quantum mechanics[1]

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I offer here some background for Chapter 3 of J. J. Sakurai, *Modern Quantum Mechanics*.

1 The rotation group

A rotation can be described by giving a matrix R such that a vector v gets transformed to a vector $\bar{v}$ under the rotation, with

$$\bar{v}_i = R_{ij}\ v_j \quad . \tag{1}$$

In these notes, I use the summation convention, under which repeated indices are summed. Here, we sum over j from 1 to 3. Rotations preserve inner products: $\bar{u} \cdot \bar{v} = u \cdot v$ for any vectors u and v. For this reason, we must have

$$u_i v_i = \bar{u}_i \bar{v}_i = R_{ik} u_k R_{il} v_l \tag{2}$$

so

$$R_{ik} R_{il} = \delta_{kl} \quad . \tag{3}$$

That is

$$R^T R = 1 \quad . \tag{4}$$

This implies also that $(\det R)^2 = 1$, which implies that $\det R$ must be either $+1$ or -1. The matrices with $R^T R = 1$ that one can reach by continuously modifying the unit matrix must have $\det R = 1$. We call these the "rotation" matrices. The matrices with $R^T R = 1$ and $\det R = -1$ are a matrix product of a parity transformation $R = -1$ and a rotation matrix.

The set of matrices with $R^T R = 1$ is called $O(3)$ and, if we require additionally that $\det R = 1$, we have $SO(3)$.

The rotation matrices $SO(3)$ form a *group*: matrix multiplication of any two rotation matrices produces a third rotation matrix; there is a matrix 1 in $SO(3)$ such that $1M = M$; for each M in $SO(3)$ there is an inverse matrix M^{-1} such that $M^{-1}M = MM^{-1} = 1$.

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2 Representation of the rotation group

In quantum mechanics, for every $R \in SO(3)$ we can rotate states with a unitary operator[3] $U(R)$. The operator must be unitary so that inner products between states stay the same under rotation. If we apply two rotations, we need

$$U(R_2 R_1) = U(R_2)U(R_1) \ . \tag{5}$$

To make this work, we need

$$\begin{aligned} U(1) &= 1 \ , \\ U(R^{-1}) &= U(R)^{-1} \ . \end{aligned} \tag{6}$$

We say that the operators $U(R)$ form a *representation* of $SO(3)$.[4]

3 Transformation of vector operators

Suppose that we have a set of three quantum operators that make a vector. We will consider the three components of momentum, (p^1, p^2, p^3), as an example. What does "make a vector" mean?

Suppose that we have states $\big|\phi\big\rangle$ and $\big|\psi\big\rangle$. Under a rotation R, these get transformed to

$$\begin{aligned} \big|\bar\phi\big\rangle &= U(R)\big|\phi\big\rangle \ , \\ \big|\bar\psi\big\rangle &= U(R)\big|\psi\big\rangle \ . \end{aligned} \tag{7}$$

Experiments that measure momenta involve inner products $\big\langle\phi\big|p^i\big|\psi\big\rangle$. If we rotate the states, we need to get the same inner products as with the original states but rotated with the matrix R:

$$\big\langle\bar\phi\big|p^i\big|\bar\psi\big\rangle = R_{ij}\big\langle\phi\big|p^j\big|\psi\big\rangle \ . \tag{8}$$

That is

$$\big\langle\phi\big|U(R)^{-1}p^i U(R)\big|\psi\big\rangle = R_{ij}\big\langle\phi\big|p^j\big|\psi\big\rangle \ . \tag{9}$$

For this to work for any states, we need

$$U(R)^{-1}p^i U(R) = R_{ij}\, p^j \ . \tag{10}$$

[3] Sakurai uses the notation $\mathcal{D}(R)$.

[4] Actually, we will weaken this a bit as we find out more: we can also allow $U(R_2R_1) = -U(R_2)U(R_1)$.

We will come back to this shortly.

Exercise 3.1 If you apply Eq. (10) to the case in which R is a rotation through an angle $\pi/4$ about the x-axis, what do you get for $U(R)^{-1}p^i U(R)$ for $i = 1, 2, 3$?

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4 Infinitesimal generators of rotations

Of special interest is the rotation $R(\psi, \vec{n})$ that gives a rotation through angle ψ about an axis in the direction of the vector $\vec{n}$. For a rotation through angle ψ about the z-axis, simple geometric considerations give

$$R = \begin{pmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{11}$$

That is

$$R_{ij} = -\sin\psi\, \epsilon_{ij3} + \cos\psi\, (\delta_{ij} - \delta_{i3}\delta_{j3}) + \delta_{i3}\delta_{j3} \quad . \tag{12}$$

Another way to write this is

$$R_{ij} = -\sin\psi\, \epsilon_{ijk} n_k + \cos\psi\, (\delta_{ij} - n_i n_j) + n_i n_j \quad , \tag{13}$$

where $\vec{n}$ is a unit vector in the 3-direction: $n_i = \delta_{i3}$. Written this way, the result generalizes to a rotation about of the three coordinate axes or, indeed, about any axis,

$$n = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \quad . \tag{14}$$

If we rotate through an infinitesimal angle $\delta\psi$, R must be infinitesimally close to the unit matrix. We can expand $R(\delta\psi, \vec{n})$ to first order in the three infinitesimal parameters $(\delta\psi\, n_1, \delta\psi\, n_2, \delta\psi\, n_3)$. Using Eq. (13), we have

$$R(\delta\psi, \vec{n})_{ij} \sim 1 - \delta\psi\ \epsilon_{ijk} n_k \quad . \tag{15}$$

We choose to write this as

$$R(\delta\psi, \vec{n})_{ij} \sim 1 - i\,\delta\psi\ n_k (\mathcal{J}^k)_{ij} \quad . \tag{16}$$

Here the $\mathcal{J}^k$ are three matrices, the *infinitesimal generators* of $SO(3)$:

$$(\mathcal{J}^k)_{ij} = -i\, \epsilon_{kij} \quad . \tag{17}$$

Here ϵ_{ijk} is the completely antisymmetric tensor with $\epsilon_{123} = +1$. One can easily verify that the infinitesimal generators obey the commutation relations

$$[\mathcal{J}^i, \mathcal{J}^j] = i\epsilon_{ijk}\mathcal{J}^k \quad . \tag{18}$$

If we multiply two rotations about the same axis, we have

$$R(\psi_2, \vec{n})\, R(\psi_1, \vec{n}) = R(\psi_1 + \psi_2, \vec{n}) \quad . \tag{19}$$

Taking $\psi_1 \equiv \psi$ and taking $\psi_2 \equiv \delta\psi$ to be infinitesimal, we have

$$[1 - i\delta\psi\; n^i \mathcal{J}^i]\, R(\psi, \vec{n}) \sim R(\psi + \delta\psi, \vec{n}) \quad . \tag{20}$$

This gives

$$\frac{d}{d\psi}\, R(\psi, \vec{n}) = -i\, n^i \mathcal{J}^i\; R(\psi, \vec{n}) \tag{21}$$

Solving this differential equation with the boundary condition $R(0, \vec{n}) = 1$ gives

$$R(\psi, \vec{n}) = \exp(-i\psi\, n^i \mathcal{J}^i) \quad . \tag{22}$$

I assert that any rotation is a rotation through some angle about some axis. Thus we are able to write any rotation as an exponential of the infinitesimal generators $\mathcal{J}^i$.

You may have thought that it is obvious that any rotation R is a rotation through some angle about some axis, but it is perhaps less than obvious. Here is a proof. What we need to show is that there is a vector n such that $R_{ij}n_j = n_i$. We know that R is a real matrix with $R^T R = 1$. Thus $R^\dagger R = 1$, so that R is also a unitary matrix. Thus it has three (possibly complex) eigenvectors with eigenvalues of the form $e^{i\phi_j}$. But since R is real, if $e^{i\phi}$ is an eigenvalue then so is $e^{-i\phi}$. Thus, of the three eigenvalues, two of them can be a pair of matching complex phase factors, $e^{i\phi}$ and $e^{-i\phi}$. Since there are three eigenvalues, the other one of them must obey $e^{i\phi} = e^{-i\phi}$, so it must be $+1$ or -1. But also $\det R = 1$, so the third eigenvalue must be $+1$. Finally, if the corresponding eigenvector is n, $Rn = n$, then also $Rn^* = n^*$. Thus n must be a phase factor times n^*. By adjusting the phase of n, we can choose it to be a real vector. Thus there is a real vector n such that $Rn = n$. The eigenvector n is the rotation axis. Once we know the rotation axis, we can construct the rotation angle by considering what R does to vectors that are orthogonal to the rotation axis.

Exercise 4.1 By expanding the right hand sides of Eq. (22) and Eq. (13) in powers of ψ, show that they match. You will need to work out $(\vec{\mathcal{J}} \cdot \vec{n})^N$ for any power N in order to do this.

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5 Representation of the generators

Moving now to the quantum state space, we note that $U(R(\delta\phi, \vec{n}))$ for infinitesimal $\delta\phi$ must be infitesimally close to the unit operator. Expanding $U(R(\delta\phi, \vec{n}))$ in the three infinitesimal parameters $(\delta\phi\, n^1, \delta\phi\, n^2, \delta\phi\, n^3)$, we have

$$U(R(\delta\phi, \vec{n})) \sim 1 - i\delta\phi\; n^i J^i \quad . \tag{23}$$

Here the J^i are three operators, the infinitesimal generators of the representation of $SO(3)$. We will find that these operators have the same commutation relations as the original generator matrices $\mathcal{J}^i$, but it takes a little analysis to show that.

First, we ask what is the representation of $R(\phi, \vec{n})$ for a finite rotation. If we multiply two rotations about the same axis and use the group representation rule, we have

$$U(R(\delta\phi, \vec{n}))\, U(R(\phi, \vec{n})) \sim U(R(\phi + \delta\phi, \vec{n})) \quad . \tag{24}$$

Thus

$$[1 - i\delta\phi\; n^i J^i]\, U(R(\phi, \vec{n})) \sim U(R(\phi + \delta\phi, \vec{n})) \quad . \tag{25}$$

This gives

$$\frac{d}{d\phi}\, U(R(\phi, \vec{n})) = -i\, n^i J^i\; U(R(\phi, \vec{n})) \tag{26}$$

Solving this differential equation with the boundary condition $U(R(0, \vec{n})) = 1$ gives

$$U(R(\phi, \vec{n})) = \exp(-i\phi\, n^i J^i) \quad . \tag{27}$$

This allows us to represent a finite rotation. We can use this to find out how the generators themselves transform under a finite rotation.

6 Transformation of the generators

Consider what happens if you rotate through an angle ϕ about some axis, then multiply by a generator matrix, then apply the inverse rotation. That is, consider the quantity

$$\mathcal{J}^j(\phi) = R(-\phi,\vec{n})\mathcal{J}^j R(\phi,\vec{n}) \tag{28}$$

To discover what this is, differentiate with respect to ϕ:

$$\begin{aligned}
\frac{d}{d\phi}\mathcal{J}^j(\phi) &= \frac{d}{d\phi}R(-\phi,\vec{n})\mathcal{J}^j R(\phi,\vec{n}) \\
&= R(-\phi,\vec{n})[in^i\mathcal{J}^i\mathcal{J}^j - \mathcal{J}^j in^i\mathcal{J}^i]R(\phi,\vec{n}) \\
&= i\,n^i R(-\phi,\vec{n})[\mathcal{J}^i,\mathcal{J}^j]R(-\phi,\vec{n}) \\
&= -\ n^i\epsilon_{ijk}R(-\phi,\vec{n})\mathcal{J}^k R(\phi,\vec{n}) \\
&= -\,i\,n^i[\mathcal{J}^i]_{jk}\mathcal{J}^k(\phi)\ \ .
\end{aligned} \tag{29}$$

This is a differential equation for $\mathcal{J}^j(\phi)$. The boundary condition at $\phi = 0$ is $\mathcal{J}^j(0) = \mathcal{J}^j$. Evidently, the solution is

$$\mathcal{J}^j(\phi) = \exp(-i\,\phi\,n^i\mathcal{J}^i)_{jk}\mathcal{J}^k = R(\phi,\vec{n})_{jk}\mathcal{J}^k\ \ . \tag{30}$$

We conclude that

$$R(-\phi,\vec{n})\mathcal{J}^j R(\phi,\vec{n}) = R(\phi,\vec{n})_{jk}\mathcal{J}^k \tag{31}$$

for all ϕ. If we denote $R(\phi,\vec{n})$ by simply R, this is

$$R^{-1}\mathcal{J}^j R = R_{jk}\mathcal{J}^k\ \ . \tag{32}$$

Compare this to Eq. (10). It says that the generator matrices $\mathcal{J}^j$ transform like the components of a vector.

We can prove Eq. (32) in a different way, which is also instructive. Recall the definition of the determinant of any matrix M:

$$\epsilon_{ijk}\det M = M_{ii'}M_{jj'}M_{kk'}\,\epsilon_{i'j'k'}\ \ . \tag{33}$$

For a rotation matrix R, we have $\det R = 1$, so

$$\epsilon_{ijk} = R_{ii'}R_{jj'}R_{kk'}\,\epsilon_{i'j'k'}\ \ . \tag{34}$$

This is an interesting result in its own right.[5] For our present purposes, using $R^T = R^{-1}$, we can rewrite it as

$$R^{-1}_{j'j}\,\epsilon_{ijk}\,R_{kk'} = R_{ii'}\,\epsilon_{i'j'k'} \quad . \tag{35}$$

Using $\epsilon_{ijk} = i(\mathcal{J}^i)_{jk}$, this is

$$R^{-1}_{j'j}\,(\mathcal{J}^i)_{jk}\,R_{kk'} = R_{ii'}\,(\mathcal{J}^{i'})_{j'k'} \quad . \tag{36}$$

That is, in a notation using matrix multiplication,

$$R^{-1}\,\mathcal{J}^i\,R = R_{ii'}\,\mathcal{J}^{i'} \quad . \tag{37}$$

This is Eq. (32).

Consider now a finite rotation R, followed by a rotation through angle θ about one axis, say the j axis, followed by the inverse of the finite rotation. Call the resulting matrix $A(\theta)$:

$$A(\theta) = R^{-1}\exp(-i\theta\mathcal{J}^j)R \quad . \tag{38}$$

We can determine what $A(\theta)$ is by writing a differential equation for it and using Eq. (32):

$$\begin{aligned} i\,\frac{d}{d\theta}A(\theta) &= R^{-1}\mathcal{J}^j\exp(-i\theta\mathcal{J}^j)R \\ &= R^{-1}\mathcal{J}^jRR^{-1}\exp(-i\theta\mathcal{J}^j)R \\ &= R^{-1}\mathcal{J}^jR\;A(\theta) \\ &= R_{jk}\mathcal{J}^kA(\theta) \quad . \end{aligned} \tag{39}$$

The solution of this differential equation with boundary condition $A(0) = 1$ is

$$A(\theta) = \exp(-i\theta R_{jk}\mathcal{J}^k) \quad . \tag{40}$$

Thus we have proved

$$R^{-1}\exp(-i\theta\mathcal{J}^j)R = \exp(-i\theta R_{jk}\mathcal{J}^k) \quad . \tag{41}$$

[5] As we will discuss later, we can transform vectors with $\bar{v}_i = R_{ii'}v_{i'}$ and we can transform objects with more indices, "tensors," with more rotation matrices, $\bar{T}_{ijk} = R_{ii'}R_{jj'}R_{kk'}\,T_{i'j'k'}$. Thus we find that the tensor with components ϵ_{ijk} is invariant under rotations.

This equation says that if we rotate with R, then rotate through angle θ about the j axis, then rotate back with R^{-1} we get a rotation through angle θ with a rotated $\mathcal{J}$ matrix. Equivalently, we get a rotation through angle θ about a rotated axis.

We have discovered a rule that gives, explicitly, the product of a certain combination of finite rotation matrices. We can now apply our hard won knowledge to the quantum rotation operators. Using the group composition law, we have

$$U(R)^{-1}U(\exp(-i\theta\mathcal{J}^j))U(R) = U(\exp(-i\theta R_{jk}\mathcal{J}^k)) \ . \tag{42}$$

We know from Eq. (27) that

$$\begin{aligned} U(\exp(-i\theta\mathcal{J}^j)) &= \exp(-i\theta J^j) \ , \\ U(\exp(-i\theta R_{jk}\mathcal{J}^k)) &= \exp(-i\theta R_{jk} J^k) \ . \end{aligned} \tag{43}$$

Thus

$$U(R)^{-1}\exp(-i\theta J^j)U(R) = \exp(-i\theta R_{jk} J^k)) \ . \tag{44}$$

If we differentiate this with respect to θ, we find

$$U(R)^{-1}\, J^j\, U(R) = R_{jk}\, J^k \ . \tag{45}$$

This is the quantum analogue of Eq. (32). If we compare this to Eq. (10), we see that this rule can be interpretated as saying that the quantum operators J_k are components of a vector operator.

7 The commutation relations

If we let $R = \exp(-i\delta\phi\, n_i \mathcal{J}^i)$ and expand Eq. (45) to first order in $\delta\phi$, we have

$$[1 + i\delta\phi\, n^i J^i] J^j [1 - i\delta\phi\, n^i J^i] \sim \left\{\delta_{jk} - i\delta\phi\, n^i [\mathcal{J}^i]_{jk}\right\} J^k \ . \tag{46}$$

Thus, using $(\mathcal{J}^i)_{jk} = -i\,\epsilon_{ijk}$

$$J^j + i\delta\phi\, n^i [J^i, J^j] = J^j - \delta\phi\, n^i \epsilon_{ijk} J^k \ . \tag{47}$$

Matching the coefficients of $\delta\phi\, n^i$ on both sides of this equation we have

$$[J^i, J^j] = i\epsilon_{ijk} J^k \quad . \tag{48}$$

Thus the quantum generators obey the same commutation relations as the generator matrices that we started with.

We may also note that if we use Eq. (10) for the components of the momentum operator, we have

$$[1 + i\delta\phi\, n^i J^i] p^j [1 - i\delta\phi\, n^i J^i] \sim \left\{ \delta_{jk} - i\delta\phi\, n^i [\mathcal{J}^i]_{jk} \right\} p^k \quad . \tag{49}$$

so

$$[J^i, p^j] = i\epsilon_{ijk} p^k \quad . \tag{50}$$

This is the infinitesimal rotation form of the statement that the components of p transform as a vector.

Exercise 7.1 Consider the quantum mechanics of a spinless particle. Do the components of $\vec{L} = \vec{x} \times \vec{p}$ have the right commutation relations to be the quantum generators of the rotation group?

Exercise 7.2 Consider the quantum mechanics of a spinless particle. Do the components of $\vec{L} = \vec{x} \times \vec{p}$ have the right commutation relations with the components of $\vec{x}$ and $\vec{p}$ so that $\vec{x}$ and $\vec{p}$ transform as vectors?

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8 The spin 1/2 representation

We have already seen the spin 1/2 representation of the rotation group, with generators

$$J^i = \frac{1}{2}\, \sigma^i \quad . \tag{51}$$

This is the simplest example of three hermitian matrices that obey the commutation relations (48).

Exercise 8.1 The rotation operators $U(R)$ for this representation can be written as 2×2 matrices (using the conventional basis for the σ^i matrices, in which σ^3 is diagonal). Consider a rotation $U(R(\psi, \vec{n}))$ through angle ψ about an axis

$$\vec{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \quad . \tag{52}$$

Starting with eq. (27), show that

$$U(R(\psi, \vec{n})) = \cos(\psi/2)\, 1 - i\sin(\psi/2)\, \vec{\sigma}\cdot\vec{n} \quad . \tag{53}$$

Exercise 8.2 The eigenvectors of S^3 in the spin 1/2 representation are

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad . \tag{54}$$

You can find eigenvectors of $\vec{S}\cdot\vec{n}$ with

$$\vec{n} = (\sin\beta\cos\alpha, \sin\beta\sin\alpha, \cos\beta) \tag{55}$$

by defining

$$\chi(\vec{n}, \pm) = U(R(\alpha, \hat{z}))U(R(\beta, \hat{y}))\, \chi_\pm \quad . \tag{56}$$

Here $\hat{x}, \hat{y}, \hat{z}$ are unit vectors in the directions of the coordinate axes. You could also use

$$\chi'(\vec{n}, \pm) = U(R(\alpha, \hat{z}))\, U(R(\beta, \hat{y}))\, U(R(-\alpha, \hat{z}))\, \chi_\pm \quad . \tag{57}$$

Find these vectors explicitly. Are these both really eigenvectors of $\vec{S}\cdot\vec{n}$? How do they differ?

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9 Reducible and irreducible representations

Let $\mathcal{V}$ be the space of quantum mechanical state vectors for whatever system we are thinking about. Then the operators $U(R)$ with the properties defined in the previous sections constitute a *representation* of the rotation group.

Similarly, suppose that there is a subspace $\mathcal{V}_1$ of $\mathcal{V}$ such that $U(R)\big|\psi\big\rangle \in \mathcal{V}_1$ when $\big|\psi\big\rangle \in \mathcal{V}_1$. In this case, we can also consider the subspace $\mathcal{V}_1^\perp$ consisting of all vectors $\big|\phi\big\rangle$ that are orthogonal to every vector in $\mathcal{V}_1$. Then $U(R)\big|\phi\big\rangle \in \mathcal{V}_1^\perp$ when $\big|\phi\big\rangle \in \mathcal{V}_1^\perp$. This follows from the fact that $U(R)$ is unitary. To prove it, let $\big|\phi\big\rangle \in \mathcal{V}_1^\perp$. Let $\big|\psi\big\rangle$ be any vector in $\mathcal{V}_1$ and define $\big|\psi'\big\rangle = U(R)^{-1}\big|\psi\big\rangle$. Then $\big|\psi'\big\rangle \in \mathcal{V}_1$, so that $\big\langle\psi'\big|\phi\big\rangle = 0$. Thus

$$\big\langle\psi\big|U(R)\big|\phi\big\rangle = \big\langle\psi'\big|\phi\big\rangle = 0 \ . \tag{58}$$

Thus $U(R)\big|\phi\big\rangle \in \mathcal{V}_1^\perp$.

We say that the space $\mathcal{V}_1$ is invariant under rotations and that the operators $U(R)$ acting on $\mathcal{V}_1$ form a representation of the rotation group.

It may be that there is a subspace $\mathcal{V}_{1,1}$ of $\mathcal{V}_1$ that is invariant under rotations. Then the complementary subspace, $\mathcal{V}_{1,1}^\perp$, consisting of all vectors in $\mathcal{V}_1$ that are orthogonal to every vector in $\mathcal{V}_{1,1}$ is also invariant under rotations. Any vector $\big|\psi\big\rangle \in \mathcal{V}_1$ can be decomposed into a sum $\big|\psi\big\rangle = \big|\psi_\mathrm{a}\big\rangle + \big|\psi_\mathrm{b}\big\rangle$ with $\big|\psi_\mathrm{a}\big\rangle \in \mathcal{V}_{1,1}$ and $\big|\psi_\mathrm{b}\big\rangle \in \mathcal{V}_{1,1}^\perp$. Then $U(R)\big|\psi_\mathrm{a}\big\rangle \in \mathcal{V}_{1,1}$ and $U(R)\big|\psi_\mathrm{b}\big\rangle \in \mathcal{V}_{1,1}^\perp$. Thus the problem of studying what $U(R)$ does to vectors in $\mathcal{V}_1$ is reduced to the two smaller problems of studying what $U(R)$ does to vectors in $\mathcal{V}_{1,1}$ and in $\mathcal{V}_{1,1}^\perp$. We say that in this case, the representation of the rotation group on $\mathcal{V}_1$ is *reducible*.

In the contrary case that there is no subspace of $\mathcal{V}_1$ that is invariant under the rotation group, we say that the representation is *irreducible*. To study possible representations of the rotation group, we should look for the irreducible representations.

10 The irreducible representations

What does an irreducible representation of the rotation group look like? To find out, we examine the action of the infinitesimal generators J_i. We can do that by choosing a suitable basis for our invariant subspace $\mathcal{V}_1$. We cannot choose a basis in which all three of the J_i are diagonal because the three J_i

do not commute with each other. The best that we can do is to choose a basis in which J_z is diagonal. We choose to call the eigenvalues m.

We note that $\vec{J}^{\,2}$ commutes with all of the generators. Therefore we can choose a basis in which $\vec{J}^{\,2}$ is diagonal. The situation is even better than that. Let $|\psi\rangle \in \mathcal{V}_1$ and $\vec{J}^{\,2}|\psi\rangle = \lambda|\psi\rangle$. Then, since $\vec{J}^{\,2}$ commutes with all of the generators of rotations, we have

$$\vec{J}^{\,2}U(R)|\psi\rangle = U(R)\vec{J}^{\,2}|\psi\rangle = \lambda U(R)|\psi\rangle \quad . \tag{59}$$

That is, the subspace of $\mathcal{V}_1$ consisting of vectors with eigenvalue λ is invariant under rotations. Since the representation is irreducible, this subspace must be all of $\mathcal{V}_1$. That is, every vector in $\mathcal{V}_1$ has $\vec{J}^{\,2}|\psi\rangle = \lambda|\psi\rangle$.

The eigenvalue λ must be non-negative since $\vec{J}^{\,2}$ is a sum of squares of operators. It will prove convenient to define a non-negative number j such that $\lambda = j(j+1)$.

With these conventions, the eigenvectors are $|j,m\rangle$ with

$$\vec{J}^2|j,m\rangle = j(j+1)|j,m\rangle, \quad J_z|j,m\rangle = m|j,m\rangle \quad . \tag{60}$$

We can learn something about the eigenvalues by using the commutation relations. Let

$$J_\pm = J_x \pm iJ_y \quad . \tag{61}$$

Then

$$[J_z, J_\pm] = \pm J_\pm \quad . \tag{62}$$

That is

$$J_z J_\pm = J_\pm(J_z \pm 1) \quad . \tag{63}$$

Now define

$$|j,m,\pm\rangle = J_\pm|j,m\rangle \quad . \tag{64}$$

From Eq. (63), we have

$$J_z|j,m,\pm\rangle = (m \pm 1)|j,m,\pm\rangle \quad . \tag{65}$$

That is, applying $J_\pm$ to $|j,m\rangle$ gives a vector with J_z eigenvalue one larger or one less than m or else it gives zero.

To learn more, we note that

$$\begin{aligned}
\big\langle j,m,\pm\big|j,m,\pm\big\rangle &= \big\langle j,m\big|J_\mp J_\pm\big|j,m\big\rangle \\
&= \big\langle j,m\big|J_x^2 + J_y^2 \pm i[J_x,J_y]\big|j,m\big\rangle \\
&= \big\langle j,m\big|J_x^2 + J_y^2 + J_z^2 - J_z^2 \mp J_z\big|j,m\big\rangle \\
&= \big\langle j,m\big|\vec{J}^{\,2} - J_z(J_z \pm 1)\big|j,m\big\rangle \\
&= j(j+1) - m(m\pm 1) \quad .
\end{aligned} \tag{66}$$

The left hand side of this could be zero, but it cannot be negative. Thus

$$m(m\pm 1) \le j(j+1) \quad . \tag{67}$$

For $m > 0$ the most restrictive of these two inequalities is

$$m(m+1) \le j(j+1) \quad . \tag{68}$$

That is

$$m \le j \quad . \tag{69}$$

For $m < 0$ the most restrictive of these two inequalities is

$$(-m)(-m+1) \le j(j+1) \quad . \tag{70}$$

That is

$$-m \le j \quad . \tag{71}$$

Combining these, we have

$$-j \le m \le j \quad . \tag{72}$$

Now think about what would happen if there were an m value larger than $-j$ but smaller than $-j+1$. Applying J_- to the corresponding state $\big|j,m\big\rangle$, we would get a non-zero state with an m value smaller than $-j$. We see that this cannot happen. Similarly, if there were an m value larger than $-j+1$ but smaller than $-j+2$, we would reach a state that cannot exist by applying J_- twice. The only way out is that the smallest m value is precisely $m = -j$. Then

$$\big\langle j,-j,-\big|j,-j,-\big\rangle = j(j+1) - (-j)(-j-1) = 0 \quad . \tag{73}$$

That is

$$J_-\big|j,-j\big\rangle = 0 \quad . \tag{74}$$

Similarly, the largest m value must be precisely $m = +j$. Then

$$J_+ \big| j, j \big\rangle = 0 \ . \tag{75}$$

The other eigenvectors can be constructed by applying J_+ as many times as needed to $\big| j, -j \big\rangle$. There is an arbitrary phase factor that we need to fix. We can define $\big| j, m+1 \big\rangle$ to be a positive real constant times $J_+ \big| j, m \big\rangle$. The value of the positive real constant is then determined by the requirement that $\big| j, m+1 \big\rangle$ be normalized, combined with Eq. (66). This gives

$$J_+ \big| j, m \big\rangle = \sqrt{j(j+1) - m(m+1)}\, \big| j, m+1 \big\rangle \ . \tag{76}$$

Then

$$\begin{aligned} J_- \big| j, m \big\rangle &= [j(j+1) - m(m-1)]^{-1/2}\, J_- J_+ \big| j, m-1 \big\rangle \\ &= [j(j+1) - m(m-1)]^{-1/2}\, [\vec{J}^{\,2} - J_z(J_z+1)] \big| j, m-1 \big\rangle \\ &= [j(j+1) - m(m-1)]^{-1/2}\, [j(j+1) - m(m-1)] \big| j, m-1 \big\rangle \\ &= \sqrt{j(j+1) - m(m-1)} \big| j, m-1 \big\rangle \ . \end{aligned} \tag{77}$$

The range of m is $-j \le m \le j$. Since m increases in integer steps, $+j$ must differ from $-j$ by an integer. That is, $2j$ is an integer. Thus the value of j can be 0, 1/2, 1, 3/2, ...

Summary of this. The value of j can be 0, 1/2, 1, 3/2, ...; then m takes the $2j+1$values $-j, -j+1, \dots, j-1, j$. The eigenvector with the largest and smallest value of m satisfy

$$J_+ \big| j, j \big\rangle = 0, \quad J_- \big| j, -j \big\rangle = 0 \ . \tag{78}$$

The other eigenvectors can be constructed using $J_\pm$:

$$\begin{aligned} J_+ \big| j, m \big\rangle &= \sqrt{j(j+1) - m(m+1)}\, \big| j, m+1 \big\rangle \ , \\ J_- \big| j, m \big\rangle &= \sqrt{j(j+1) - m(m-1)}\, \big| j, m-1 \big\rangle \ . \end{aligned} \tag{79}$$

11 Orbital angular momentum

For a particle with position $\vec{x}$ and momentum $\vec{p}$, the operators $L_i = \epsilon_{ijk} x_j p_k$ have the commutation relations

$$[L_i, L_j] = i\epsilon_{ijk}\, L_k \ . \tag{80}$$

Thus they generate a representation of $SO(3)$. Additionally,

$$\begin{aligned} [L_i, x_j] &= i\epsilon_{ijk}\, x_k \quad , \\ [L_i, p_j] &= i\epsilon_{ijk}\, p_k \quad , \end{aligned} \tag{81}$$

so that this $SO(3)$ is *the* $SO(3)$ that rotates $\vec{x}$ and $\vec{p}$. We call $\vec{L}$ the orbital angular momentum. There can be an additional part of the angular momentum operator, the spin angular momentum, which rotates the internal state of the particle.

To find out about orbital angular momentum, we write $\vec{L}$ using cartesian coordinates x, y, z and transform to polar coordinates r, θ, ϕ. This gives

$$\begin{aligned} L_+ &= e^{i\phi}\,\frac{\partial}{\partial\theta} + i\,\frac{\cos\theta}{\sin\theta}\,e^{i\phi}\,\frac{\partial}{\partial\phi} \quad , \\ L_- &= -\,e^{-i\phi}\,\frac{\partial}{\partial\theta} + i\,\frac{\cos\theta}{\sin\theta}\,e^{-i\phi}\,\frac{\partial}{\partial\phi} \quad , \\ L_z &= -\,i\,\frac{\partial}{\partial\phi} \quad . \end{aligned} \tag{82}$$

Exercise 11.1 Derive Eq. (82).

With this result, we also derive

$$\vec{L}^{\,2} = -\frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2} - \frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) \quad . \tag{83}$$

Exercise 11.2 Derive Eq. (83).

Consider now the space of state vectors $\big|\psi\big\rangle$ for a particle confined to a unit sphere. That is, the wave functions are $\big\langle\theta,\phi\big|\psi\big\rangle$ with normalization

$$\big\langle\phi\big|\psi\big\rangle = \int_{-1}^{1} d\cos\theta \int_{-\pi}^{\pi} d\phi\ \big\langle\phi\big|\theta,\phi\big\rangle\big\langle\theta,\phi\big|\psi\big\rangle \quad . \tag{84}$$

Of course, particles are not normally confined to a unit sphere, but in applications, we just add another coordinate r. We seek to decompose this space into angular momentum eigenstates $\big|l,m\big\rangle$ with

$$\begin{aligned}
\vec{L}^{\,2}\big|l,m\big\rangle &= l(l+1)\big|l,m\big\rangle \ , \\
L_z\big|l,m\big\rangle &= m\big|l,m\big\rangle \ , \\
L_+\big|l,m\big\rangle &= \sqrt{l(l+1)-m(m+1)}\,\big|l,m+1\big\rangle \ , \\
L_-\big|l,m\big\rangle &= \sqrt{l(l+1)-m(m-1)}\,\big|l,m-1\big\rangle \ .
\end{aligned} \tag{85}$$

We will call the wave functions

$$\big\langle\theta,\phi\big|l,m\big\rangle = Y_l^m(\theta,\phi) \ . \tag{86}$$

This is easy. First, the ϕ dependence has to be

$$Y_l^m(\theta,\phi) \propto e^{im\phi} \tag{87}$$

so that $L_z\big|l,m\big\rangle = m\big|l,m\big\rangle$. We should start with $m = l$ (or $m = -l$, but Sakurai starts with $m = +l$). Then we want

$$L_+\big|l,l\big\rangle = 0 \ . \tag{88}$$

That is

$$\left[\frac{\partial}{\partial\theta} + i\,\frac{\cos\theta}{\sin\theta}\,\frac{\partial}{\partial\phi}\right] Y_l^l(\theta,\phi) = 0 \tag{89}$$

Given the ϕ dependence, this is

$$\left[\frac{\partial}{\partial\theta} - l\,\frac{\cos\theta}{\sin\theta}\right] Y_l^l(\theta,\phi) = 0 \tag{90}$$

The solution of this is

$$Y_l^l(\theta,\phi) \propto [\sin\theta]^l e^{il\phi} \tag{91}$$

We need to normalize this correctly:

$$Y_l^l(\theta,\phi) = \left[\frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}\right]\ \sqrt{(2l)!}\ [\sin\theta]^l e^{il\phi} \tag{92}$$

The factor $(-1)^l$ is conventional.

Now to get the other $Y_l^m(\theta,\phi)$, we simply apply L_- enough times to reach the m that we want. To see in a simple way how this works, let $\vec{x}$ be the unit vector

$$\vec{x} = (x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \ . \tag{93}$$

Then we can consider the Y_l^m to be functions of $\vec{x}$. Define three simple functions

$$\begin{aligned} f_\pm &= \mp \frac{1}{\sqrt{2}}\,(x \pm iy) \\ f_0 &= z \end{aligned} \tag{94}$$

Then

$$\begin{aligned} L_- f_+ &= \sqrt{2}\, f_0 \ \ , \\ L_- f_0 &= \sqrt{2}\, f_- \ \ , \\ L_- f_- &= 0 \ \ . \end{aligned} \tag{95}$$

Exercise 11.3 Verify Eq. (95).

We have seen that Y_l^l is proportional to $(f_+)^l$. Applying L_-, we get a constant times $(f_+)^{l-1} f_0$. Applying L_- again, we get a constant times $(l-1)(f_+)^{l-2}(f_0)^2 + (f_+)^{l-2}(f_+ f_-)$. In general, we always get a constant times a sum of terms, where each term has l powers of the fs. There are m factors of f_+ together with $l-m$ factors of fs in the form of either f_0 or $f_+ f_-$. After l applications of L_-, we get Y_l^0. This consists of terms with l factors of fs either in the form f_0 or $f_+ f_-$. Note that $f_+ f_- = (f_0^2 - 1)/2$. If we make this substitution, we see that what we have is a polynomial in $\cos\theta$. Applying L_- more times, we get negative m. We get $-m$ factors of f_- together with $l+m$ factors of fs in the form of either f_0 or $f_+ f_-$. The process ends for $m = -l$, for which we have a constant times $(f_-)^l$. If we apply L_- to this, we get zero.

The result of this process can be written in the standard form

$$\begin{aligned} Y_l^m(\theta,\phi) = {} & \left[\frac{(-1)^l}{2^l l!} \sqrt{\frac{2l+1}{4\pi}} \right] \sqrt{\frac{(l+m)!}{(l-m)!}} \\ & \times e^{im\phi} \frac{1}{[\sin\theta]^m} \left(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta} \right)^{l-m} [\sin\theta]^{2l} \ \ . \end{aligned} \tag{96}$$

If we write Y_l^m this way, we see that it is right for $m = l$ and that L_- applied to Y_l^m gives Y_l^{m-1} with the right normalization. With a little thought, you can see that this is

$$Y_l^m(\theta,\phi) = const.\, e^{im\phi}\,[\sin\theta]^m\, f_{m,l}(\cos\theta) \quad , \tag{97}$$

where $f_{m,l}(\cos\theta)$ is a polynomial in $\cos\theta$ with highest power $[\cos\theta]^{l-m}$. When we get to $m = 0$ we have simply a polynomial in $\cos\theta$ with highest power $[\cos\theta]^l$. This polynomial is called the Legendre polynomial, $P_l(\cos\theta)$. With the conventional normalization $P_l(1) = 1$, the result is

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta) \quad , \tag{98}$$

For negative m, we can start with Y_l^{-l}, and apply L_+ as many times as needed. This amounts to

$$Y_l^{-m}(\theta,\phi) = (-1)^m\, Y_l^m(\theta,\phi)^* \quad . \tag{99}$$

The $(-1)^m$ arises from the change in sign in the $\partial/\partial\theta$ term in L_+ compared to L_-.

Exercise 11.4 Construct the Y_l^m for $l = 2$. Specifically, first find Y_2^2 and Y_2^{-2} using $L_+\big|2,2\big\rangle = 0$ and $L_-\big|2,-2\big\rangle = 0$, respectively. Check that Eq. (92) gets the normalization right. Then construct Y_2^1 and Y_2^0 by applying L_- to Y_2^2 and construct Y_2^{-1} and Y_2^0 by applying L_+ to Y_2^{-2}. This constructs Y_2^0 twice. Make sure that you get the same result both ways.

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12 More on spin 1/2

Let us look some more at the spin 1/2 representation. We have already seen the spin 1/2 representation of the rotation group, with generators

$$J^i = \frac{1}{2}\,\sigma^i \quad . \tag{100}$$

The generator matrices correspond to basis vectors

$$\chi_+ = \begin{pmatrix}1\\0\end{pmatrix} \quad , \qquad \chi_- = \begin{pmatrix}0\\1\end{pmatrix} \quad . \tag{101}$$

These have eigenvalues of J_z equal to $+1/2$ for χ_+ and $-1/2$ for χ_-. Thus the vector $\big|j,m\big\rangle = \big|1/2,+1/2\big\rangle$ corresponds to χ_+, at least up to a phase, while $\big|j,m\big\rangle = \big|1/2,-1/2\big\rangle$ corresponds to χ_-, at least up to a phase. The standard phase convention is the $J_\pm$ transforms $\big|j,m\big\rangle$ into $\big|j,m\pm 1\big\rangle$ with no phase factor. We can check the phase factors:

$$J_+ = \frac{1}{2}[\sigma_x + i\sigma_y] = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad . \tag{102}$$

Thus

$$J_+\chi_- = \chi_+ \quad . \tag{103}$$

Similarly,

$$J_-\chi_+ = \chi_- \quad . \tag{104}$$

Thus χ_+ and χ_- are related by the right phase to be $\big|1/2,+1/2\big\rangle$ and $\big|1/2,-1/2\big\rangle$.

We can note something else about the spin 1/2 representation. Consider a rotation about any axis through an angle 2π:

$$U(2\pi,\vec{n}) = \exp(-i\,2\pi\,\vec{n}\cdot\vec{\sigma}/2) \quad . \tag{105}$$

Using the result of Exercise 8.1, we have

$$U(2\pi,\vec{n}) = -1 \quad . \tag{106}$$

On the other hand, the O(3) rotation matrix for a rotation through angle 2π is the unit 3×3 matrix. Thus a single SO(3) rotation matrix corresponds to two rotation matrices in the spin 1/2 representation. Indeed, any SO(3) rotation matrix corresponds to two rotation matrices in the spin 1/2 representation. For this reason, it is not exactly true that $U(R)$ is a function of R: for the spin 1/2 representation, $U(R)$ is determined by R only up to a sign.

To be precise, we should say that the 3×3 matrix R is determined uniquely by the 2×2 matrix U. The matrices U are 2×2 unitary matrices with determinant 1.[6] They form a group called SU(2), which is called the "universal covering group" of SO(3). What we have been calling representations of SO(3) are, more properly, representations of SU(2). When we talk about what happens in a small neighborhood of the unit matrix, there is no distinction between SU(2) and SO(3). But when we look at the global structure of the groups, there is a difference.

[6]Their determinant is 1 because if $U = \exp A$ where $A^\dagger = A$, then $\det U = \exp(\mathrm{Tr}A)$. The trace of each of the σ_i is zero, so $\det\exp(-i\phi\,\vec{n}\cdot\vec{\sigma}/2) = 1$.

13 Products of representations

If we have one vector space that carries the spin j_1 representation of the rotation group and another that carries the spin j_2 representation, we can form the tensor product of the two vector spaces. This means that we form the vector space with basis elements

$$\big|j_1, j_2, m_1, m_2\big\rangle = \big|j_1, m_1\big\rangle \otimes \big|j_2, m_2\big\rangle \ . \tag{107}$$

The vectors in this space represent physically the combined j_1 and j_2 systems. The general vector in the tensor product space is a linear combination of these basis states. This product representation is called the $j_1 \otimes j_2$ representation and is reducible. The rotations are represented by

$$\begin{aligned}&\big\langle j_1, j_2, m_1', m_2'\big|U(R)\big|j_1, j_2, m_1, m_2\big\rangle \\ &\qquad = \big\langle j_1, m_1'\big|U_1(R)\big|j_1, m_1\big\rangle \otimes \big\langle j_2, m_2'\big|U_2(R)\big|j_2, m_2\big\rangle \ .\end{aligned} \tag{108}$$

That is, the combined rotation operator is the product of the individual rotation operators, each operating on its own factor in the tensor product space.

If we now expand $U(R)$, $U_1(R)$ and $U_2(R)$ for an infinitesimal rotation, and keep the first order terms, we find

$$\begin{aligned}&\big\langle j_1, j_2, m_1', m_2'\big|J_i\big|j_1, j_2, m_1, m_2\big\rangle \\ &\qquad = \big\langle j_1, m_1'\big|J_{i,1}\big|j_1, m_1\big\rangle \otimes \big\langle j_2, m_2'\big|j_2, m_2\big\rangle \\ &\qquad\quad + \big\langle j_1, m_1'\big|j_1, m_1\big\rangle \otimes \big\langle j_2, m_2'\big|J_{i,2}\big|j_2, m_2\big\rangle \ .\end{aligned} \tag{109}$$

That is, the combined infinitesimal generator of rotations about the i axis is the sum of the infinitesimal generators for the two systems. We usually write this as

$$J_i = J_{i,1} + J_{i,2} \ \ , \tag{110}$$

although

$$J_i = J_{i,1} \otimes 1 + 1 \otimes J_{i,2} \tag{111}$$

would be more precise.

14 Spin 1/2 times spin 1/2

Consider the tensor product of two spin 1/2 representations, $1/2 \otimes 1/2$. We can think about the vectors in this space as having two spin 1/2 indices, so that we represent a vector as ψ^{ij}, where i and j take values $\pm 1/2$. Under a rotation U (or R), the vector ψ changes into $\tilde{\psi}$, where

$$\tilde{\psi}^{ij} = U^{ii'} U^{jj'} \psi^{i'j'} \quad . \tag{112}$$

This is a 9 dimensional representation of SU(2) (or SO(3)). But it is reducible. We can write any two index vector ψ as a sum of an antisymmetric part and an antisymmetric part:

$$\psi^{ij} = \psi_{\rm A}^{ij} + \psi_{\rm S}^{ij} \quad , \tag{113}$$

where

$$\psi_{\rm A}^{ij} = -\psi_{\rm A}^{ji} \tag{114}$$

and

$$\psi_{\rm S}^{ij} = +\psi_{\rm S}^{ji} \quad . \tag{115}$$

The set of all antisymmetric ψ constitutes a subspace of the $1/2 \otimes 1/2$ space and the set of all symmetric ψ also constitutes a subspace of the $1/2 \otimes 1/2$. Evidently, both of these subspaces are invariant under rotations: if ψ in Eq. (112) is symmetric, then so is $\tilde{\psi}$ and if ψ is antisymmetric, then so is $\tilde{\psi}$. Thus the $1/2 \otimes 1/2$ representation is reducible.

The antisymmetric subspace is one dimensional: the only vector in it has the form $\lambda \epsilon^{ij}$, where ϵ^{ij} is the antisymmetric tensor having indices that take two values, with $\epsilon^{1/2,-1/2} = -\epsilon^{-1/2,1/2} = 1$ and $\epsilon^{1/2,1/2} = \epsilon^{-1/2,-1/2} = 0$. Since this subspace has only one dimension, it is irreducible. The only irreducible representation of the rotation group that is one dimensional is the $j = 0$ representation. Thus the antisymmetric subspace carries the $j = 0$ representation of the rotation group.

We should check that this is consistent. Since the antisymmetric subspace has only one basis vector, namely ϵ^{ij}, we must have

$$U^{ii'} U^{jj'} \epsilon^{i'j'} = \lambda \epsilon^{i'j'} \quad . \tag{116}$$

For the $j = 0$ representation, every vector in the space should be invariant. That is, λ should be 1. Is that so? Yes, because

$$U^{ii'} U^{jj'} \epsilon^{i'j'} = \det U \ \epsilon^{ij} \tag{117}$$

and $\det U = 1$.

The symmetric subspace is three dimensional, since $3 = 4 - 1$. Is it reducible? Consider that it contains a vector with J_z eigenvalue $m = 1$, namely (using the ket notation) $\big|1/2, +1/2\big\rangle\big|1/2, +1/2\big\rangle$. To get $m = 1$, we need a representation with $j \geq 1$. All of the representations with $j > 1$ have dimension greater than 3, so they don't work. Thus the only possibility for the representation carried by the symmetric space is the $j = 1$ representation, which has precisely three dimensions. Thus the symmetric subspace carries the irreducible $j = 1$ representation of the rotation group.

In fact, it is easy to construct the three standard basis vectors of the $j = 1$ representation:

$$\begin{aligned} \big|1, +1\big\rangle &= \big|1/2, +1/2\big\rangle\big|1/2, +1/2\big\rangle \;\; , \\ \big|1, 0\big\rangle &= \frac{1}{\sqrt{2}}\left[\big|1/2, +1/2\big\rangle\big|1/2, -1/2\big\rangle + \big|1/2, -1/2\big\rangle\big|1/2, +1/2\big\rangle\right] \;\; , \\ \big|1, -1\big\rangle &= \big|1/2, -1/2\big\rangle\big|1/2, -1/2\big\rangle \;\; . \end{aligned} \tag{118}$$

Using $J_i = J_{i,1} \otimes 1 + 1 \otimes J_{i,2}$, we see that the vectors $\big|1, m\big\rangle$ have the indicated J_z eigenvalues and that $J_\pm$ relates one of them to another with the right phase.

In this notation, the $j = 0$ vector is

$$\big|0, 0\big\rangle = \frac{1}{\sqrt{2}}\left[\big|1/2, +1/2\big\rangle\big|1/2, -1/2\big\rangle - \big|1/2, -1/2\big\rangle\big|1/2, +1/2\big\rangle\right] \;\; . \tag{119}$$

15 Spin 1 times spin 1

Consider the tensor product $1 \otimes 1$. In a standard vector index notation, the objects in the tensor product space have components T^{ij}, where i and j run from 1 to 3. (In the Dirac notation with unit vectors in the 1,2,3 directions as basis vectors, this is $\big\langle i, j\big|T\big\rangle$.) The $1 \otimes 1$ representation decomposes to

$$1 \otimes 1 = 0 \oplus 1 \oplus 2 \;\; . \tag{120}$$

We can exhibit this explicitly in the vector index notation:

$$T^{ij} = s\,\frac{1}{3}\,\delta^{ij} + \epsilon^{ijk} v_k + \tilde{T}^{ij} \;\; . \tag{121}$$

Here s is a scalar, the "0" representation, given by

$$s = \delta_{kl} T^{kl} \;\; . \tag{122}$$

Next, v is a vector, the "1" representation, given by

$$v_k = \frac{1}{2}\,\epsilon_{klm} T^{km} \quad . \tag{123}$$

Finally, $\tilde{T}^{ij}$ is a traceless, symmetric tensor. This is what remains after we have removed the trace and the antisymmetric part. It must carry the "2" representation. Explicitly

$$\tilde{T}^{ij} = \frac{1}{2}[T^{ij} + T^{ji}] - \frac{1}{3}\,\delta^{ij}\;\delta_{kl} T^{kl} \quad . \tag{124}$$

16 Products of two representations in general

In general, if we have one vector space that carries the spin j_1 representation of the rotation group and another that carries the spin j_2 representation, we can form the tensor product of the two vector spaces, with basis elements

$$\big|j_1, j_2, m_1, m_2\big\rangle = \big|j_1, m_1\big\rangle \otimes \big|j_2, m_2\big\rangle \quad . \tag{125}$$

This product representation is called the $j_1 \otimes j_2$ representation and is reducible.

To find out how to reduce the product representation, we recall that

$$J_i = J_{i,1} \otimes 1 + 1 \otimes J_{i,2} \quad . \tag{126}$$

The combined space carries representations j with

$$j = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2 \quad . \tag{127}$$

The basis elements for these representations are states $\big|j, m\big\rangle$. Because of Eq. (126), the state $\big|j, m\big\rangle$ must be a linear combination of product states $\big|j_1, j_2, m_1, m_2\big\rangle$ with $m_1 + m_2 = m$. Let us use this to determine which representations occur.

Draw a little picture in the m_1-m_2 plane, with dots at the allowed values of m_1 and m_2. There are no dots for $m_1 + m_2 > j_1 + j_2$, so no representations with $j > j_1 + j_2$ can appear.

There is one dot at $m_1 = j_1$, $m_2 = j_2$. Thus the representation $j = j_1 + j_2$ must appear in the product space and it must appear once.

There are two dots for $m_1 + m_2 = j_1 + j_2 - 1$. That is, the space of vectors with J_z eigenvalues equal to $m = j_1 + j_2 - 1$ is two dimensional.

One vector in this space is $\big|j_1+j_2, j_1+j_2-1\big\rangle$. There must be one more vector with J_z eigenvalues equal to $m = j_1+j_2-1$, the vector orthogonal to $\big|j_1+j_2, j_1+j_2-1\big\rangle$. This has to be the vector $\big|j_1+j_2-1, j_1+j_2-1\big\rangle$, so the representation $j = j_1+j_2-1$ must occur and it must occur precisely once.

There are three dots for $m_1+m_2 = j_1+j_2-2$. That is, the space of vectors with J_z eigenvalues equal to $m = j_1+j_2-2$ is three dimensional. As before, all but one of these dimensions is accounted for by the representations that we have already found, so there has to be one vector $\big|j_1+j_2-2, j_1+j_2-2\big\rangle$. That is, the representation $j = j_1+j_2-2$ must occur and it must occur precisely once.

This argument stops working when we get to $j = |j_1-j_2|$. Then when we go to values of m_1+m_2 that are smaller than $j = |j_1-j_2|$, we do not get more dots. (Try this, with your picture.) Thus we do not get representations j with $j < |j_1-j_2|$.

One describes this by saying

$$j_1 \otimes j_2 = |j_1-j_2| \oplus (|j_1-j_2|+1) \oplus \cdots \oplus (j_1+j_2) \ . \tag{128}$$

What this means is that any vector in the product space can be expanded as

$$\big|\psi\big\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{j} \big|j,m\big\rangle\big\langle j,m\big|\psi\big\rangle \ . \tag{129}$$

This may be compared to

$$\big|\psi\big\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \big|j_1,j_2,m_1,m_2\big\rangle\big\langle j_1,j_2,m_1,m_2\big|\psi\big\rangle \ . \tag{130}$$

The relationship between these two is obtained from

$$\big|j,m\big\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \big|j_1,j_2,m_1,m_2\big\rangle\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle \ . \tag{131}$$

The $\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle$ are called the Clebsch-Gordan coefficients. The non-zero coefficients have m_1, m_2 and m in the proper ranges and $m = m_1+m_2$. They can be calculated by using the recursion relations

$$\begin{aligned}
&\sqrt{j(j+1)-m(m+1)}\,\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle \\
&\quad = \sqrt{j_1(j_1+1)-m_1(m_1+1)}\,\big\langle j_1,j_2,m_1+1,m_2\big|j,m+1\big\rangle \\
&\qquad + \sqrt{j_2(j_2+1)-m_2(m_2+1)}\,\big\langle j_1,j_2,m_1,m_2+1\big|j,m+1\big\rangle
\end{aligned} \tag{132}$$

and

$$
\begin{aligned}
&\sqrt{j(j+1)-m(m-1)}\,\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle \\
&\quad=\sqrt{j_1(j_1+1)-m_1(m_1-1)}\,\big\langle j_1,j_2,m_1-1,m_2\big|j,m-1\big\rangle \\
&\qquad+\sqrt{j_2(j_2+1)-m_2(m_2-1)}\,\big\langle j_1,j_2,m_1,m_2-1\big|j,m-1\big\rangle \ .
\end{aligned}
\tag{133}
$$

You can easily derive these by putting the J_+ or J_- operators between states and using Eq. (126) to write the matrix element in two ways. (Please demonstrate this for yourself.)

One also needs the normalization condition,

$$
\begin{aligned}
1 &= \sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} |\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle|^2 \\
&= \sum_{m_1=\min(-j_1,m-j_2)}^{\max(j_1,m+j_2)} |\big\langle j_1,j_2,m_1,m-m_1\big|j,m\big\rangle|^2 \ .
\end{aligned}
\tag{134}
$$

With the recursion relations and the normalization condition, you can derive the values of any Clebsch-Gordan coefficients that you want. (By convention, the Clebsch-Gordan coefficients are real. There is a sign for each j that is not fixed by the normalization condition. You have to apply some convention to fix this sign.)

Exercise 16.1 Consider the Clebsch-Gordan coefficients $\big\langle j_1,j_2,m_1,m_2\big|j,m\big\rangle$ for combining spin $j_1=5$ with spin $j_2=2$ to make spin $j=4$. Calculate $\big\langle 5,2,-2,1\big|4,-1\big\rangle$ and $\big\langle 5,2,1,-1\big|4,0\big\rangle$.

---

17 Spin j from $2j$ copies of spin 1/2

We can construct the spin j representation from the product of $2j$ spin 1/2 representations. Using a component spinor notation with spinors ξ^i with $i=+,-$, we consider the product of spinor spaces with $2j$ factors. An element of this space has components

$$
\psi^{i_1 i_2 \dots i_{2j}} \tag{135}
$$

Let us take the symmetric part of this

$$[S\psi]^{i_1 i_2 \ldots i_{2j}} = \frac{1}{(2j)!} \sum_{\pi \in S_{2j}} \psi^{i_{\pi(1)} i_{\pi(2)} \ldots i_{\pi(2j)}} \quad . \tag{136}$$

The S stands for this symmetrizing operation, while S_{2j} is the group of permutations π of $2j$ objects.

The standard basis vectors for this space is

$$\psi(m)^{i_1 i_2 \ldots i_{2j}} = [S\psi_m]^{i_1 i_2 \ldots i_{2j}} \quad , \tag{137}$$

where

$$\psi_m^{i_1 i_2 \ldots i_{2j}} = c(m)\, \delta_+^{i_1} \cdots \delta_+^{i_{j+m}} \delta_-^{i_{j+m+1}} \cdots \delta_-^{i_{2j}} \quad . \tag{138}$$

Here there are $j+m$ factors δ_+^i and $j-m$ factors δ_-^i. The normalization factor is

$$c(m) = \sqrt{\frac{(2j)!}{(j+m)!(j-m)!}} \quad . \tag{139}$$

(You should verify this.) This basis vector is an eigenvector of J_z with eigenvalue m. The possible values of m run from $-j$ to j. Thus we have the spin j representation of the rotation group.

The action of a rotation R on this basis vector is easily found using the rotation matrices $U(R)$ for the spin 1/2 representation:

$$\psi \to \hat{\psi} \quad , \tag{140}$$

where

$$\hat{\psi}(m)^{i_1 i_2 \ldots i_{2j}} = U^{i_1 j_1} \cdots U^{i_{2j} j_{2j}} \psi(m)^{j_1 \cdots j_{2j}} \tag{141}$$

That is

$$\begin{aligned} \hat{\psi}(m)^{i_1 i_2 \ldots i_{2j}} &= \frac{c(m)}{(2j)!} \sum_{\pi \in S_{2j}} U^{i_1 j_1} \cdots U^{i_{2j} j_{2j}} \psi_m^{j_{\pi(1)} \cdots j_{\pi(2j)}} \\ &= \frac{c(m)}{(2j)!} \sum_{\pi \in S_{2j}} U^{i_{\pi(1)} j_{\pi(1)}} \cdots U^{i_{\pi(2j)} j_{\pi(2j)}} \psi_m^{j_{\pi(1)} \cdots j_{\pi(2j)}} \\ &= \frac{c(m)}{(2j)!} \sum_{\pi \in S_{2j}} U^{i_{\pi(1)} j_1} \cdots U^{i_{\pi(2j)} j_{2j}} \psi_m^{j_1 \cdots j_{2j}} \\ &= \frac{c(m)}{(2j)!} \sum_{\pi \in S_{2j}} U^{i_{\pi(1)} +} \cdots U^{i_{\pi(j+m)} +} U^{i_{\pi(j+m+1)} -} \cdots U^{i_{\pi(2j)} -} \end{aligned} \tag{142}$$

The matrix element of this with $\psi(m')$ gives

$$\langle j, m' | U(R) | j, m \rangle \tag{143}$$

in the spin j representation. (Note that I am using the same symbol, U for matrices in the spin-1/2 representation and operators in the spin-j representation. This should not cause confusion since it is easy to tell which is which.) That is

$$\begin{aligned}\langle j, m' | U(R) | j, m \rangle &= \psi^*(m')^{i_1 \cdots i_{2j}} \hat{\psi}(m)^{i_1 \dots i_{2j}} \\ &= \psi_{m'}^{i_1 \cdots i_{2j}} \hat{\psi}(m)^{i_1 \dots i_{2j}} \\ &= \frac{c(m)c(m')}{(2j)!} \sum_{\pi \in S_{2j}} \delta_+^{i_1} \cdots \delta_+^{i_{j+m'}} \delta_-^{i_{j+m'+1}} \cdots \delta_-^{i_{2j}} \\ &\quad \times U^{i_{\pi(1)}+} \dots U^{i_{\pi(j+m)}+} U^{i_{\pi(j+m+1)}-} \dots U^{i_{\pi(2j)}-} \quad .\end{aligned} \tag{144}$$

Thus there are $2j$ factors of U^{ij} with $j + m'$ of the i indices being $+$ and $j - m'$ of the i indices being $-$, while $j + m$ of the j indices are $+$ and $j - m$ of the j indices are $-$. The $+$ and $-$ indices are placed in all permutations relative to each other.

You might think this is ugly. But note that you know the two by two matrices $U(R)$ and if you have a computer you can easily put together the required permutations and sums.

Exercise 17.1 Let R be the rotation through angle ψ about the axis n with polar angles θ, ϕ. Consider the spin $j = 2$ representation of the rotation group. Using the standard basis for angular momentum eigenstates, the operator $U(R)$ for this representation corresponds to a matrix $\langle 2, m' | U(R) | 2, m \rangle$. Evaluate $\langle 2, 1 | U(R) | 2, 0 \rangle$. Please state your result as a function of ψ, θ, and ϕ. Then give a numerical answer for $\psi = \pi/6$, $\theta = \pi/3$, and $\phi = \pi/4$.

---

18 Transformation property of the Clebsch-Gordan coefficients

We have been writing our Clebsch-Gordan coefficients as

$$\langle j_1, j_2, m_1, m_2 | j, m \rangle \quad . \tag{145}$$

For this section, let us use

$$\left\langle j,m \middle| j_1,j_2,m_1,m_2 \right\rangle \ . \tag{146}$$

This is the same thing, since the coefficients are real. This way is more convenient for the Wigner-Eckart theorem.

Note that for any rotation R

$$\left\langle j,m \middle| j_1,j_2,m_1,m_2 \right\rangle = \left\langle j,m \middle| U(R)^{-1}U(R) \middle| j_1,j_2,m_1,m_2 \right\rangle \ . \tag{147}$$

We have (using the summation convention for repeated indices)

$$U(R)\big|j_1,j_2,m_1,m_2\big\rangle = \big|j_1,j_2,m_1',m_2'\big\rangle \mathcal{D}^{(j_1)}(R)_{m_1'm_1}\mathcal{D}^{(j_2)}(R)_{m_2'm_2} \tag{148}$$

and

$$\big\langle j,m\big|U(R)^{-1} = \big\langle j,m'\big|\mathcal{D}^{(j)}(R)^*_{m'm} \ . \tag{149}$$

Thus

$$\begin{aligned}\big\langle j,m\big|j_1,j_2,m_1,m_2\big\rangle = {}& \mathcal{D}^{(j)}(R)^*_{m'm}\mathcal{D}^{(j_1)}(R)_{m_1'm_1}\mathcal{D}^{(j_2)}(R)_{m_2'm_2} \\ & \times \big\langle j,m'\big|j_1,j_2,m_1',m_2'\big\rangle \ .\end{aligned} \tag{150}$$

If we take infinitesimal rotations, we will get $m = m_1 + m_2$ and the recursion relations that we solved to get the Clebsch-Gordan coefficients. We know that the recursion relations provided a solution (for fixed j_1, j_2 and j) that is unique up to the normalization. Therefore, if there are some coefficients $C(j,m;j_1,j_2,m_1,m_2)$ that obey

$$\begin{aligned}C(j,m;j_1,j_2,m_1,m_2) = {}& \mathcal{D}^{(j)}(R)^*_{m'm}\mathcal{D}^{(j_1)}(R)_{m_1'm_1}\mathcal{D}^{(j_2)}(R)_{m_2'm_2} \\ & \times C(j,m';j_1,j_2,m_1',m_2') \ ,\end{aligned} \tag{151}$$

then the coefficients C must be the Clebsch-Gordan coefficients up to the normalization:

$$C(j,m;j_1,j_2,m_1,m_2) = \lambda(j,j_1,j_2)\left\langle j,m \middle| j_1,j_2,m_1,m_2 \right\rangle \ . \tag{152}$$

19 Irreducible tensor operators

An irreducible tensor operator $T^{(l)}_m$ is an operator on the quantum space that has the rotational covariance property

$$U(R)^{-1}T^{(l)}_m U(R) = T^{(l)}_{m'}\,\mathcal{D}^{(l)}(R^{-1})_{m'm} \ . \tag{153}$$

We will see below why we might be interested in such an object.

One way to construct such an irreducible tensor operator is to start with a cartesian tensor operator $T^{i_1 \cdots i_N}$, where the indices are ordinary 3-vector indices that take values 1,2,3. That is, the components of T are operators on the quantum space with the rotational covariance property

$$U(R)^{-1} T^{i_1 \cdots i_N} U(R) = R_{i_1,j_1} \cdots R_{i_N,j_N} \, T^{j_1 \cdots j_N} \quad . \tag{154}$$

Suppose that we have basis tensors $u(l,m)^{i_1 \cdots i_N}$ that make the standard basis vectors for the l-representation of the rotation group that occurs within the space of N-th rank tensors. That is

$$R_{i_1,j_1} \cdots R_{i_N,j_N} u(l,m)^{j_1 \cdots j_N} = u(l,m')^{i_1 \cdots i_N} \; \mathcal{D}^{(l)}(R)_{m'm} \quad . \tag{155}$$

If we have the basis tensors, we can define

$$T_m^{(l)} = u(l,m)^{i_1 \cdots i_N} \; T^{i_1 \cdots i_N} \quad . \tag{156}$$

I claim that the simple procedure of contracting the basis vectors with T constructs irreducible tensor operators from the cartesian tensor operators T. To see this, we write

$$\begin{aligned} U(R)^{-1} T_m^{(l)} U(R) &= u(l,m)^{i_1 \cdots i_N} \; U(R)^{-1} T^{i_1 \cdots i_N} U(R) \\ &= u(l,m)^{i_1 \cdots i_N} \; R_{i_1,j_1} \cdots R_{i_N,j_N} \; T^{j_1 \cdots j_N} \\ &= R^{-1}_{j_1,i_1} \cdots R^{-1}_{j_N,i_N} \; u(l,m)^{i_1 \cdots i_N} \; T^{j_1 \cdots j_N} \\ &= u(l,m')^{j_1 \cdots j_N} \; \mathcal{D}^{(l)}(R^{-1})_{m'm} T^{j_1 \cdots j_N} \\ &= T_{m'}^{(l)} \; \mathcal{D}^{(l)}(R^{-1})_{m'm} \quad . \end{aligned} \tag{157}$$

A special case occurs for

$$T^{i_1 \cdots i_N} = V^{i_1} V^{i_2} \cdots V^{i_N} \tag{158}$$

made from a single vector operator (for example the position operator). To see what to do with this, consider what the functions $Y_m^l(\theta, \phi)$ look like. We can think of θ, ϕ as the polar coordinates of a unit vector $\vec{n}$. Thus we can think of the spherical harmonics as functions of $\vec{n}$, $Y_l^m(\vec{n})$. These functions are polynomials in the components of $\vec{n}$. Specifically, $Y_l^m(\vec{n})$ has l factors of the components of $\vec{n}$. To see this, recall the construction using Eq. (95). With this insight, we can form $Y_l^m(V)$ as the same polynomial in the components of $\vec{V}$. Then the $Y_l^m(V)$ for fixed l and varying m are linear combinations of the components of the tensor in Eq. (158) with l factors of V.

Then (writing RV for the vector $\hat{V}$ with components $\hat{V}^i = R_{ij}V^j$),

$$\begin{aligned} U(R)^{-1}Y_l^m(V)U(R) &= Y_l^m(RV) \\ &= Y_l^{m'}(V)\ \mathcal{D}^{(l)}(R^{-1})_{m'm} \quad . \end{aligned} \tag{159}$$

Note that we have R^{-1} on the second line because the rotated version of a function f evaluated at V is $f(R^{-1}V)$, so

$$Y_l^m(R^{-1}V) = Y_l^{m'}(V)\ \mathcal{D}^{(l)}(R)_{m'm} \quad . \tag{160}$$

Thus in Eq. (159), we need to exchange R and R^{-1}. From, Eq. (159), we see that $Y_l^m(V)$ has the right transformation law to make an irreducible tensor operator.

Irreducible tensor operators are useful for describing the electromagnetic properties of atoms. For instance, the static electric multipole moments of a classical charge distribution are

$$\tilde{q}_{l,m} = \int d\boldsymbol{x}'\ Y_l^m(\theta',\phi')(r')^l\rho(\boldsymbol{x}');\ . \tag{161}$$

(This is adapted from eq. (4.3) in J.D. Jackson, *Classical Electrodynamics*. My $\tilde{q}_{l,m}$ is Jackson's $(-1)^m q_{l,-m}$.) This is the classical version. In quantum mechanics for particles bound to a force center, we would measure the operator

$$\tilde{q}_{l,m} = \sum_{i=1}^{N} q_i Y_l^m(x_i);\ . \tag{162}$$

where we sum over particles i, x_i is the position operator for the ith particle, and q_i is the charge of the ith particle. Note that $Y_l^m(x_i)$ is an irreducible tensor operator as we have defined it. Similar, but more complicated, formulas apply for radiation from atoms. See Jackson, section 9.10.

20 The Wigner-Eckart theorem

With the preparation that we have in the previous sections, the Wigner-Eckart theorem is pretty simple. It concerns matrix elements of irreducible tensor operators. We consider

$$\langle\alpha,j,m|T_{m_2}^{(j_2)}|\beta,j_1,m_1\rangle \quad . \tag{163}$$

Here $|\beta, j_1, m_1\rangle$ for $m_1 \in \{-j_1, \ldots, +j_1\}$ are quantum states that transform according to the j_1 representation of the rotation group. The index m_1 labels the eigenvalue of J_z. We assume that the states for different m_1 are connected by the raising and lowering operators in the standard way. The index β labels any additional quantum numbers that represent characteristics of the states that are invariant under rotation. Similarly $\langle\alpha, j, m|$ for $m \in \{-j, \ldots, +j\}$ are quantum states that transform according to the j representation of the rotation group. The index m labels the eigenvalue of J_z. We assume that the states for different m are connected by the raising and lowering operators in the standard way. The index α labels any additional quantum numbers that represent characteristics of the states that are invariant under rotation. Finally $T^{(j_2)}_{m_2}$ for $m_2 \in \{-j_2, \ldots, +j_2\}$ are the components of an irreducible tensor operator that transform according to the j_2 representation of the rotation group in the standard way discussed previously.

To analyze this, we write

$$\begin{aligned}&\langle\alpha, j, m|T^{(j_2)}_{m_2}|\beta, j_1, m_1\rangle \\ &\qquad = \langle\alpha, j, m|U(R)^{-1}\, U(R)T^{(j_2)}_{m_2}\, U(R)^{-1}U(R)|\beta, j_1, m_1\rangle \;.\end{aligned} \tag{164}$$

Then

$$U(R)|\beta, j_1, m_1\rangle = |\beta, j_1, m_1'\rangle \mathcal{D}^{(j_1)}(R)_{m_1' m_1} \tag{165}$$

and

$$\langle\alpha, j, m|U(R)^{-1} = \langle\alpha, j, m'|\mathcal{D}^{(j)}(R)^*_{m'm} \;. \tag{166}$$

Furthermore

$$U(R)T^{(j_2)}_{m_2}\, U(R)^{-1} = T^{(j_2)}_{m_2'}\; \mathcal{D}^{(j_2)}(R)_{m_2' m_2} \;. \tag{167}$$

Thus

$$\begin{aligned}\langle\alpha, j, m|T^{(j_2)}_{m_2}|\beta, j_1, m_1\rangle &= \mathcal{D}^{(j)}(R)^*_{m'm}\mathcal{D}^{(j_1)}(R)_{m_1' m_1}\mathcal{D}^{(j_2)}(R)_{m_2' m_2} \\ &\qquad \times \langle\alpha, j, m|T^{(j_2)}_{m_2}|\beta, j_1, m_1\rangle \;.\end{aligned} \tag{168}$$

This is the same as the transformation law for the Clebsch-Gordan coefficients. Therefore we can conclude that our matrix elements of a tensor operator are equal to the corresponding Clebsch-Gordan coefficients times a normalizing factor that is independent of m_1, m_2 and m:

$$\langle\alpha, j, m|T^{(j_2)}_{m_2}|\beta, j_1, m_1\rangle = \lambda(\alpha, j; j_2; \beta, j_1)\,\langle j, m|j_1, j_2, m_1, m_2\rangle \;. \tag{169}$$

This result is conventionally written in the form

$$\langle\alpha, j, m\big|T^{(j_2)}_{m_2}\big|\beta, j_1, m_1\rangle = \frac{\langle\alpha, j\big|\big|T^{(j_2)}\big|\big|\beta, j_1\rangle}{\sqrt{2j_1+1}} \langle j_1, j_2, m_1, m_2\big|j, m\rangle \quad . \tag{170}$$

The normalizing factor $\langle\alpha, j\big|\big|T^{(j_2)}\big|\big|\beta, j_1\rangle$ is sometimes called the reduced matrix element.

21 The hydrogen atom

Let's consider finding the energy levels of the hydrogen atom as an example of using angular momentum. The hamiltonian is[7]

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r} \quad . \tag{171}$$

With a straightforward change of variables, we can write this as

$$H = -\frac{1}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\vec{L}^2\right] - \frac{e^2}{r} \quad . \tag{172}$$

Here $\vec{L}$ is the orbitial angular momentum operator, $\vec{x}\times\vec{p}$. Using spherical coordinates,

$$\vec{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\left(\frac{\partial}{\partial\phi}\right)^2 \quad . \tag{173}$$

To find the eigenvalues and eigenvectors of H, we recognize that H is invariant under rotations. Thus it commutes with $\vec{L}$. Because of that, we can find simultaneous eigenvectors of H, $\vec{L}^2$, and L_z. Thus we look for state vectors $\big|n, l, m\rangle$ with

$$\begin{aligned} H\big|n,l,m\rangle &= E(n,l,m)\big|n,l,m\rangle \quad , \\ \vec{L}^2\big|n,l,m\rangle &= l(l+1)\big|n,l,m\rangle \quad , \\ \vec{L}_z\big|n,l,m\rangle &= m\big|n,l,m\rangle \quad . \end{aligned} \tag{174}$$

[7] In SI units, there is an $\hbar$ in the definition of the momentum operator and the potential energy is $e^2/(4\pi\epsilon_0 r)$. However we choose units such that $\hbar = 1$ and also such that $4\pi\epsilon_0 = 1$. Another convention, which I prefer, is $\epsilon_0 = 1$, so that the potential is $e^2/(4\pi)$. However, I choose here $4\pi\epsilon_0 = 1$ so that there is no $1/(4\pi)$ in the Coulomb potential and we remain close to the notation of Sakurai.

(We will see that the energies E depend on l but not on m.) The corresponding wave functions have the form

$$\psi_{n,l,m}(r,\theta,\phi) = R(r) Y_l^m(\theta,\phi) \quad . \tag{175}$$

We need

$$\begin{split}\left\{ -\frac{1}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\vec{L}^2\right] - \frac{e^2}{r}\right\} R(r) Y_l^m(\theta,\phi) \\ = E\, R(r) Y_l^m(\theta,\phi) \quad .\end{split} \tag{176}$$

When it operatates on Y_l^m, $\vec{L}^2$ gives $l(l+1)$. Thus

$$\begin{split}\left\{ -\frac{1}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2}\right] - \frac{e^2}{r}\right\} R(r) Y_l^m(\theta,\phi) \\ = E\, R(r) Y_l^m(\theta,\phi) \quad .\end{split} \tag{177}$$

We can cancel the factors of Y_l^m, giving

$$\left\{ -\frac{1}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{2m\,r^2} - \frac{e^2}{r}\right\} R(r) = E\, R(r) \quad . \tag{178}$$

Now we have an ordinary differential equation for $R(r)$. To solve it in a standard way,[8] one often defines $u(r) = rR(r)$. This gives

$$\left\{ -\frac{1}{2m}\left(\frac{\partial}{\partial r}\right)^2 + \frac{l(l+1)}{2m\,r^2} - \frac{e^2}{r}\right\} u(r) = E\, u(r) \quad . \tag{179}$$

Written this way, the equation looks a little simpler. We can simplify it further by changing variables from r to

$$\rho = \sqrt{-2mE}\; r \quad . \tag{180}$$

(Note that $E < 0$.) Then

$$\left\{ \left(\frac{\partial}{\partial \rho}\right)^2 - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1\right\} u = 0 \quad , \tag{181}$$

[8] I follow the book by Griffiths, *Introduction to Quantum Mehanics*. My treatment is pretty abbreviated, so see Griffiths for more details.

where

$$\rho_0 = e^2 \sqrt{\frac{2m}{-E}} \quad . \tag{182}$$

It is useful to define a new variable v related to u by

$$u = \rho^{l+1} e^{-\rho}\, v \quad . \tag{183}$$

The differential equation for v is

$$\left\{ \rho \left(\frac{\partial}{\partial \rho} \right)^2 + 2[(l+1) - \rho] \frac{\partial}{\partial \rho} + [\rho_0 - 2(l+1)] \right\} v = 0 \quad . \tag{184}$$

Now one looks for a solution in which v is a polynomial in ρ:

$$v = \sum_{J=0}^{J_{\max}} C_J \rho^J \quad . \tag{185}$$

If we can find a polynomial that solves the differential equation, then it is a suitable energy eigenfunction, being well behaved at both $\rho = 0$ and $\rho = \infty$. The differential equation gives

$$C_{J+1} = \frac{2(J+l+1) - \rho_0}{(J+1)[J+2(l+1)]}\, C_J \quad . \tag{186}$$

Now, $v(\rho)$ is supposed to be a polynomial, so the series needs to terminate somewhere.[9] The solution will terminate at some $J_{\max}$ if

$$\rho_o = 2n \quad , \tag{187}$$

where

$$n = J_{\max} + l + 1 \quad . \tag{188}$$

Thus what we need is

$$e^2 \sqrt{\frac{2m}{-E}} = 2n \quad , \tag{189}$$

$$E = -\frac{me^4}{2} \frac{1}{n^2} \quad . \tag{190}$$

For a given value of l, the lowest value of the "principle quantum number" n is obtained with $J_{\max} = 0$,

$$n_{\min} = l + 1 \quad . \tag{191}$$

[9] If it is not a polynomial and the series goes on forever, you do get a solution, but the solution blows up for $\rho \to \infty$, so that it does not give a normalizable solution.

22 Bell's inequality

Bell's inequality is nicely discussed in Sakurai. Here, I present only the quantum calculation. We consider a $j = 0$ state of two spin 1/2 particles,

$$\big|\psi\big\rangle = \frac{1}{\sqrt{2}}\left(\big|\vec{n}, +1/2\big\rangle \otimes \big|\vec{n}, -1/2\big\rangle - \big|\vec{n}, -1/2\big\rangle \otimes \big|\vec{n}, +1/2\big\rangle\right) \quad . \tag{192}$$

Here $\big|\vec{n}, \pm 1/2\big\rangle$ are the eigenvectors of $\vec{S}\cdot\vec{n}$ in a standard basis where we can use any choice of quantization axis $\vec{n}$ that we want.

We now ask what happens if the first particle comes to the laboratory of Alice and the second particle comes to the laboratory of Bob. Alice measures the spin of her particle along a direction $\vec{n}_A$ that she chooses. Bob measures the spin of his particle along a direction $\vec{n}_B$ that he chooses. We seek the probability that Alice gets $+1/2$ for her measurement and Bob gets $+1/2$ for his measurement. This probability is[10]

$$\begin{aligned}
P(\vec{n}_A, +1/2; \vec{n}_B, +1/2) &= \Big|\big(\big\langle\vec{n}_A, +1/2\big| \otimes \big\langle\vec{n}_B, +1/2\big|\big)\big|\psi\big\rangle\Big|^2 \\
&= \Big|\big(\big\langle\vec{n}_A, +1/2\big| \otimes \big\langle\vec{n}_B, +1/2\big|\big) \\
&\quad\times \frac{1}{\sqrt{2}}\Big(\big|\vec{n}_B, +1/2\big\rangle \otimes \big|\vec{n}_B, -1/2\big\rangle \\
&\quad\quad - \big|\vec{n}_B, -1/2\big\rangle \otimes \big|\vec{n}_B, +1/2\big\rangle\Big)\Big|^2 \\
&= \Big|\big(\big\langle\vec{n}_A, +1/2\big| \otimes \big\langle\vec{n}_B, +1/2\big|\big) \\
&\quad\times \frac{-1}{\sqrt{2}}\big|\vec{n}_B, -1/2\big\rangle \otimes \big|\vec{n}_B, +1/2\big\rangle\Big|^2 \\
&= \frac{1}{2}\Big|\big\langle\vec{n}_A, +1/2\big|\vec{n}_B, -1/2\big\rangle\Big|^2
\end{aligned} \tag{193}$$

To evaluate the inner product, we can choose a reference frame with $\vec{n}_A$ along the z-axis and $\vec{n}_B$ in the z, y-plane, rotated from the z-axis by an angle θ. Then

$$\big|\vec{n}_B, -1/2\big\rangle = \exp(-i\theta S_x)\big|\vec{n}_A, -1/2\big\rangle \tag{194}$$

[10] We choose to use $\vec{n}_B$ for our quantization axis to write the singlet state.

In a spinor notation, this is

$$\begin{aligned}\xi(\vec{n}_B,-1/2) &= \big(\cos(\theta/2) - i\sin(\theta/2)\sigma_x\big)\begin{pmatrix}0\\1\end{pmatrix}\\ &= \begin{pmatrix}-i\sin(\theta/2)\\ \cos(\theta/2)\end{pmatrix} \quad .\end{aligned} \tag{195}$$

The inner product of this with

$$\xi(\vec{n}_A,+1/2) = \begin{pmatrix}1\\0\end{pmatrix} \tag{196}$$

is

$$\big\langle \vec{n}_A,+1/2\big|\vec{n}_B,-1/2\big\rangle = -i\sin(\theta/2) \quad . \tag{197}$$

The phase factor -1 is not significant here since our spinors are defined only up to a phase.

This gives

$$P(\vec{n}_A,+1/2;\vec{n}_B,+1/2) = \frac{1}{2}\,\sin^2(\theta/2) \quad . \tag{198}$$

There is a way to do this calculation so that the irrelevant phase factors never appear. We have

$$\begin{aligned}\Big|\big\langle \vec{n}_A,+1/2\big|\vec{n}_B,-1/2\big\rangle\Big|^2 = \mathrm{Tr}\Big[&\Big(\big|\vec{n}_A,+1/2\big\rangle\big\langle\vec{n}_A,+1/2\big|\Big)\\ &\times\Big(\big|\vec{n}_B,-1/2\big\rangle\big\langle\vec{n}_B,-1/2\big|\Big)\Big] \quad .\end{aligned} \tag{199}$$

Here we are regarding $\big|\vec{n}_A,+1/2\big\rangle\big\langle\vec{n}_A,+1/2\big|$ and $\big|\vec{n}_B,-1/2\big\rangle\big\langle\vec{n}_B,-1/2\big|$ as operators, namely projection operators, and we take the trace of the product of these operators. Now using a 2×2 matrix representation, we have

$$\begin{aligned}\big|\vec{n}_A,+1/2\big\rangle\big\langle\vec{n}_A,+1/2\big| &= \frac{1}{2}\,[1+\vec{n}_A\cdot\vec{\sigma}] \quad ,\\ \big|\vec{n}_B,-1/2\big\rangle\big\langle\vec{n}_B,-1/2\big| &= \frac{1}{2}\,[1-\vec{n}_B\cdot\vec{\sigma}] \quad .\end{aligned} \tag{200}$$

You can prove this by noting that if you apply $[1+\vec{n}_A\cdot\vec{\sigma}]$ to an eigenvector of $\vec{n}_A\cdot\vec{\sigma}$ with eigenvalue $+1$, you get the eignevector back again, while if you apply it to an eigenvector with eigenvalue -1, you get zero. That is the defining property of the projection operator.

With this representation, we have

$$
\begin{aligned}
\left|\left\langle \vec{n}_A, +1/2 \middle| \vec{n}_B, -1/2 \right\rangle\right|^2 &= \frac{1}{4}\mathrm{Tr}\Big[\,(1+\vec{n}_A\cdot\vec{\sigma})\,(1-\vec{n}_B\cdot\vec{\sigma})\,\Big] \\
&= \frac{1}{4}\mathrm{Tr}\Big[1+\vec{n}_A\cdot\vec{\sigma}-\vec{n}_B\cdot\vec{\sigma} \\
&\qquad\qquad - i(\vec{n}_A\times\vec{n}_B)\cdot\vec{\sigma}-\vec{n}_A\cdot\vec{n}_B\Big] \\
&= \frac{1}{2}\big[1-\vec{n}_A\cdot\vec{n}_B\big] \\
&= \sin^2(\theta_{AB}/2) \quad .
\end{aligned}
\tag{201}
$$

This again gives the result (198).

Exercise 22.1 Suppose that Alice and Bob play with spin 1 particles. From two spin 1 particles, with states $\big|\vec{n},+1\big\rangle$, $\big|\vec{n},0\big\rangle$ and $\big|\vec{n},-1\big\rangle$, we can make a spin 0 state. Since the spin 0 state is an eigenstate of $\vec{S}\cdot\vec{n}$ with eigenvalue 0, it must be a combination of the form

$$
\big|\psi\big\rangle = \alpha\big|\vec{n},+1\big\rangle\otimes\big|\vec{n},-1\big\rangle+\beta\big|\vec{n},0\big\rangle\otimes\big|\vec{n},0\big\rangle+\gamma\big|\vec{n},-1\big\rangle\otimes\big|\vec{n},+1\big\rangle \quad . \tag{202}
$$

Find the coefficients α, β and γ (up to an overall phase).

Exercise 22.2 We now ask what happens if the first particle comes to the laboratory of Alice and the second particle comes to the laboratory of Bob. Alice measures the spin of her particle along a direction $\vec{n}_A$ that she chooses. Bob measures the spin of his particle along a direction $\vec{n}_B$ that he chooses. We seek the probability $P(\vec{n}_A,+1;\vec{n}_B,+1)$ that Alice gets $+1$ for her measurement and Bob gets $+1$ for his measurement. Calculate this probability in quantum mechanics. Does your answer make sense when the angle θ_{AB} between the two axes goes to zero? Does your answer make sense when θ_{AB} goes to π?
