

Ph195b lecture notes for 3/11/02

More on Clebsch-Gordon coefficients

Let's recall the general scenario for addition of two angular momenta. We have a quantum system A whose state lives in a Hilbert space H_A and a quantum system B whose state lives in a Hilbert space H_B . Let $\vec{\mathbf{J}}^A$ and $\vec{\mathbf{J}}^B$ be the angular momentum operators on the respective Hilbert spaces, and let

$$\vec{\mathbf{J}} = \vec{\mathbf{J}}^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes \vec{\mathbf{J}}^B$$

be the 'total' angular momentum operator on the tensor product space $H_{AB} = H_A \otimes H_B$. This tensor product on the state space induces a natural tensor product representation for the rotation group,

$$\begin{aligned} (\hat{n}, \varphi) &\mapsto \exp\left(\frac{-i}{\hbar} \hat{n} \cdot \vec{\mathbf{J}}^A \varphi\right) \otimes \exp\left(\frac{-i}{\hbar} \hat{n} \cdot \vec{\mathbf{J}}^B \varphi\right) \\ &= \exp\left(\frac{-i}{\hbar} \hat{n} \cdot \left(\vec{\mathbf{J}}^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes \vec{\mathbf{J}}^B\right) \varphi\right) \\ &\equiv \exp\left(\frac{-i}{\hbar} \hat{n} \cdot \vec{\mathbf{J}} \varphi\right). \end{aligned}$$

As Merzbacher succinctly puts it, however, the problem of the addition of two angular momenta consists of obtaining the eigenvalues j, m of \mathbf{J}_z and \mathbf{J}^2 , as well as their eigenvectors $\{|j; m\rangle\}$ in terms of the tensor products $\{|j_A; m_A\rangle \otimes |j_B; m_B\rangle\}$ of eigenvectors of $\mathbf{J}_z^A, (\mathbf{J}^A)^2$ and $\mathbf{J}_z^B, (\mathbf{J}^B)^2$.

Introducing the more compact notation

$$|j_A j_B m_A m_B\rangle \equiv |j_A; m_A\rangle \otimes |j_B; m_B\rangle,$$

we thus seek expansions of the form

$$\begin{aligned} |j; m\rangle &= \sum_{m_A, m_B} C(j_A j_B; m_A m_B | j; m) |j_A j_B m_A m_B\rangle \\ &= \sum_{m_A, m_B} \langle j_A j_B m_A m_B | j; m\rangle |j_A j_B m_A m_B\rangle. \end{aligned}$$

This serves to cleanly define the Clebsch-Gordon coefficients $C(j_A j_B; m_A m_B | j; m)$. From this definition, it should be clear that we can 'solve' an arbitrary case of addition of angular momenta if we have at our disposal a table of C-G coefficients! In the last lecture we used techniques from group representation theory to derive C-G coefficients for the particular case $j_A = 1/2, j_B = 1$.

In terms of the matrix S we derived last time, we know that the vector \vec{c} representing a state in the $\{|j; m\rangle\}$ ('coupled') basis may be written in terms of the vector \vec{u} that represents the same state in the $\{|j_A j_B m_A m_B\rangle\}$ ('uncoupled') basis as

$$\vec{c} = S \vec{u}.$$

Here \vec{u} and \vec{c} are to be thought of as column vectors, and S as a square matrix (actually this S corresponds to what we called S^{-1} last time). Conversely,

$$\vec{u} = S^{-1} \vec{c},$$

where $S^{-1} = S^\dagger = (S^T)^*$ (the complex-conjugate transpose of S) since we are assuming a linear change of basis. Hence, for particular values of m_A, m_B, j, m we have

$$\begin{aligned} C(j_A j_B; m_A m_B | j; m) &= [\vec{u}(j_A j_B; m_A m_B)]^* \cdot [S^\dagger \vec{c}(j; m)] \\ &= [\vec{u}(j_A j_B; m_A m_B)]^\dagger S^\dagger \vec{c}(j; m) \\ &= \left([\vec{c}(j; m)]^\dagger S \vec{u}(j_A j_B; m_A m_B) \right)^*, \end{aligned}$$

where $\vec{u}(j_A j_B; m_A m_B)$ is the vector representing $|j_A j_B m_A m_B\rangle$ in the uncoupled basis, $\vec{c}(j; m)$ is the vector representing $|j; m\rangle$ in the coupled basis, and \cdot denotes the familiar “dot” (scalar) product between vectors. Note that in our example from last time, we were working with real representations and therefore found that

$$\begin{aligned} C(j_A j_B; m_A m_B | j; m) &= \left([\vec{c}(j; m)]^\dagger S \vec{u}(j_A j_B; m_A m_B) \right)^* \\ &= [\vec{c}(j; m)]^\dagger S \vec{u}(j_A j_B; m_A m_B) \\ &= \vec{c}(j; m) \cdot S \vec{u}(j_A j_B; m_A m_B). \end{aligned}$$

It is important to note that the C-G coefficients can be derived via operator algebra alone (see Merzbacher pp. 428-429). We took the rather more abstract, and far more interesting (but somewhat more laborious) route through group representation theory.

Properties of C-G coefficients

Following Merzbacher, we can proceed to derive some important properties of the Clebsch-Gordon coefficients. Looking at the defining expansion

$$|j; m\rangle = \sum_{m_A, m_B} C(j_A j_B; m_A m_B | j; m) |j_A j_B m_A m_B\rangle,$$

we note that by applying $\mathbf{J}_z = \mathbf{J}_z^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes \mathbf{J}_z^B$ to both sides of the equation, we obtain

$$m\hbar |j; m\rangle = \sum_{m_A, m_B} C(j_A j_B; m_A m_B | j; m) (m_A + m_B) \hbar |j_A j_B m_A m_B\rangle.$$

Hence, it must be the case that $C(j_A j_B; m_A m_B | j; m) = 0$ unless

$$m = m_A + m_B.$$

Likewise, this implies that in general $C(j_A j_B; m_A m_B | j; m) = 0$ unless

$$j_A + j_B \geq j.$$

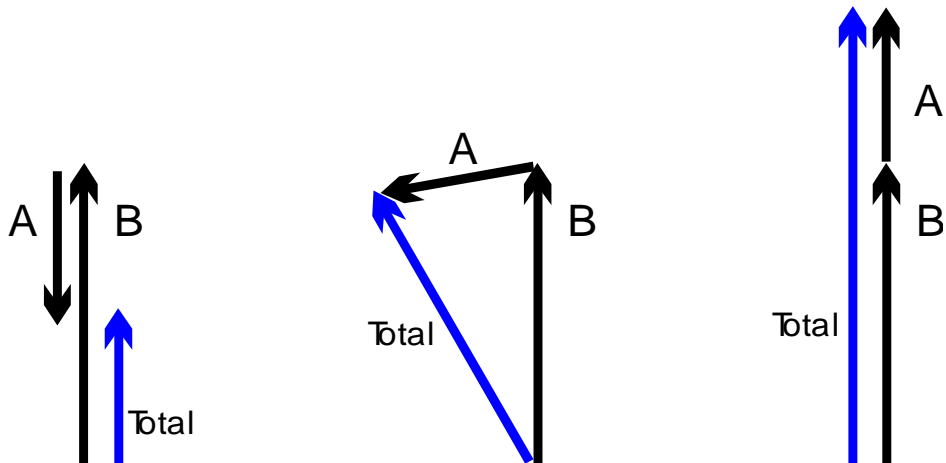
It turns out that through the algebraic derivation of C-G coefficients, one can also show that $C(j_A j_B; m_A m_B | j; m) = 0$ unless

$$j \geq |j_A - j_B|,$$

leading to the *triangular condition*,

$$|j_A - j_B| \leq j \leq j_A + j_B.$$

This can be understood by noting that in some abstract sense, what we are really trying to do here is investigate the addition of angular momentum ‘vectors’:



Using tables and symmetries

Last time we noted that the C-G coefficients have important symmetries, such as

$$\begin{aligned}
 C(j_A j_B; m_A m_B | j m) &= \\
 C(ab; \alpha \beta | c(\alpha + \beta)) &= (-1)^{a+b-c} C(ba; \beta \alpha | c(\alpha + \beta)) \\
 &= (-1)^{a+b-c} C(ab; (-\alpha)(-\beta) | c(-\alpha - \beta)) \\
 &= C(ba; (-\beta)(-\alpha) | c(-\alpha - \beta)).
 \end{aligned}$$

These are often necessary for using tables of C-G coefficients. For example, here's one from Quantum Theory of Angular Momentum, by D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii (World Scientific, 1988) [pp. 284-289]:

Table 8.11.
Numerical Values of the Clebsch-Gordan Coefficients.

| a | α | b | β | $C_{\alpha\alpha b\beta}^{0\alpha+\beta}$ | | a | α | b | β | $C_{\alpha\alpha b\beta}^{1/2\alpha+\beta}$ | |
|-----|----------|-----|---------|---|-----------|-----|----------|-----|---------|---|-----------|
| 0 | 0 | 0 | 0 | 1 | 1.000000 | 5/2 | 5/2 | 2 | -2 | $1/\sqrt{3}$ | 0.577350 |
| 1/2 | 1/2 | 1/2 | -1/2 | $1/\sqrt{2}$ | 0.707107 | 5/2 | 3/2 | 2 | -1 | $-2/\sqrt{3 \cdot 5}$ | -0.516398 |
| 1 | 1 | 1 | -1 | $1/\sqrt{3}$ | 0.577350 | 5/2 | 3/2 | 2 | -2 | $1/\sqrt{3 \cdot 5}$ | 0.258199 |
| 1 | 0 | 1 | 0 | $-1/\sqrt{3}$ | -0.577350 | 5/2 | 1/2 | 2 | 0 | $1/\sqrt{5}$ | 0.447214 |
| 3/2 | 3/2 | 3/2 | -3/2 | 1/2 | 0.500000 | 5/2 | 1/2 | 2 | -1 | $-\sqrt{2/3 \cdot 5}$ | -0.365148 |
| 3/2 | 1/2 | 3/2 | -1/2 | -1/2 | -0.500000 | 3 | 3 | 5/2 | -5/2 | $\sqrt{2/7}$ | 0.534522 |
| 2 | 2 | 2 | -2 | $1/\sqrt{5}$ | 0.447214 | 3 | 2 | 5/2 | -3/2 | $-\sqrt{5/3 \cdot 7}$ | -0.487950 |
| 2 | 1 | 2 | -1 | $-1/\sqrt{5}$ | -0.447214 | 3 | 2 | 5/2 | -5/2 | $1/\sqrt{3 \cdot 7}$ | 0.218218 |
| 2 | 0 | 2 | 0 | $1/\sqrt{5}$ | 0.447214 | 3 | 1 | 5/2 | -1/2 | $2/\sqrt{3 \cdot 7}$ | 0.436436 |
| 5/2 | 5/2 | 5/2 | -5/2 | $1/\sqrt{2 \cdot 3}$ | 0.408248 | 3 | 1 | 5/2 | -3/2 | $-\sqrt{2}/\sqrt{3 \cdot 7}$ | -0.308607 |
| 5/2 | 3/2 | 5/2 | -3/2 | $-1/\sqrt{2 \cdot 3}$ | -0.408248 | 3 | 0 | 5/2 | 1/2 | $-1/\sqrt{7}$ | -0.377964 |
| 5/2 | 1/2 | 5/2 | -1/2 | $1/\sqrt{2 \cdot 3}$ | 0.408248 | | | | | | |
| 3 | 3 | 3 | -3 | $1/\sqrt{7}$ | 0.377964 | a | α | b | β | $C_{\alpha\alpha b\beta}^{1\alpha+\beta}$ | |
| 3 | 2 | 3 | -2 | $-1/\sqrt{7}$ | -0.377964 | 1/2 | 1/2 | 1/2 | 1/2 | 1 | 1.000000 |
| 3 | 1 | 3 | -1 | $1/\sqrt{7}$ | 0.377964 | 1/2 | 1/2 | 1/2 | -1/2 | $1/\sqrt{2}$ | 0.707107 |
| 3 | 0 | 3 | 0 | $-1/\sqrt{7}$ | -0.377964 | 1 | 1 | 0 | 0 | 1 | 1.000000 |
| | | | | | | 1 | 0 | 0 | 0 | 1 | 1.000000 |
| a | α | b | β | $C_{\alpha\alpha b\beta}^{1/2\alpha+\beta}$ | | 1 | 1 | 1 | 0 | $1/\sqrt{2}$ | 0.707107 |
| 1/2 | 1/2 | 0 | 0 | 1 | 1.000000 | 1 | 1 | 1 | -1 | $1/\sqrt{2}$ | 0.707107 |
| 1 | 1 | 1/2 | -1/2 | $\sqrt{2/3}$ | 0.816497 | 1 | 0 | 1 | 0 | 0 | 0.000000 |
| 1 | 0 | 1/2 | 1/2 | $-1/\sqrt{3}$ | -0.577350 | 3/2 | 3/2 | 1/2 | -1/2 | $\sqrt{3/2}$ | 0.866025 |
| 3/2 | 3/2 | 1 | -1 | $1/\sqrt{2}$ | 0.707107 | 3/2 | 1/2 | 1/2 | 1/2 | -1/2 | -0.500000 |
| 3/2 | 1/2 | 1 | 0 | $-1/\sqrt{3}$ | -0.577350 | 3/2 | 1/2 | 1/2 | -1/2 | $1/\sqrt{2}$ | 0.707107 |
| 3/2 | 1/2 | 1 | -1 | $1/\sqrt{2 \cdot 3}$ | 0.408248 | 3/2 | 3/2 | 3/2 | -1/2 | $\sqrt{3/2 \cdot 5}$ | 0.547723 |
| 2 | 2 | 3/2 | -3/2 | $\sqrt{2/5}$ | 0.632456 | 3/2 | 3/2 | 3/2 | -3/2 | $3/(2\sqrt{5})$ | 0.670820 |
| 2 | 1 | 3/2 | -1/2 | $-\sqrt{3/2 \cdot 5}$ | -0.547723 | 3/2 | 1/2 | 3/2 | 1/2 | $-\sqrt{2/5}$ | -0.632456 |
| 2 | 1 | 3/2 | -3/2 | $1/\sqrt{2 \cdot 5}$ | 0.316228 | 3/2 | 1/2 | 3/2 | -1/2 | $-1/(2\sqrt{5})$ | -0.223607 |
| 2 | 0 | 3/2 | 1/2 | $1/\sqrt{5}$ | 0.447214 | 2 | 2 | 1 | -1 | $\sqrt{3/5}$ | 0.774597 |
| | | | | | | 2 | 1 | 1 | 0 | $-\sqrt{3/2 \cdot 5}$ | -0.547723 |

Let's say we want to check $C(1/2 1; (-1/2) 0 | 1/2 (-1/2))$, which we calculated last time to be $-1/\sqrt{3}$. In their notation, we want the case $a = 1/2, \alpha = -1/2, b = 1, \beta = 0, c = 1/2, \gamma = -1/2$. However, they only list $a = 1, \alpha = 0, b = 1/2, \beta = 1/2, c = 1/2, \gamma = 1/2$. But this is equal to the coefficient we want, by symmetry, so our answer is verified.

Addition of three or more angular momenta

There are unfortunately a number of important physical scenarios in which one needs to couple together three or more angular momentum systems. For example, to get the total 'spin' of an atom one needs to add together the intrinsic spin of the nucleus, electron spin(s), and electron orbital angular momenta – recall we said that silver atoms used for the Stern-Gerlach experiment had overall spin 1/2, for example. We are not going to worry about this in any detail (yet), but it is worth having a brief look at the definitions of some C-G-like objects that you may someday encounter.

With three angular momenta j_1, j_2, j_3 there are three distinct 'schemes' for the overall coupling. Following the notation of Varshalovich *et al*, these are

$$\text{I) } j_1 + j_2 = j_{12}, \quad j_{12} + j_3 = j,$$

$$\text{II) } j_2 + j_3 = j_{23}, \quad j_1 + j_{23} = j,$$

$$\text{III) } j_1 + j_3 = j_{13}, \quad j_{13} + j_2 = j.$$

With scheme I, we ultimately produce coupled basis kets

$$|j_1 j_2 (j_{12}) j_3 |j; m\rangle = \sum_{m_1, m_2, m_3} \left(\begin{array}{c} \left[\begin{array}{c} \sum_{m_{12}} C(j_{12} j_3; m_{12} m_3 | j; m) \\ \times C(j_1 j_2; m_1 m_2 | j_{12}; m_{12}) \end{array} \right] \\ \times |j_3; m_3\rangle \otimes |j_2; m_2\rangle \otimes |j_1; m_1\rangle. \end{array} \right)$$

Likewise, scheme II produces

$$|j_1 j_2 j_3 (j_{23}) |j; m\rangle = \sum_{m_1, m_2, m_3} \left(\begin{array}{c} \left[\begin{array}{c} \sum_{m_{23}} C(j_1 j_{23}; m_1 m_{23} | j; m) \\ \times C(j_2 j_3; m_2 m_3 | j_{23}; m_{23}) \end{array} \right] \\ \times |j_3; m_3\rangle \otimes |j_2; m_2\rangle \otimes |j_1; m_1\rangle \end{array} \right),$$

and something similar holds for scheme III. The *Wigner 6j symbols* $\left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{array} \right\}$ are used to convert between these representations, e.g.,

$$\langle j_1 j_2 (j_{12}) j_3 j; m | j_1 j_2 j_3 (j_{23}) j; m \rangle = (-1)^{j_1 + j_2 + j_3 + j} \sqrt{(2j_{12} + 1)(2j_{23} + 1)} \times \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{array} \right\}.$$

These are related (by a simple phase factor) to the *Racah coefficients* $W(abed; cf)$:

$$\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \end{array} \right\} \equiv (-1)^{a+b+d+e} W(abed; cf).$$

The *Wigner 3jm symbols* $\left(\begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right)$ represent the overall amplitude for three angular momenta to be coupled to yield zero angular momentum:

$$\left(\begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right) = (-1)^{j_1 - j_2 + j_3} \sum_{j', m'} C(j_1 j_2; m_1 m_2 | j'; m') C(j' j_3; m' m_3 | 0; 0).$$

Interestingly, these are related to the Clebsch-Gordon coefficients and are often used in place of them:

$$\left(\begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right) = (-1)^{j_3 + m_3 + 2j_1} \frac{1}{\sqrt{2j_3 + 1}} C(j_1 j_2; (-m_1) (-m_2) | j_3; m_3),$$

$$C(j_1 j_2; m_1 m_2 | j_3; m_3) = (-1)^{j_1 - j_2 + m_3} \sqrt{2j_3 + 1} \left(\begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{array} \right).$$

The Wigner 3jm's have some useful symmetry properties, such as symmetry under cyclic

permutations of the columns.

Finally, it is worth noting that there exist *Wigner 9j symbols* (also known as *Fano coefficients*), and *Wigner 12j symbols*. These play analogous roles to that of the $6j$ symbols when converting between coupling schemes for 4 or 5 angular momenta.

Spins vs. orbital angular momenta

In case it hasn't otherwise become clear, I wanted to end with some general indications of how various values of j can arise in typical quantum system such as atoms.

Electrons, protons, and neutrons have intrinsic spin $1/2$. We know that the orbital angular momentum of any particle, on the other hand, is only allowed to have j equal to a non-negative integer. When multiple protons and neutrons are coupled together to make an atomic nucleus, their intrinsic spins and orbital angular momenta can add to yield total j that is either an integer or a half-integer. Likewise, the total angular momentum of the atom electron 'cloud' can be integer or half integer, and this adds together with the nuclear j to yield an integer or half-integer total j for the atom. The total angular momentum of a composite system is generally referred to as the system's overall spin.

Roughly speaking, the total spin of an atom depends on the relative orientations of the intrinsic spins of each of its constituent particles, as well as the relative orientations of the angular momentum vectors of all the orbital degrees of freedom. Hence an atom's spin depends on its 'internal state,' as we'll see explicitly next term. For example ^{133}Cs , with its electrons in their orbital ground state, can have overall $j = 4$ or $j = 3$ depending on whether the total electron spin of $1/2$ is parallel or opposite to its total nuclear spin of $7/2$.

Spherical tensor operators and the Wigner-Eckart Theorem

(Merzbacher §17.7)

Let's intuitively define a vector operator $\vec{\mathbf{A}} \leftrightarrow \{\mathbf{A}_x, \mathbf{A}_y, \mathbf{A}_z\}$ as a set of three Hilbert-space operators whose expectation values transform under rotations like a coordinate-space vector. Recalling that inner products between vectors are preserved under spatial rotations, we must have

$$\langle \vec{\mathbf{A}} \rangle \leftrightarrow \begin{pmatrix} \langle \mathbf{A}_x \rangle \\ \langle \mathbf{A}_y \rangle \\ \langle \mathbf{A}_z \rangle \end{pmatrix},$$

$$\langle \Psi | \vec{\mathbf{A}} | \Psi \rangle \cdot \hat{e} = \langle \Psi' | \vec{\mathbf{A}} | \Psi' \rangle \cdot \hat{e}',$$

where \hat{e} is a unit vector in the coordinate space and primed objects are the images of

unprimed objects after the rotation. If we let U_R denote the Hilbert-space representation of a spatial rotation R ,

$$|\Psi'\rangle = U_R|\Psi\rangle, \quad \hat{e}' = R\hat{e}.$$

Since

$$\begin{aligned} \langle \Psi' | \vec{\mathbf{A}} | \Psi' \rangle \cdot \hat{e}' &= \langle \mathbf{A}_x \rangle e'_x + \langle \mathbf{A}_y \rangle e'_y + \langle \mathbf{A}_z \rangle e'_z \\ &= \langle \Psi' | \vec{\mathbf{A}} \cdot \hat{e}' | \Psi' \rangle \end{aligned}$$

and

$$\langle \Psi | \vec{\mathbf{A}} | \Psi \rangle \cdot \hat{e} = \langle \Psi' | U_R \vec{\mathbf{A}} \cdot \hat{e} U_R^\dagger | \Psi' \rangle,$$

we must have

$$\begin{aligned} U_R \vec{\mathbf{A}} \cdot \hat{e} U_R^\dagger &= \vec{\mathbf{A}} \cdot \hat{e}', \\ U_R \vec{\mathbf{A}} U_R^\dagger \cdot \hat{e} &= \vec{\mathbf{A}} \cdot \hat{e}'. \end{aligned}$$

Merzbacher gives us a nice parametrization of the matrix R that represents a spatial rotation by clockwise angle φ around an axis \hat{n} ,

$$R = \begin{pmatrix} (1 - n_x^2) \cos \varphi + n_x^2 & n_x n_y (1 - \cos \varphi) - n_z \sin \varphi & n_x n_z (1 - \cos \varphi) + n_y \sin \varphi \\ n_y n_x (1 - \cos \varphi) + n_z \sin \varphi & (1 - n_y^2) \cos \varphi + n_y^2 & n_y n_z (1 - \cos \varphi) - n_x \sin \varphi \\ n_z n_x (1 - \cos \varphi) + n_y \sin \varphi & n_z n_y (1 - \cos \varphi) - n_x \sin \varphi & (1 - n_z^2) \cos \varphi + n_z^2 \end{pmatrix}.$$

Hence with $\hat{e}' = R\hat{e}$ we see that

$$U_R \mathbf{A}_j U_R^\dagger = \sum_i \mathbf{A}_i R_{ij}.$$

To write it another way,

$$\begin{pmatrix} \mathbf{A}_x \\ \mathbf{A}_y \\ \mathbf{A}_z \end{pmatrix} \mapsto R(\hat{n}, \varphi) \begin{pmatrix} \mathbf{A}_x \\ \mathbf{A}_y \\ \mathbf{A}_z \end{pmatrix}$$

under the spatial rotation (\hat{n}, φ) , which shows that the transformation of a vector operator under rotation follows (or induces) a linear representation of the rotation group.

Of course, we know what the Hilbert-space representation U_R looks like as well, from which we can infer

$$\exp\left(-\frac{i}{\hbar} \varphi \hat{n} \cdot \vec{\mathbf{J}}\right) \vec{\mathbf{A}} \exp\left(+\frac{i}{\hbar} \varphi \hat{n} \cdot \vec{\mathbf{J}}\right) = R \vec{\mathbf{A}}.$$

As Merzbacher points out, taking φ to be infinitesimal and expanding both the operator exponentials and the rotation matrix R to first order gives the convenient relation

$$[\vec{\mathbf{A}}, \hat{n} \cdot \vec{\mathbf{J}}] = i\hbar \hat{n} \times \vec{\mathbf{A}}$$

that is necessarily satisfied for arbitrary \hat{n} by any vector operator $\vec{\mathbf{A}}$.

This notion of a vector operator can be generalized to define *spherical tensor operators*, with a vector operator being a rank-1 spherical tensor operator. We have previously seen that the rotation group has linear representations on vector spaces of various dimension, and the vector operators pick out the representation with dimension $3 = (2j + 1)$ (hence rank

$j = 1$). For arbitrary (non-negative) integer rank k , we define

$$U_R \mathbf{T}_k^q U_R^\dagger = \sum_{q'=-k}^k \mathbf{T}_k^{q'} D_{q'q}^{(k)}(R).$$

Here $D_{q'q}^{(k)}(R)$ denotes the (q', q) matrix element of the k -dimensional linear representation of the rotation R . Keep in mind that we have implicitly fixed some underlying Hilbert space, on which \mathbf{T}_k^q acts and which defines the U_R representation.

For rank 1, it is straightforward to explicitly compute the spherical tensor components of an arbitrary vector operator with Cartesian components $(\mathbf{A}_x, \mathbf{A}_y, \mathbf{A}_z)$:

$$\mathbf{T}_1^{+1} = -\frac{1}{\sqrt{2}}(\mathbf{A}_x + i\mathbf{A}_y)$$

$$\mathbf{T}_1^0 = \mathbf{A}_z,$$

$$\mathbf{T}_1^{-1} = \frac{1}{\sqrt{2}}(\mathbf{A}_x - i\mathbf{A}_y).$$

An important example of a vector operator is the position operator $\vec{\mathbf{r}}$ for particle motion in 3D, whose spherical tensor components are evidently

$$\left(-\frac{\mathbf{x} + i\mathbf{y}}{\sqrt{2}}, \mathbf{z}, \frac{\mathbf{x} - i\mathbf{y}}{\sqrt{2}} \right).$$

It is again convenient to consider infinitesimal rotations, now in the definition of spherical tensor operators, yielding the necessary and sufficient condition

$$[\hat{\mathbf{n}} \cdot \vec{\mathbf{J}}, \mathbf{T}_k^q] = \sum_{q'=-k}^k \mathbf{T}_k^{q'} \langle kq' | \hat{\mathbf{n}} \cdot \vec{\mathbf{J}} | kq \rangle,$$

which in turn can be reduced to

$$[\mathbf{J}_z, \mathbf{T}_k^q] = q\hbar\mathbf{T}_k^q,$$

$$[\mathbf{J}_+, \mathbf{T}_k^q] = \sqrt{(k-q)(k+q+1)}\hbar\mathbf{T}_k^{q+1},$$

$$[\mathbf{J}_-, \mathbf{T}_k^q] = \sqrt{(k+q)(k-q+1)}\hbar\mathbf{T}_k^{q-1}.$$

It should be clear that knowing the decomposition of an operator into spherical tensor components can thus be quite useful in dealing with problems that have rotational symmetry.

Given that spherical tensor operators have such nice transformation properties under rotations of the coordinate space, it seems convenient to ask the following question (Merzbacher): "If T_k^q is an irreducible tensor operator, how much information about its matrix elements in the angular momentum basis can be inferred?" As it turns out, quite a lot! The answer is summarized in the famous *Wigner-Eckart theorem* (see pp. 432-435 for the derivation):

$$\langle \alpha' j' m' | T_k^q | \alpha j m \rangle = \langle j k m q | j k j' m' \rangle \langle \alpha' j' || T_k^q || \alpha j \rangle.$$

If α and α' denote the set of quantum numbers necessary in addition to j, m to fully specify a basis state, this shows that the matrix elements of a spherical tensor operator are

proportional to Clebsch-Gordan coefficients $\langle jkmq | jk'j' m' \rangle$. The constant of proportionality characterizes the aspects of T_k^q that are not pinned down by rotational symmetry, and is known as the reduced matrix element.

Central potentials and the radial equation

For spherically symmetric (central) potentials $V(r)$, the 3D Schrödinger Equation with

$$\mathbf{H} = \frac{\vec{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

has stationary solutions of the form

$$\begin{aligned}\mathbf{H}\psi_E(\vec{r}) &= E\psi_E(\vec{r}), \\ \psi_E(\vec{r}) &= R_E(r)Y_l^m(\theta, \varphi).\end{aligned}$$

Here $Y_l^m(\theta, \varphi)$ are the spherical harmonics we saw previously. Since \mathbf{H} is rotationally symmetric it commutes with both \mathbf{L}^2 and \mathbf{L}_z , hence we may choose the energy eigenstates to be eigenstates of total angular momentum and \mathbf{L}_z as well. The function $R_E(r)$ contains the radial behavior of ψ , and reflects the influence of a particular potential energy term $V(r)$.

Using

$$\vec{\mathbf{p}} \leftrightarrow i\hbar\vec{\nabla}$$

in the position representation and the form of ∇^2 in spherical coordinates, one can show (Merzbacher 11.111) that the kinetic energy term

$$\frac{\vec{\mathbf{p}}^2}{2m} \leftrightarrow \frac{\mathbf{L}^2\hbar^2}{2mr^2} - \frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right),$$

where $\vec{\mathbf{L}} = \vec{r} \times \vec{\mathbf{p}}$ is the operator for orbital angular momentum. Hence the stationary form of the 3D Schrödinger Equation may be written

$$\left[-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2\hbar^2}{2mr^2} + V(r) \right] \psi_E(\vec{r}) = E\psi_E(\vec{r}).$$

Substituting in the separated form involving spherical harmonics,

$$\left[-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right] R_E(r) = ER_E(r),$$

since $Y_l^m(\theta, \varphi)$ is an eigenfunction of \mathbf{L}^2 with eigenvalue $l(l+1)$.

It is often convenient to introduce one more transformation, by defining

$$u(r) = rR_E(r).$$

This now satisfies the *radial equation*

$$-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right] u = Eu,$$

which looks like the 1D Schrödinger Equation with an extra potential energy term $l(l+1)\hbar^2/2mr^2$, corresponding to a centrifugal barrier. Having made these transformations, we are now free to think of the problem of finding eigenstates for a central potential as being equivalent to that of solving the 1D radial equation. An important difference however is that r (unlike x) is never negative, so we must be careful about the boundary condition on u as $r \rightarrow 0$. Clearly we would like $u(0) = 0$ for finiteness of ψ at the origin, but later on we will see

that there are some requirements on its functional form as well.

Solution of the radial equation for a free particle

In the absence of a real potential energy term (as opposed to the centrifugal one), it turns out that the radial equation can be morphed into something whose solutions are clearly Bessel functions. Starting from the original

$$\left[-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right] R_E(r) = ER_E(r),$$

we first introduce the scaling

$$\rho = \sqrt{\frac{2mE}{\hbar^2}} r = kr.$$

With this, we have

$$\frac{d^2 R}{d\rho^2} + \frac{2}{\rho} \frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2} \right] R = 0.$$

Inserting the ansatz

$$R = \frac{J(\rho)}{\sqrt{\rho}},$$

we obtain

$$\frac{d^2 J}{d\rho^2} + \frac{1}{\rho} \frac{dJ}{d\rho} + \left[1 - \frac{(l+1/2)^2}{\rho^2} \right] J = 0,$$

which is *Bessel's equation*. The solutions of this equation that are well-behaved at $r = 0$ are the cylindrical Bessel functions $J_{l+1/2}(\rho)$. Hence the radial components of the stationary wave functions can be written

$$R(\rho) = C j_l(\rho)$$

where C is a normalization constant and $j_l(\rho)$ is a *spherical Bessel function*

$$j_l(\rho) \equiv \sqrt{\frac{\pi}{2\rho}} J_{l+1/2}(\rho).$$

Thus we end up with free-particle solutions

$$\psi_{klm}(\vec{r}) = C j_l(kr) Y_l^m(\theta, \varphi),$$

where

$$E = \frac{\hbar^2 k^2}{2m}.$$

It should be noted that these energy eigenstates for the free particle (like plane waves) are not normalizable, as the asymptotic form of the spherical Bessel functions is

$$j_l(\rho) \simeq \frac{\cos[\rho - (l+1)\pi/2]}{\rho}, \quad (\rho \gg l)$$

and we thus will have an integrand in the normalization integral that goes like

$$\rho^2 d\rho |R(\rho)|^2 \sim d\rho \cos^2(\rho).$$

The spherical square well potential

Next we move on to the 3D version of a potential well, with $V(r) = -V_0$ for $r < a$ and $V(r) = 0$ for $r > a$ (with $V_0 > 0$). Just as in the 1D case, we must solve the radial equation within regions of constant $V(r)$ and then match solutions at the boundary:

$$\begin{aligned} -\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} R &= (E + V_0) R \quad \text{for } r < a, \\ -\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} R &= ER \quad \text{for } r > a. \end{aligned}$$

Bound states of the spherical square well will have $-V_0 \leq E \leq 0$.

Inside the well region ($r < a$) we can use the above results with $E \rightarrow E + V_0$,

$$R(r) = A j_l \left(\sqrt{\frac{2m(E + V_0)}{\hbar^2}} r \right) \quad \text{for } r < a.$$

Outside the well ($r > a$) we should be more careful. Since we are now dealing with a bound state problem, we should expect the eigenstates to be normalizable. The trick is that Bessel's equation admits additional solutions besides the $j_l(\rho)$, which are singular at the origin but may be admissible in a region that does not include $r = 0$. For $a < r \leq \infty$, the radial solutions of choice are spherical Hankel functions of the first kind. Recall that for bound states we have $E < 0$ and therefore outside the well

$$k = i \sqrt{\frac{-2mE}{\hbar^2}} \equiv i\kappa,$$

and the corresponding solutions are

$$R(r) = B h_l^{(1)} \left(i \sqrt{\frac{-2mE}{\hbar^2}} r \right).$$

As in the 1D case we match solutions at the boundary $r = a$. Note that we have a total of three constraints (continuity of ψ , continuity of ψ' , overall normalization) in two unknowns (A and B). Hence we can match the logarithmic derivative to find the energy spectrum and worry about normalization separately. This leads to

$$\sqrt{\frac{\alpha^2 - \kappa^2}{\kappa^2}} \frac{j_l'(\sqrt{\alpha^2 - \kappa^2} a)}{j_l(\sqrt{\alpha^2 - \kappa^2} a)} = \frac{h_l^{(1)'}(\kappa a)}{h_l^{(1)}(\kappa a)}$$

as an equation for the allowed discrete energy eigenvalues, where $\alpha^2 \equiv 2mV_0/\hbar^2$.