Chapter 1. Quantum Mechanics for Scattering

Contents

1 Postulates of quantum mechanics

1.1 4 fundamental postulates

There is no generally adopted system of postulates of quantum mechanics. Here, we treat four postulates following *Introductory Quantum Mechanics, 4th Ed. by R. L. Liboff (Addison Wesley, 2003).*

Postulate I - To any self-consistently and well-defined observable A in physics, there corresponds an operator (call it $\hat{A}$) such that measurement of A yields a which are eigenvalue of $\hat{A}$. The eigenvalue equation for observables becomes

$$\hat{A}\varphi = a\varphi$$

where φ is the eigenfunction of $\hat{A}$ corresponding to a.

Postulate II - Measurement of the observable A that yields the value a leaves the system in the state φ_a, where φ_a is the eigenfunction of $\hat{A}$ that corresponds to the eigenvalue of a.

Postulate III - The state of a system at any instant time may be represented by a state ft ψ which is analytic. If a system is in the state $\psi(\vec{r}, t)$, the average of any physical observable C at a time t,

$$< C >= \int \psi^* \hat{C} \psi d\vec{r}$$

which is called the expectation value.

Postulate IV - The state function $\psi(\vec{r}, t)$ develops in time according to the equation

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r}, t) = \hat{H}\psi(\vec{r}, t)$$

which is called the time-dependent Schrödinger Equation (TDSE). The operator $\hat{H}$ is the Hamiltonian operator.

1.2 Position, momentum, and energy operators

(a) The position operator: $\hat{x}$

$$\begin{aligned} \hat{x} &= x \\ \hat{x}\varphi_{x_0} &= x_0\varphi_{x_0}, \\ \varphi_{x_0} &= \delta(x - x_0) \end{aligned}$$

x_0: Possible values that measurement of $\hat{x}$ will yield
φ : $|\varphi|^2 dx$ is the probability of finding the particle with x_1 in the interval x and $x + dx$.

(b) The momentum operator : $\hat{p_x}$

$$\begin{aligned} \hat{p_x} &= \frac{\hbar}{i}\frac{\partial}{\partial x} \\ \frac{\hbar}{i}\frac{\partial \varphi}{\partial x} &= p_x\varphi \\ \varphi_k(x) &= Ae^{ip_x x/\hbar} = Ae^{ikx} \end{aligned}$$

p_x: Possible values that measurement of $\hat{p_x}$ will yield
φ : $|\varphi|^2 dx$ is the probability of finding the particle with p_x in the interval x and $x + dx$.

Here $k \equiv p_x/\hbar = p/\hbar$ or $p = \hbar k$. It is a periodic function with a wavelength of $\lambda = 2\pi/k$, which is equivalent to the de Broglie wavelength. Remember that $\varphi_k(x)$ and $\hbar k$ are in a continuum.

(c) The energy operator: $\hat{H}$

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$$
$$\hat{H}\varphi = E\varphi$$

This is the *time independent Schrödinger equation.*

For a free particle, ($V = 0$, purely kinetic, no boundary)

$$\hat{H} = \frac{p_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} = E\varphi, \quad \text{or} \quad \varphi_{xx} + k^2\varphi = 0$$

where the subscript x denotes differentiation, and

$$k^2 = \frac{2mE}{\hbar^2}$$

Thus the eigenfunction and eigenvalue become, respectively,

$$\begin{aligned} \varphi(x) &= Ae^{ikx} + Be^{-ikx} \\ E &= \frac{\hbar^2 k^2}{2m} \end{aligned}$$

Note that $\varphi(x)$ and $\frac{\hbar^2 k^2}{2m}$ are also in a continuum.

It is interesting to note that with a known momentum eigenfunction $\varphi(x)$ and its eigenvalues $\hbar k$,

$$\hat{H}\varphi = \frac{\hat{p}}{2m}\hat{p}\varphi = \frac{\hat{p}}{2m}\hbar k\varphi = \frac{\hbar k}{2m}\hat{p}\varphi = \frac{\hbar^2 k^2}{2m}\varphi$$

Thus, φ is a simultaneous eigenfunction of $\hat{p}$ and $\hat{H}$ for a free particle. Physically if the free particle is in this state, measurement of p will definitely yield $\hbar k$, and measurement of E will definitely yield $\frac{\hbar^2 k^2}{2m}$.

1.3 Uncertainty principle

Suppose that measurement of the momentum yields $\hbar k$. What does measurement of x find in this state? To answer this question, remember that Born postulated that the probability density of finding the particle between x and $x + dx$ is, $|\varphi_k|^2 = |A|^2 =$ constant, which means that the probability density is the same for all x. In other words, It is equally, likely to find the particle an any point from $-\infty$ to ∞.

If the free particle is again in this state, then we can measure momentum definitely, but position indefinitely. Thus $\Delta p \to 0$ and $\Delta x \to \infty$. It follows the Uncertainty Principle.

We can also establish the uncertainty relation between complementary variables E and t. Measure energy definitely. Thus $\Delta E \to 0$. Uncertainty principle says the energy and the time that takes to measure E are complementary.

$$\Delta E\ \Delta t \geq \hbar \quad \text{or} \quad \Delta t \geq \frac{\hbar}{\Delta E} \to \infty$$

How do we understand this situation? To measure E, we need an energy measuring set. A particle should interact with the apparatus. Uncertainty principle teaches us that we must wait indefinite time before we detect E.

The uncertainty Δt is infinite in the present case, since there is an infinite uncertainty in x.

1.4 Measurements of x, p, and E, and their uncertainties:

A free particle with a mass m are in the following states,

$$\begin{array}{lrcl} (a) & \psi_a(x) & = & A\ \exp(ik_0x) \\ (b) & \psi_b(x) & = & B\ \delta(x-x_0) \end{array}$$

What values and uncertainties of x, p, and E does one measure in each state?

(a) $\psi_a(x) = A\ \exp(ik_0x)$

(1) Measurement values

x : One measures $x = x'$. Note that it is independent of the initial state (Post I).

p : Since the state is an eigenfunction of the momentum operator, one gets $p = \hbar k_0$ (Post II).

E : With the same reason, $E = \hbar^2 k_0^2/2m$.

(2) Uncertainties

x : One gets any value of x' with the equal probability since $|\psi_a|^2 = A^2 =$ constant. It implies $\Delta x = \infty$.

p : One measures a momentum $p = \hbar k_0$ definitely, and thus $\Delta p = 0$

E : One measures an energy $E = \hbar^2 k_0^2/2m$ definitely but any time of t, and thus $\Delta E = 0$, and $\Delta t = \infty$.

(b) $\psi_b(x) = B\ \delta(x - x_0)$

(1) Measurement values

x : One measures $x = x_0$ definitely. Remember that $B\ \delta(x - x_0)$ is the eigenstate of $\hat{x}$.

p : One gets any value of $p = \hbar k'$.

E : $E = \hbar^2 k'^2/2m$.

(2) Uncertainties

x : One measures a position $x = x_0$ definitely, and thus $\Delta x = 0$

p : One gets any value of k' with the equal probability. It implies $\Delta p = \infty$.

E : One measures an energy $E = \hbar^2 k'^2/2m$ indefinitely but a definite time of t, and thus $\Delta E = \infty$, and $\Delta t = 0$.

2 The Schrödinger wave equation for a particle

2.1 Geometrical interpretation of the one-dimensional wave functions

The 1-D Schrödinger equation becomes

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\varphi(x) = E\varphi(x)$$

or

$$\varphi_{xx} = -k^2(x)\varphi$$

where

$$\begin{aligned} \frac{\hbar^2 k^2}{2m} &= E - V(x) = T \\ \varphi_x &= \frac{\partial \varphi}{\partial x}, \quad \varphi_{xx} = \frac{\partial^2 \varphi}{\partial x^2} \end{aligned}$$

and T denotes the kinetic energy of the system.

The geometrical Interpretation of $\varphi(x), \varphi_x(x), \varphi_{xx}(x)$ can be summarized as

⊙ φ > 0 Upper half-plane
$= 0$ x-axis
< 0 Lower half-plane

⊙ φ_x > 0 Positive slope at x
$= 0$ Parallel to x-axis
< 0 Negative slope at x

⊙ φ_{xx} > 0 Concave upward curvature at x
$= 0$ No curvature
< 0 Concave downward curvature

We thus conclude geometrically that

⊙ $T > 0$: For $\varphi > 0$, $\varphi_{xx} < 0$
Concave downward in the upper plane.
: For $\varphi < 0$, $\varphi_{xx} > 0$
Concave upward in the lower plane.
⇒ Oscillatory pattern is possible.
⇒ Bigger T, faster oscillation.

⊙ $T < 0$: For $\varphi > 0$, $\varphi_{xx} > 0$
Concave upward in the upper plane.
: For $\varphi < 0$, $\varphi_{xx} < 0$
Concave downward in the lower plane.
⇒ No match between two planes.
Growing or decaying pattern
⇒ Bigger $|T|$, faster grow or decay .

⊙ $T = 0$: $\varphi_{xx} = 0 \rightarrow \varphi_x = \text{const.}$
Should be matched at the turning point.

2.2 Schrödinger equation for a free particle in the 3-D Cartesian coordinates

The time-independent Schrödinger equation (TISE) for a free particle in the three dimensional Cartesian coordinates can be written

$$\hat{H}\varphi = -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\varphi = E\varphi$$

We set, since x, y and z are independent each other,

$$\varphi = X(x)Y(y)Z(z)$$

and then TISE becomes

$$\frac{X_{xx}}{X} + \frac{Y_{yy}}{Y} + \frac{Z_{zz}}{Z} = -k^2, \qquad E = \frac{\hbar^2 k^2}{2m}$$

or

$$-\frac{X_{xx}}{X} = k^2 + (\frac{Y_{yy}}{Y} + \frac{Z_{zz}}{Z}) = k_x^2.$$

The left hand side of the equation is a function only of x, while the middle term is a function of y and z. The only way for the equality to hold for all (x, y, z) is to be a constant in both sides, calling k_x^2. It gives

$$X_{xx} + k_x^2 X = 0, \quad X = A_x e^{ik_x x}$$

Similarly,

$$Y_{yy} + k_y^2 Y = 0, \quad Y = A_y e^{ik_y y}$$
$$Z_{zz} + k_z^2 Z = 0, \quad Z = A_z e^{ik_z z}$$

We then obtain the eigenfunctions by combining together

$$\varphi = A_x A_y A_z e^{i(k_x + k_y + k_z)} = Ae^{i\mathbf{k}\cdot\mathbf{r}}$$

where the position vector $\mathbf{r}$ and the wave vector $\mathbf{k}$ have components,

$$\mathbf{r} = (x, y, z), \qquad \mathbf{k} = (k_x, k_y, k_z)$$

The eigenvalues are

$$E_k = \frac{\hbar^2 k^2}{2m}$$

The corresponding time dependent solution is

$$\varphi(\mathbf{r}, t) = Ae^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}, \quad E_k = \hbar\omega$$

This solution represents a propagating plane wave, since it is constant on the surfaces $\mathbf{k}\cdot\mathbf{r} =$ constant. This surface is normal to $\mathbf{k}$, because the perpendicular distance from any point on this surface $r_{\|} = \mathbf{k}\cdot\mathbf{r}/k$ is constant.

The normalization constant can be obtained by using the 3-D δ function

$$< \varphi_{\mathbf{k}} | \varphi_{\mathbf{q}} > \;\; = \;\; |A|^2 \int\int\int \varphi_{\mathbf{k}}^* \varphi_{\mathbf{q}} d\mathbf{r} = \delta(\mathbf{k} - \mathbf{q})$$

The 3-D δ function is defined as

$$\begin{aligned}\delta(\mathbf{r}-\mathbf{r_1}) &= \delta(x-x_1)\delta(y-y_1)\delta(z-z_1)\\ &= \frac{1}{(2\pi)^3}\int\int\int \exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r_1})]d\mathbf{k}\\ \varphi_{\mathbf{k}}(\mathbf{r},t) &= \frac{1}{(2\pi)^{3/2}}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\end{aligned}$$

The free particle wavepacket can be obtained by the superposition

$$\begin{aligned}\psi(\mathbf{r},t) &= \frac{1}{(2\pi)^{3/2}}\int\int\int b(\mathbf{r},t)e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}d\mathbf{k}\\ b(\mathbf{k},t) &= \frac{1}{(2\pi)^{3/2}}\int\int\int \psi(\mathbf{r},t)e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}d\mathbf{r}\end{aligned}$$

where $E_k = \hbar^2k^2/2m = \hbar\omega$ and the integration should be carried over 3-dimensional volume elements. We also have

$$\begin{aligned}\int \psi^*\psi\ d\mathbf{r} &= \int\int b^*(\mathbf{q},t)b(\mathbf{k},t)\ d\mathbf{k}d\mathbf{q}\ \frac{1}{(2\pi)^3}\int e^{i[(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}-\omega t]}\ d\mathbf{r}\\ &= \int\int b^*(\mathbf{q},t)b(\mathbf{k},t)\delta(\mathbf{k}-\mathbf{q})\ d\mathbf{k}d\mathbf{q}\\ &= \int b^*b\ d\mathbf{k}\end{aligned}$$

$b^*b\ d\mathbf{k} = P(\mathbf{k})d\mathbf{k}$ is the probability that $\hbar k$ in the volume $\hbar^3 d\mathbf{k}$ is observed.

If the probability amplitude $b(\mathbf{k},t)$ is peaked about $\mathbf{k_0}$, the packet propagates with the group velocity

$$\mathbf{v}_g = \nabla_{\mathbf{k}}\omega(k)|_{\mathbf{k}=\mathbf{k}_0}$$

where $\nabla_{\mathbf{k}}$ is written for the gradient with respect to $\mathbf{k}$. For a free packet, $E_k = \hbar\omega = \hbar^2k^2/2m$, we thus obtain

$$\mathbf{v}_g = \frac{\hbar\mathbf{k}_0}{2m} = \mathbf{v}_{classical}$$

This is the classical velocity of a particle moving with momentum $\hbar\mathbf{k}_0$.

2.3 A free particle in spherical coordinates

2.3.1 Hamiltonian

We first show that the Hamiltonian for a free particle in spherical coordinates

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{\mathbf{L}}^2}{2mr^2}$$

where the radial momentum is defined as

$$\hat{p}_r = \frac{1}{2}(\frac{1}{r}\hat{\mathbf{r}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\frac{1}{r})$$

and $\mathbf{L}$ is the angular momentum operator.

We calculate

$$\begin{aligned}
\hat{p}_r\varphi &= \frac{1}{2}(\frac{1}{r}\hat{\mathbf{r}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\frac{1}{r})\varphi \\
&= \frac{-i\hbar}{2}(\frac{1}{r}\hat{\mathbf{r}}\cdot\hat{\nabla} + \hat{\mathbf{p}}\cdot\hat{\nabla}\frac{1}{r})\varphi \\
&= \frac{-i\hbar}{2}(\frac{\partial\varphi}{\partial r} + \nabla\varphi\cdot\hat{e}_r + \varphi\nabla\cdot\hat{e}_r) \\
&= \frac{-i\hbar}{2}(\frac{\partial\varphi}{\partial r} + \frac{\partial\varphi}{\partial r}\hat{e}_r\cdot\hat{e}_r + \frac{2\varphi}{r}) \\
&= -i\hbar(\frac{\partial\varphi}{\partial r} + \frac{\varphi}{r}) \\
&= -i\hbar\frac{1}{r}\frac{\partial}{\partial r}(r\varphi)
\end{aligned}$$

where $\hat{e}_r$ is the unit radius vector. We have used

$$\nabla\cdot\mathbf{r}r^{n-1} = (n+2)r^{n-1}, \qquad \nabla\cdot\mathbf{r}r^{-1} = \frac{2}{r}$$

We thus have $\hat{p}_r^2$ and $\hat{L}^2$ (See I-5.)

$$\begin{aligned}
\hat{p}_r^2 &= -\hbar^2(\frac{1}{r}\frac{\partial}{\partial r}r\frac{1}{r}\frac{\partial}{\partial r}r) \\
&= -\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r \\
\hat{L}^2 &= -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]
\end{aligned}$$

The Hamiltonian is then obtained

$$\begin{aligned}
\hat{H} &= -\frac{\hbar^2}{2m}\nabla^2 \\
&= -\frac{\hbar^2}{2m}\{\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]\} \\
&= \frac{\hat{p}_r^2}{2m} + \frac{\hat{\mathbf{L}}^2}{2mr^2}
\end{aligned}$$

2.3.2 Radial momentum operator

We can establish the following properties of the radial momentum, $\hat{p}_r$;

(a) Hermitian

$$\begin{aligned}\hat{p}_r^\dagger &= \frac{1}{2}(\frac{1}{r}\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}+\hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\frac{1}{r})^\dagger \\ &= \frac{1}{2}(\hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\frac{1}{r}+\frac{1}{r}\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}) \\ &= \hat{p}_r\end{aligned}$$

since $\hat{p}$, $\hat{r}$ and $1/r$ are Hermitian.

(b)$[\hat{r},\hat{p}_r]=i\hbar$.

$$\begin{aligned}[\hat{r},\hat{p}_r]\varphi(r) &= -i\hbar[\hat{r},\frac{1}{r}\frac{\partial}{\partial r}r]\varphi(r) \\ &= -i\hbar[\varphi+r\frac{\partial\varphi}{\partial r}-\frac{1}{r}(2r\varphi+r^2\frac{\partial\varphi}{\partial r})] \\ &= i\hbar\varphi\end{aligned}$$

(c) $<\varphi|\hat{p}_r\psi>=<\hat{p}_r\varphi|\psi>$ implies $\tilde{\varphi}=r\varphi=0$ and $\tilde{\psi}=r\psi=0$ at $r=0$ and $r\to\infty$.

$$\begin{aligned}<\varphi|\hat{p}_r\psi> &= -i\hbar\int d\Omega\int drr^2\varphi^*\frac{1}{r}\frac{\partial}{\partial r}r\psi \\ &= -i\hbar\int_{4\pi}d\Omega\int_0^\infty dr\tilde{\varphi}^*\frac{\partial}{\partial r}\tilde{\psi} \\ &= -i\hbar\int_{4\pi}d\Omega[(\tilde{\varphi}^*\tilde{\psi})|_0^\infty+i\hbar\int_{4\pi}d\Omega\int_0^\infty dr\tilde{\varphi}^*\frac{\partial}{\partial r}\tilde{\psi}] \\ <\hat{p}_r\varphi|\psi> &= i\hbar\int d\Omega\int drr^2(\frac{1}{r}\frac{\partial}{\partial r}r\varphi^*)\psi \\ &= i\hbar\int d\Omega\int_0^\infty dr\tilde{\varphi}^*\frac{\partial}{\partial r}\tilde{\psi}\end{aligned}$$

The equality of two brackets holds when

$$(\tilde{\varphi}^*\tilde{\psi})|_0^\infty=0$$

It implies that $\tilde{\varphi}=r\varphi=0$ and $\tilde{\psi}=r\psi=0$ at $r=0$ and $r\to\infty$.

2.3.3 Kinetic energy operator

The kinetic energy operator

$$\hat{T}=-\frac{\hbar^2}{2m}\nabla^2$$

is Hermitian in the space of square integrable functions.

We attempt to prove $<\varphi|\hat{T}\psi>=<\hat{T}^\dagger\varphi|\psi>=<\hat{T}\varphi|\psi>$, where φ and ψ are the square integrable functions.

$$\begin{aligned}I &= -\frac{\hbar^2}{2m}\int_V[\varphi^*\nabla^2\psi-(\nabla^2\varphi^*)\psi]d\mathbf{r} \\ &= -\frac{\hbar^2}{2m}\int_V\nabla\cdot[\varphi^*\nabla\psi-(\nabla\varphi^*)\psi]d\mathbf{r} \\ &= -\frac{\hbar^2}{2m}\int_S[\varphi^*\nabla\psi-(\nabla\varphi^*)\psi]\cdot d\mathbf{S}\end{aligned}$$

To obtain the third step, we use *Green's theorem*. The volume V is enclosed by the surface S. It will vanish if φ and ψ, and their derivatives vanish sufficiently strongly on the boundary, which will be the case where the wave functions fall off quickly (exponentially) as we go to infinite distance such that they are square integrable. It follows that the kinetic energy operator is Hermitian for functions in the space of square integrable functions.

2.3.4 Angular momentum operator

(a) Commutator Relations

We can obtain the following commutator relations between angular momenta by using $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and the basic commutator relations $[\hat{x}, \hat{p}_x] = i\hbar$ and so on,
(1) $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$, or $\hat{\mathbf{L}} \times \hat{\mathbf{L}} = i\hbar\hat{\mathbf{L}}$,
(2) $[\hat{L}_i, \hat{L}^2] = 0$, or $[\hat{\mathbf{L}}, \hat{L}^2] = 0$.

In (1), ϵ_{ijk} stands for the following totally anti-symmetric tensor: $\epsilon_{ijk} = 0$ if any two indices are equal, and $\epsilon_{ijk} = +1$ or (-1) if the indices i, j, k can be obtained from 1, 2, 3 by an even (or an odd) number of permutations. The indices 1, 2, 3 stands for the $x-, y-, z-$components of vectors, and repeated suffixes are to be summed over. It is often called the Levi-Civita symbol.

(3) $[L_i, x_k] = i\hbar\epsilon_{ikl}x_l$
(4) $[\hat{L}_i, \hat{x}_j] = [\hat{x}_i, \hat{L}_j]$
(5) $[L_i, p_k] = i\hbar\epsilon_{ikl}p_l$
(6) $[\hat{L}_i, \hat{p}_j] = [\hat{p}_i, \hat{L}_j]$
(7) $[\hat{L}^2, \hat{\mathbf{r}}] = -2i\hbar(\hat{\mathbf{L}} \times \hat{\mathbf{r}} - i\hbar\hat{\mathbf{r}}) = 2i\hbar(\hat{\mathbf{r}} \times \hat{\mathbf{L}} - i\hbar\hat{\mathbf{r}})$
(8) $[\hat{\mathbf{L}}, \hat{r}^2] = 0$
(9) $[\hat{L}^2, \hat{\mathbf{p}}] = -2i\hbar(\hat{\mathbf{L}} \times \hat{\mathbf{p}} - i\hbar\hat{\mathbf{p}}) = 2i\hbar(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - i\hbar\hat{\mathbf{p}})$
(10) $[\hat{\mathbf{L}}, \hat{p}^2] = 0$
(11) $[\hat{\mathbf{L}}, \hat{\mathbf{r}}] = i\hbar \begin{pmatrix} 0 & \hat{z} & -\hat{y} \\ -\hat{z} & 0 & \hat{x} \\ \hat{y} & -\hat{x} & 0 \end{pmatrix}$
(12) $[\hat{\mathbf{L}}, \hat{\mathbf{p}}] = i\hbar \begin{pmatrix} 0 & \hat{p}_z & -\hat{p}_y \\ -\hat{p}_z & 0 & \hat{p}_x \\ \hat{p}_y & -\hat{p}_x & 0 \end{pmatrix}$
(13) $[\hat{\mathbf{r}}, \mathbf{e} \cdot \hat{\mathbf{L}}] = i\hbar\mathbf{e} \times \hat{\mathbf{r}}$
(14) $[\hat{\mathbf{p}}, \mathbf{e} \cdot \hat{\mathbf{L}}] = i\hbar\mathbf{e} \times \hat{\mathbf{p}}$,
where $\mathbf{e}$ is a unit vector in an arbitrary but fixed direction.
(15) $[\hat{\mathbf{L}} \cdot \hat{\mathbf{A}}, \hat{\mathbf{L}}] = i\hbar\hat{\mathbf{L}} \times \hat{\mathbf{A}}$,
where $\mathbf{A}$ is a constant operator.
(16) $[\hat{L}_i, \hat{V}_j] = i\hbar\epsilon_{ijk}\hat{V}_k$,
where $\mathbf{V}$ is a vector operator.
(17) $[\hat{\mathbf{L}}, \hat{\mathbf{L}} \times \hat{\mathbf{L}}] = -\hbar^2 \begin{pmatrix} 0 & \hat{L}_z & -\hat{L}_y \\ -\hat{L}_z & 0 & \hat{L}_x \\ \hat{L}_y & -\hat{L}_x & 0 \end{pmatrix}$
(18) $[\hat{L}_x^2, \hat{L}_y^2] = [\hat{L}_y^2, \hat{L}_z^2] = [\hat{L}_z^2, \hat{L}_x^2]$
(19) $[\hat{A}^2, \hat{L}^2] = 0$
if $[\hat{A}, \hat{L}_x] = [\hat{A}, \hat{L}_y] = [\hat{A}, \hat{L}_z] = 0$

(b) Hermiticity of $\hat{L}_i$ and $\hat{L}^2$.

$\hat{L}_i$ and $\hat{L}^2$ are Hermitian.

(c) Angular momentum operators in the spherical coordinates.

Employing the transformation equations between the Cartesian and spherical coordinates

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}$$

We express the Cartesian components of angular momentum operators, $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$, and the square $\hat{L}^2$ in the spherical coordinates.

$$r^2 = x^2 + y^2 + z^2, \quad \cos\theta = \frac{z}{r}, \quad \tan\phi = \frac{y}{x}$$

$$\begin{aligned} \frac{\partial\theta}{\partial x} &= \frac{\cos\phi\cos\theta}{r}, \qquad \frac{\partial\phi}{\partial x} = -\frac{y}{x^2}\cos^2\phi, \\ \frac{\partial\theta}{\partial y} &= \frac{\sin\phi\cos\theta}{r}, \qquad \frac{\partial\phi}{\partial y} = \frac{1}{x}\cos^2\phi, \\ \frac{\partial\theta}{\partial z} &= -\frac{\sin\theta}{r}, \qquad \frac{\partial\phi}{\partial z} = 0 \\ \frac{\partial r}{\partial x} &= \frac{x}{r}, \qquad \frac{\partial r}{\partial y} = \frac{y}{r}, \qquad \frac{\partial r}{\partial z} = \frac{z}{r} \end{aligned}$$

$$\begin{aligned} \hat{L}_x &= -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}) \\ &= i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}) \\ \hat{L}_y &= -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}) \\ &= i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}) \\ \hat{L}_z &= -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \\ &= -i\hbar\frac{\partial}{\partial\phi} \\ \hat{L}^2 &= -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}) \\ &= -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}] \end{aligned}$$

2.4 Eigenvalues and eigenfunctions angular momentum

2.4.1 Eigenvalues of angular momentum

Employing the commutator relations $[\hat{J}_i, \hat{J}_j] = i\hbar\hat{J}_k$ and $[\hat{J}_i, \hat{J}^2] = 0$, we obtain the eigenvalues of angular momentum operators $\hat{J}^2$ and J_z. Here we denote $\hat{J}$ as the orbital angular momentum $\hat{L}$, the spin angular momentum $\hat{S}$, or the total angular momentum (**J=L+S**) $\hat{J}$.

We first define the ladder operators

$$\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y$$

and then have commutator relations

$$\begin{aligned}
[\hat{J}_z, \hat{J}_\pm] &= [\hat{J}_z, \hat{J}_x \pm i\hat{J}_y] = i\hbar\hat{J}_y \pm i(-i\hbar\hat{J}_x) \\
&= \pm\hbar\hat{J}_\pm \\
[\hat{J}^2, \hat{J}_\pm] &= [\hat{J}^2, \hat{J}_x \pm i\hat{J}_y] = [\hat{J}^2, \hat{J}_x] \pm i[\hat{J}^2, \hat{J}_y] \\
&= 0 \\
\hat{J}_\pm\hat{J}_\mp &= (\hat{J}_x \pm i\hat{J}_y)(\hat{J}_x \mp i\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 \mp i[\hat{J}_x, \hat{J}_y] \\
&= \hat{J}_x^2 + \hat{J}_y^2 \pm \hbar\hat{J}_z \\
\hat{J}^2 &= \hat{J}_\pm\hat{J}_\mp + \hat{J}_z^2 \mp \hat{J}_z \\
[\hat{J}_\pm, \hat{J}_\mp] &= \hat{J}_x^2 + \hat{J}_y^2 \pm \hbar\hat{J}_z - \hat{J}_x^2 - \hat{J}_y^2 - (\mp\hbar\hat{J}_z) \\
&= \pm 2\hbar J_z
\end{aligned}$$

We set an eigenvalue equation for $\hat{J}_z$

$$\hat{J}_z\varphi_m = m\hbar\varphi_m$$

and evaluate

$$\begin{aligned}
\hat{J}_z\hat{J}_+\varphi_m &= (\hbar\hat{J}_+ + \hat{J}_+\hat{J}_z)\varphi_m = (\hbar\hat{J}_+ + \hat{J}_+ m\hbar)\varphi_m \\
&= (m+1)\hbar\hat{J}_+\varphi_m \\
\hat{J}_+\varphi_m &= \varphi_{m+1} \quad \text{(not normalized yet)}
\end{aligned}$$

$\hat{J}_+\varphi_m$ is an eigenfunction of $\hat{J}_z$ with the eigenvalue of $(m+1)\hbar$. Applying $\hat{J}_+$ again gives

$$\hat{J}_+(\hat{J}_+\varphi_m) = \hat{J}_+\varphi_{m+1} = \varphi_{m+2}$$

and so on. Similarly

$$\hat{J}_-\varphi_m = \varphi_{m-1}, \quad \hat{J}_-\varphi_{m-1} = \varphi_{m-2}$$

Therefore, we have found a scheme of generating a sequence of eigenfunctions of $\hat{J}_z$ from φ_m, with successive values of m differing by unity,

$$(..., \varphi_{m-2}, \varphi_{m-1}, \varphi_m, \varphi_{m+1}, \varphi_{m+2}, ...)$$

Now the commutator relation $[\hat{J}^2, \hat{J}_z] = 0$ leads that φ_m can also be an eigenfunction of $\hat{J}^2$,

$$\hat{J}^2\varphi_m = \hbar^2 K^2\varphi_m$$

$[\hat{J}^2, \hat{J}_\pm] = 0$ leads

$$\begin{aligned}
\hat{J}_+\hat{J}^2\varphi_m &= \hbar^2K^2(\hat{J}_+\varphi_m) = \hat{J}^2(\hat{J}_+\varphi_m) \\
&= \hat{J}^2\varphi_{m+1}
\end{aligned}$$

φ_{m+1} is an eigenfunction of $\hat{J}^2$ with the eigenvalue of $\hbar^2 K^2$. It implies that there are a lot of degeneracy!!

Now let us count the degeneracy. We have

$$\begin{aligned} < J^2 >= \hbar^2 K^2 &= < J_x^2 > + < J_y^2 > + < J_z^2 > \\ &= < J_x^2 > + < J_x^2 > + m^2\hbar^2 \end{aligned}$$

It yields

$$\hbar^2 K^2 \geq m^2\hbar^2 \quad \Rightarrow \quad |K| \geq |m|$$

For a given value of $K > 0$, $-K < m < K$. It means that there exist the minimum and maximum values of K, called

$$m_{min} = -K, \qquad m_{max} = K$$

and at these extremum values

$$\hat{J}_+ \varphi_{m_{max}} = 0, \qquad \hat{J}_- \varphi_{m_{min}} = 0$$

Applying $\varphi_{m_{max}}$ on $\hat{J}^2 = \hat{J}_- \hat{J}_+ + \hat{J}_z^2 + \hat{J}_z$ gives

$$\begin{aligned} \hat{J}^2 \varphi_{m_{max}} &= \hbar^2 K^2 \varphi_{m_{max}} \\ &= \hat{J}_- \hat{J}_+ \varphi_{m_{max}} + \hat{J}_z^2 \varphi_{m_{max}} + \hat{J}_z \varphi_{m_{max}} \\ &= \hbar^2 m_{max}(m_{max}+1)\varphi_{m_{max}} \\ K^2 &= m_{max}(m_{max}+1) \end{aligned}$$

Similarly, applying $\varphi_{m_{min}}$ on $\hat{J}^2 = \hat{J}_+ \hat{J}_- + \hat{J}_z^2 - \hat{J}_z$ gives

$$\begin{aligned} \hat{J}^2 \varphi_{m_{min}} &= \hbar^2 m_{min}(m_{min}-1)\varphi_{m_{min}} \\ K^2 &= m_{min}(m_{min}-1) \end{aligned}$$

Thus it yields

$$\begin{aligned} m_{max}(m_{max}+1) &= m_{min}(m_{min}-1) \\ m_{max} &= -m_{min} \equiv j \end{aligned}$$

Thus there are (2j+1)-m's for a given value of j, and the eigenstates of $\hat{J}^2$ are (2j+1)-fold degenerate.

Since m runs from $-j$ to $+j$ in units step, we obtain

$$\begin{aligned} j &= \text{integer} && \text{if } m = 0 \text{ is included} \\ j &= \frac{1}{2} \times \text{an odd integer} && \text{if } m = 0 \text{ is NOT included} \end{aligned}$$

If j is an integer, the related m values are also integers. If j is an odd multiple of one-half, the related m values are odd multiples of one-half.

We now obtain the eigenvalues of $\hat{J}^2$,

$$\begin{aligned} j &= m_{max} = -m_{min} \\ J^2 &= \hbar^2 K^2 = \hbar^2 j(j+1) \end{aligned}$$

The common eigenstates of $\hat{J}^2$ and $\hat{J}_z$ are functions of (j, m), and satisfy

$$\begin{aligned} \hat{J}^2 \varphi_{jm} &= \hbar^2 j(j+1)\varphi_{jm} \\ \hat{J}_z \varphi_{jm} &= \hbar m \varphi_{jm} \end{aligned}$$

2.4.2 Eigenfunctions of angular momentum - Spherical harmonics

There are two ways to obtain the eigenfunctions of $\hat{L}^2$ and L_z; (a) Direct solution of the eigenvalue equations

$$\begin{aligned}\hat{L}^2\varphi_{\ell m} &= \hbar^2\ell(\ell+1)\varphi_{\ell m}\\ \hat{L}_z\varphi_{\ell m} &= \hbar m\varphi_{\ell m}\end{aligned}$$

and (b) Solution from the ladder operator condition

$$\hat{L}_+\varphi_{\ell\ell} = 0$$

(a) Direct Solution

The square and z-component of orbital angular momentum operator in the spherical coordinates are

$$\begin{aligned}\hat{L}^2 &= -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]\\ \hat{L}_z &= -i\hbar\frac{\partial}{\partial\phi}\end{aligned}$$

They are functions only of angular variables (θ,ϕ). It means that the eigenfunctions may be chosen independent of r,

$$\varphi_{\ell m} \equiv Y_{\ell m}(\theta,\phi)$$

which is known to be *Spherical Harmonics*. It is normalized such that

$$\begin{aligned}\int_{4\pi}|Y_{\ell m}|^2 d\Omega &= \int_0^{2\pi}d\phi\int_0^{\pi}|Y_{\ell m}|^2\sin\theta d\theta\\ &= \int_0^{2\pi}d\phi\int_{-1}^{1}|Y_{\ell m}|^2 d\cos\theta = 1\end{aligned}$$

where Ω is the solid angle which extends to 4π.

We are now ready to obtain the eigenfunctions of $\hat{J}_z$,

$$\frac{\partial}{\partial\phi}Y_{\ell m} = imY_{\ell m}$$

This is only a function of ϕ. We thus set

$$Y_{\ell m} = \Phi_m(\phi)\Theta_{\ell m}(\theta)$$

Then we obtain

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}$$

which satisfies the normalization

$$\int_0^{2\pi}d\phi|\Phi_m(\phi)|^2 = 1$$

The index m is determined from the single valuedness of Φ, namely

$$\begin{aligned}\Phi(\phi) &= \Phi(\phi+2\pi)\\ e^{im\phi} &= e^{im(\phi+2\pi)} \quad \Rightarrow \quad e^{i2\pi m} = 1\end{aligned}$$

It yields

$$m = 0, 1, 2, ... \quad \text{(integer values)}$$

Applying $Y_{\ell m}$ on $\hat{L}^2$ gives

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta}{\partial\theta}) + [\ell(\ell+1) - \frac{m^2}{\sin^2\theta}]\Theta = 0$$

Setting $\mu \equiv \cos\theta$ yields

$$\frac{d}{d\mu}[(1-\mu^2)\frac{d\Theta}{d\mu}] + [\ell(\ell+1) - \frac{m^2}{1-\mu^2}]\Theta = 0$$

since

$$\begin{aligned}
\hat{O} &\equiv \frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} = (1-\mu^2)\frac{\partial^2}{\partial\mu^2} - 2\mu\frac{\partial}{\partial\mu} \\
&= \sin^2\theta[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta})] - 2\cos\theta(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}) \\
&= \frac{\partial^2}{\partial\theta^2} - \sin\theta\frac{\cos\theta}{\sin^2\theta}\frac{\partial}{\partial\theta} - 2\cos\theta(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}) \\
&= \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})
\end{aligned}$$

where we use

$$d\mu = -\sin\theta d\theta \quad \rightarrow \quad \frac{\partial}{\partial\mu} = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}$$

The differential equation obtained is known to be the *Associated Legendre Differential Equation.* Its solutions are *Associated Legendre Polynomials*,

$$P_{\ell m} = (-)^m(1-\mu^2)^{m/2}\frac{d^m P_\ell}{d\mu^m}$$

where P_ℓ is the Legendre polynomials

$$P_\ell(\mu) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{d\mu^\ell}(\mu^2-1)^\ell$$

which satisfies the Legendre differential equation,

$$\frac{d}{d\mu}[(1-\mu^2)\frac{dP_\ell}{d\mu}] + \ell(\ell+1)P_\ell = 0$$

The normalized $\Theta_{\ell m}$ becomes

$$\Theta_{\ell m}(\mu) = [\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}]^{1/2}P_{\ell m}(\mu)$$

The spherical harmonics is

$$Y_{\ell m}(\mu) = [\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}]^{1/2}P_{\ell m}(\cos\theta)e^{im\phi}$$

(b) Ladder Operator Method

In the ladder operator method, we have a condition

$$\begin{aligned}
\hat{L}_+ Y_{\ell\ell} &= \frac{1}{\sqrt{2\pi}}\hat{L}_+ e^{i\ell\phi}\Theta_{\ell\ell} \\
&= \frac{\hbar}{\sqrt{2\pi}}e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})e^{i\ell\phi}\Theta_{\ell\ell} \\
&= \frac{\hbar}{\sqrt{2\pi}}[e^{i(\ell+1)\phi}\frac{\partial\Theta_{\ell\ell}}{\partial\theta} + ie^{i\phi}\cot\theta(i\ell)e^{i\ell\phi}\Theta_{\ell\ell}] \\
&= \frac{\hbar}{\sqrt{2\pi}}e^{i(\ell+1)\phi}(\frac{\partial\Theta_{\ell\ell}}{\partial\theta} - \ell\cot\theta\Theta_{\ell\ell}) = 0
\end{aligned}$$

It yields

$$\frac{\partial\Theta_{\ell\ell}}{\partial\theta} = \ell\cot\theta\Theta_{\ell\ell}$$

Using a relation

$$\begin{aligned}
\ell\cot\theta &= \frac{\partial}{\partial\theta}\ln\sin^\ell\theta \\
\frac{1}{\Theta_{\ell\ell}}\frac{\partial\Theta_{\ell\ell}}{\partial\theta} &= \frac{\partial}{\partial\theta}\ln\Theta_{\ell\ell} = \frac{\partial}{\partial\theta}\ln\sin^\ell\theta \\
\Theta_{\ell\ell} &= A_{\ell\ell}\sin^\ell\theta
\end{aligned}$$

where $A_{\ell\ell}$ is the normalization constant.

$$Y_{\ell\ell} = \frac{A_{\ell\ell}}{\sqrt{2\pi}}\sin^\ell\theta e^{i\ell\phi}$$

Now operating $\hat{L}_-$ on $Y_{\ell\ell}$ generates $Y_{\ell\ell-1}$,

$$\begin{aligned}
Y_{\ell\ell-1} &= \hat{L}_- Y_{\ell\ell} = \hbar e^{-i\phi}(i\cot\theta\frac{\partial}{\partial\phi} - \frac{\partial}{\partial\theta})\frac{A_{\ell\ell}}{\sqrt{2\pi}}\sin^\ell\theta e^{i\ell\phi} \\
&= \frac{A_{\ell\ell}}{\sqrt{2\pi}}\hbar[i\cos\theta\sin^{\ell-1}(i\ell) - \ell\cos\theta\sin^{\ell-1}\theta]e^{i(\ell-1)\phi} \\
&= \frac{A_{\ell\ell-1}}{\sqrt{2\pi}}\sin^{\ell-1}\theta\cos\theta e^{i(\ell-1)\phi}
\end{aligned}$$

which agrees with the ones obtained in the direct method (a). In the similar fashion, $Y_{\ell\ell-2}$ can be generated.

$$\begin{aligned}
Y_{\ell\ell-2} &= \hat{L}_- Y_{\ell\ell-1} \\
&= \frac{A_{\ell\ell-2}}{\sqrt{2\pi}}e^{i(\ell-2)\phi}[(-\cot\theta)(\ell-1)\sin^{\ell-1}\theta\cos\theta - \sin^{\ell-2}\theta(\ell-1)\cos^2\theta + \sin^\ell\theta)] \\
&= \frac{A_{\ell\ell-2}}{\sqrt{2\pi}}e^{i(\ell-2)\phi}[-2(\ell-1)\sin^{\ell-2}\theta\cos^2\theta + \sin^\ell\theta)]
\end{aligned}$$

The normalized relations between $\hat{L}_+, \hat{L}_-$, and $\hat{L}_z$, and the states $|\ell, m>$ are

$$\begin{aligned}
\hat{L}_+|\ell m> &= \hbar[(\ell-m)(\ell+m+1)]^{1/2}|\ell, m+1> \\
\hat{L}_-|\ell m> &= \hbar[(\ell+m)(\ell-m+1)]^{1/2}|\ell, m-1> \\
\hat{L}_z|\ell m> &= \hbar m|\ell, m>
\end{aligned}$$

2.4.3 Orthonormality and parity of spherical harmonics

(a) Orthonormality of spherical harmonics

The spherical harmonics are orthonormal,

$$< Y_{\ell m} | Y_{\ell_1 m_1} >= \delta_{\ell \ell_1} \delta_{m m_1}.$$

(b) Parity of the Spherical Harmonics

The parity operator, $\hat{\mathcal{P}}$, in three dimensions is defined by the equation $\hat{\mathcal{P}} f(r, \theta, \phi) = f(r, \pi - \theta, \pi + \phi)$. Applying the parity operator $\hat{\mathcal{P}}$ on $Y_{\ell m}(\theta, \phi)$ gives

$$\begin{aligned} \hat{\mathcal{P}} Y_{\ell m} &= [\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}]^{1/2} P_{\ell m}(\cos(\pi - \theta)) e^{im(\phi+\pi)} \\ &= [\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}]^{1/2} (-)^{\ell+m} P_{\ell m}(\cos\theta) (-)^m e^{im\phi} \\ &= (-)^\ell Y_{\ell m}(\theta, \phi) \end{aligned}$$

2.4.4 Legendre polynomials

The first few Legendre Polynomials $P_\ell(\cos\theta)$

ℓ	P_ℓ
0	1
1	$\cos\theta$
2	$(3\cos^2\theta - 1)/2$
3	$(5\cos^3\theta - 3\cos\theta)/2$
4	$(35\cos^4\theta - 30\cos^2\theta + 3)/8$

The first few Associated Legendre Polynomials $P_{\ell m}(\theta)$

ℓ	m	$P_{\ell m}$
0	0	1
1	-1	$\sin\theta/2$
1	0	$\cos\theta$
1	1	$-\sin\theta$
2	-2	$\sin^2\theta/8$
2	-1	$\sin\theta\cos\theta/2$
2	0	$(3\cos^2\theta - 1)/2$
2	1	$-3\sin\theta\cos\theta$
2	2	$3\sin^2\theta$
3	-3	$\sin^3\theta/48$
3	-2	$\sin^2\theta\cos\theta/8$
3	-1	$\sin\theta(5\cos^2\theta - 1)/8$
3	0	$(5\cos^3\theta - 3\cos\theta)/2$
3	1	$-3\sin\theta(5\cos^2\theta - 1)/2$
3	2	$15\sin^2\theta\cos\theta$
3	3	$-15\sin^3\theta$

The first few Spherical Harmonics $Y_{\ell m}(\theta, \phi)$

ℓ	m	$Y_{\ell m}$
0	0	$1/\sqrt{4\pi}$
1	0	$\sqrt{3}\cos\theta/\sqrt{4\pi}$
1	±1	$\mp\sqrt{3/2}\sin\theta e^{\pm i\phi}/\sqrt{4\pi}$
2	0	$\sqrt{5}(3\cos^2\theta-1)/2\sqrt{4\pi}$
2	±1	$\mp\sqrt{5}\sqrt{6}\sin\theta\cos\theta e^{\pm i\phi}/2\sqrt{4\pi}$
2	±2	$\sqrt{5}\sqrt{3/2}\sin^2\theta e^{\pm i2\phi}/2\sqrt{4\pi}$
3	0	$2\sqrt{7}(5\cos^3\theta-3\cos\theta)/4\sqrt{4\pi}$
3	±1	$\mp\sqrt{7}\sqrt{3}\sin\theta(5\cos^2\theta-1)e^{\pm i\phi}/4\sqrt{4\pi}$
3	±2	$\sqrt{7}\sqrt{30}\sin^2\theta\cos\theta e^{\pm i2\phi}/4\sqrt{4\pi}$
3	±3	$\mp\sqrt{7}\sqrt{5}\sin^3\theta e^{\pm i3\phi}/4\sqrt{4\pi}$
4	0	$3(35\cos^4\theta-30\cos^2\theta+3)/8\sqrt{4\pi}$
4	±1	$\mp3\sqrt{20}\sin\theta(7\cos^3\theta-3\cos\theta)e^{\pm i\phi}/8\sqrt{4\pi}$
4	±2	$3\sqrt{10}\sin^2\theta(7\cos^2\theta-1)e^{\pm i2\phi}/8\sqrt{4\pi}$
4	±3	$\mp3\sqrt{140}\sin^3\theta\cos\theta e^{\pm i3\phi}/8\sqrt{4\pi}$
4	±4	$3\sqrt{35/2}\sin^4\theta e^{\pm i4\phi}/8\sqrt{4\pi}$

(a) Generating Function of the Legendre Polynomials

Employing the generating function of the Legendre polynomials

$$(1-2\mu s+s^2)^{-1/2}=\sum_{\ell=0}^{\infty}P_\ell(\mu)s^\ell$$

let us obtain $P_\ell(\mu)$ up to $\ell=2$.

The generating function is given as

$$\begin{aligned}
g(s) &= (1-2\mu s+s^2)^{-1/2}\\
g(s)|_{s=0} &= 1\\
g'(s)|_{s=0} &= -\frac{1}{2}(2s-2\mu)(1-2\mu s+s^2)^{-3/2}|_{s=0}\\
&= \mu\\
g''(s)|_{s=0} &= -(1-2\mu s+s^2)^{-3/2}+\frac{3}{4}[(2s-2\mu)^2](1-2\mu s+s^2)^{-5/2}|_{s=0}\\
&= 3\mu^2-1
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
P_0(\mu) &= g(s)|_{s=0}=1\\
P_1(\mu) &= g'(s)|_{s=0}=\mu\\
P_2(\mu) &= \frac{1}{2}g''(s)|_{s=0}=\frac{1}{2}(3\mu^2-1)
\end{aligned}$$

Next, we deduce the associated Legendre polynomials P_{2m} using the definition

$$\begin{aligned}
P_{\ell m}(\mu) &= (-1)^m(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_\ell(\mu)\\
P_{\ell 0} &= P_\ell\\
P_{\ell,-m}(\mu) &= (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_{\ell m}(\mu)
\end{aligned}$$

Thus, we obtain

$$\begin{aligned}
P_{2m}(\mu) &= (-1)^m(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_2(\mu) \\
P_{21}(\mu) &= (-1)(1-\mu^2)^{1/2}\frac{d}{d\mu}P_2(\mu) \\
&= -3(1-\mu^2)^{1/2}\mu = -3\sin\theta\cos\theta \\
P_{22}(\mu) &= (1-\mu^2)\frac{d^2}{d\mu^2}P_2(\mu) \\
&= (1-\mu^2)3\mu = 3\sin^2\theta \\
P_{\ell 0} &= P_\ell = \frac{1}{2}(3\mu^2-1) \\
P_{\ell,-m}(\mu) &= (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_{\ell m}(\mu), \\
P_{2,-1}(\mu) &= (-1)\frac{1}{2\cdot 3}(-3\sin\theta\cos\theta) \\
&= \frac{1}{2}\sin\theta\cos\theta \\
P_{2,-2}(\mu) &= \frac{1}{2\cdot 3\cdot 4}3\sin^2\theta \\
&= \frac{1}{8}\sin^2\theta
\end{aligned}$$

2.4.5 (Homework Set #1) Generation of spherical harmonics

1. Draw polar plots of $|Y_{\ell m}(\mu)|$ versus θ for $\ell = 0, 1, 2, 3$ and 4, and all accompanying m values in any plane through the z-axis by using the program "mainylm.f" (Appendix A).

$$|Y_{\ell m}(\mu)| = [\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}]^{1/2}|P_{\ell m}(\mu)|$$

Consult your figures with Figure 9.10 of Liboff.

2. Compare your numerical results with the analytic results given in the last table of in the previous subsection 2.4.4.

3. Discuss the validity of the program "mainylm.f"

3 A two-particle system under a central potential

Consider a two-particle system in which the momenta and masses of the particles are $(\mathbf{p}_1, m_1)$ and $(\mathbf{p}_2, m_2)$, respectively. The potential of interaction is a function of the radial distance between particles, called a central potential.

3.1 Hamiltonian

The transformation of two-particle system to the coordinates relative to the center of mass system can be written

$$(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2) \Rightarrow (\mathbf{r}, \mathbf{p}; \mathcal{R}, \mathcal{P})$$

where

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_2 - \mathbf{r}_1, & \mathcal{R} &= \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \\ \mathbf{r}_1 &= \mathcal{R} - \frac{m_2}{m_1 + m_2}\mathbf{r}, & \mathbf{r}_2 &= \mathcal{R} + \frac{m_1}{m_1 + m_2}\mathbf{r}, \end{aligned}$$

The momentum conservation gives

$$\mathcal{P} = \mathbf{p}_1 + \mathbf{p}_2$$

The relative momentum becomes

$$\begin{aligned} \mathbf{p} &= \mu\dot{\mathbf{r}} = \mu(\dot{\mathbf{r}}_2 - \dot{\mathbf{r}}_1) = \mu(\frac{\mathbf{p}_2}{m_2} - \frac{\mathbf{p}_1}{m_1}) \\ &= \frac{m_1}{m_1 + m_2}\mathbf{p}_2 - \frac{m_2}{m_1 + m_2}\mathbf{p}_1 \\ \mathbf{p}_1 &= -\mathbf{p} + \frac{m_1}{m_1 + m_2}\mathcal{P}, \qquad \mathbf{p}_2 = \mathbf{p} + \frac{m_2}{m_1 + m_2}\mathcal{P} \end{aligned}$$

where the reduced mass μ denotes

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

It is interesting to note that if we define the respective radii vectors relative to the center of mass as $\mathbf{r}'_1$ and $\mathbf{r}'_2$, they are related to $\mathbf{r}$ by

$$\mathbf{r}'_1 = -\frac{m_2}{m_1 + m_2}\mathbf{r}, \qquad \mathbf{r}'_2 = \frac{m_1}{m_1 + m_2}\mathbf{r}$$

Therefore, the fractional distance to the center of mass becomes

$$R = \frac{|\mathbf{r}'_2|}{|\mathbf{r}'_1|} = \frac{m_1}{m_2}$$

In case that the system is very asymmetric in masses ($m_1 \ll m_2$), like a hydrogen atom, R becomes

$$R \ll 1, \qquad \mu \approx m_1.$$

Now the Hamiltonian in the CM and relative coordinates may be written

$$\begin{aligned} H &= \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(|\mathbf{r_2} - \mathbf{r_1}|) = \frac{\mathcal{P}^2}{2M} + [\frac{\mathbf{p}^2}{2\mu} + V(r)] \\ &= H_{CM} + H_{rel} \end{aligned}$$

where we use the result of (II-1-2). Since $\mathcal{R}$ is cyclic in H_{CM}, the momentum of CM is constant. The CM point is at rest or moves uniformly.

3.2 Commutator relations and other relations

$$
\begin{aligned}
[\mathbf{p}_1, \mathbf{p}_2] &= 0 \\
[\mathbf{p}, \mathcal{P}] &= \frac{1}{m_1+m_2}[(m_1\mathbf{p}_2 - m_2\mathbf{p}_1), \mathbf{p}_1+\mathbf{p}_2] \\
&= \frac{m_1}{m_1+m_2}[\mathbf{p}_2, \mathbf{p}_1+\mathbf{p}_2] - \frac{m_2}{m_1+m_2}[\mathbf{p}_1, \mathbf{p}_1+\mathbf{p}_2] \\
&= \frac{m_1}{m_1+m_2}[\mathbf{p}_2, \mathbf{p}_1] - \frac{m_2}{m_1+m_2}[\mathbf{p}_1, \mathbf{p}_2] \\
&= 0 \\
[\hat{H}_{CM}, \hat{H}_{rel}] &= [\frac{\mathcal{P}^2}{2M}, \frac{\mathbf{p}^2}{2\mu} + V(r)] \\
&= [\frac{\mathcal{P}^2}{2M}, \frac{\mathbf{p}^2}{2\mu}] + [\frac{\mathcal{P}^2}{2M}, V(r)] = 0
\end{aligned}
$$

$$
\begin{aligned}
\frac{p^2}{2\mu} + \frac{\mathcal{P}^2}{2M} &= \frac{1}{2\mu}(\frac{m_1\mathbf{p}_2 - m_2\mathbf{p}_1}{m_1+m_2})^2 + \frac{1}{2M}(\mathbf{p}_1+\mathbf{p}_2)^2 \\
&= \frac{1}{2M}[\frac{(m_1\mathbf{p}_2 - m_2\mathbf{p}_1)^2 + m_1m_2(\mathbf{p}_1+\mathbf{p}_2)^2}{m_1m_2}] \\
&= \frac{1}{2M}[\frac{m_2M\mathbf{p}_1^2 + m_1M\mathbf{p}_2^2}{m_1m_2}] \\
&= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \\
\mu r^2 + M\mathcal{R}^2 &= \frac{m_1m_2}{M}(\mathbf{r}_2 - \mathbf{r}_1)^2 + M(\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M})^2 \\
&= \frac{1}{M}[m_1Mr_1^2 + m_2Mr_2^2] \\
&= m_1r_1^2 + m_2r_2^2
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{p}\cdot\mathbf{r} + \mathcal{P}\cdot\mathcal{R} &= (\frac{m_1\mathbf{p}_2 - m_2\mathbf{p}_1}{m_1+m_2})\cdot(\mathbf{r}_2 - \mathbf{r}_1) + (\mathbf{p}_1+\mathbf{p}_2)\cdot(\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1+m_2}) \\
&= \frac{1}{M}[(m_1+m_2)(\mathbf{p_1}\cdot\mathbf{r_1} + \mathbf{p_2}\cdot\mathbf{r_2}) + (m_2-m_2)\mathbf{p_1}\cdot\mathbf{r_2} + (m_1-m_1)\mathbf{p_2}\cdot\mathbf{r_1} \\
&= \mathbf{p_1}\cdot\mathbf{r_1} + \mathbf{p_2}\cdot\mathbf{r_2}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{L} + \mathbf{L}_{CM} &= \mathbf{r}\times\mathbf{p} + \mathcal{R}\times\mathcal{P} \\
&= (\mathbf{r}_2 - \mathbf{r}_1)\times(\frac{m_1\mathbf{p}_2 - m_2\mathbf{p}_1}{m_1+m_2}) + (\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1+m_2})\times(\mathbf{p}_1+\mathbf{p}_2) \\
&= \frac{1}{M}[(m_1+m_2)(\mathbf{r_1}\times\mathbf{p_1} + \mathbf{r_2}\times\mathbf{p_2}) + (m_1-m_1)\mathbf{r_1}\times\mathbf{p_2} + (m_2-m_2)\mathbf{r_2}\times\mathbf{p_1} \\
&= \mathbf{r_1}\times\mathbf{p_1} + \mathbf{r_2}\times\mathbf{p_2} \\
&= \mathbf{L_1} + \mathbf{L_2}
\end{aligned}
$$

3.3 Reduction to the equivalent one-body problem

The Hamiltonian of the system becomes

$$\begin{aligned}\hat{H}_{total} &= \hat{H}_{rel} + \hat{H}_{CM} \\ &= [\frac{\hat{p}^2}{2\mu} + V(r)] + [\frac{\hat{\boldsymbol{\mathcal{P}}}^2}{2M}]\end{aligned}$$

Since $\hat{H}_{rel}$ and $\hat{H}_{CM}$ are independent of one another, the total eigenfunctions and eigenvalues can be written, respectively,

$$\begin{aligned}\Psi_{total} &= \psi_{CM}(\mathcal{R})\varphi_{rel}(\mathbf{r}), \\ E_{total} &= E_{CM} + E_{rel}\end{aligned}$$

For the CM coordinates, the ψ_{CM} is just a free particle plane wave function with mass M,

$$\begin{aligned}\psi_{CM}(\mathcal{R}) &= A\exp(i\mathbf{K}\cdot\mathcal{R}), \\ E_{CM} &= \frac{\hbar^2 K^2}{2M}, \qquad \mathcal{P} = \hbar\mathbf{K}\end{aligned}$$

Thus the problem becomes now a one-body problem with mass μ in the relative coordinates.

(a) Differential equation in relative coordinates

TISE for φ_{rel} appears as, neglecting the subscript "rel",

$$\hat{H}\varphi = [\frac{\hat{p}^2}{2\mu} + V(r)]\varphi = [\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{\mathbf{L}}^2}{2\mu r^2} + V(r)]\varphi = E\varphi$$

We now set

$$\varphi(r,\theta,\phi) = R(r)Y_{\ell m}(\theta,\phi)$$

Then $R(r)$ satisfies

$$[\frac{\hat{p}_r^2}{2\mu} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)]R(r) = ER(r)$$

$$[-\frac{\hbar^2}{2\mu}(\frac{1}{r}\frac{d^2}{dr^2}r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)]R(r) = ER(r)$$

This is an ordinary, second-order, linear differential equation for $R(r)$. Furthermore, if we set

$$R(r) \equiv \frac{u(r)}{r}$$

then, $u(r)$ satisfies

$$[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)]u(r) = Eu(r)$$

This is the same Schrödinger equation as would be obtained for a fictitious one-dimensional problem in which a particle of mass μ moves in the effective potential

$$V_{eff}(r) = V(r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}$$

Note that r must be $r \geq 0$. Thus the whole problem can be said to reduce to the equivalent one-dimensional problem in the positive r-axis.

The second term in V_{eff}, called the angular momentum barrier, becomes infinitely large as $r \to 0$ and acts like a repulsive core, which for $\ell > 0$ prevents collapse of the system. There exists a turning point for a given E and inside the barrier where $E < V$, the classically forbidden region, the radial probability density $|rR(r)|^2 = |u(r)|^2$ becomes small. Because of analytic property of wavefunctions, $u(r)$ should be continuous at the turning point.

(b) General properties of solutions of $R(r)$ (or $u(r)$)

Let us examine the behavior of the solutions $R(r)$ (or $u(r)$) of the radial equation at the origin. We shall assume that as r approaches zero, the potential $V(r)$ remains finite, or at least goes infinity less rapidly than $1/r$. We consider a solution which behaves at the origin like r^s;

$$R(r) \sim Ar^s, \quad \text{as} \quad r \to 0$$

Plugging into the TISE for $R(r)$, and considering only the dominant term give

$$-s(s+1) + \ell(\ell+1) = 0 \quad \Rightarrow \quad s = \ell \text{ or } -(\ell+1)$$

The $1/r^{\ell+1}$ will be rejected because of infinity behavior, and thus $R(r) \sim Ar^\ell$ or $u(r) \sim Ar^{\ell+1}$ will be the only acceptable solution which goes to zero at the origin for all ℓ. This is valid for the free particle. (See Problem XII.11.) Consequently, we should have $u(0) = 0$.

The normalization of the wavefunctions is given by

$$< RY_{\ell m}|RY_{\ell m} >= \int_0^\infty r^2|R(r)|^2 dr = \int_0^\infty |u(r)|^2 dr = 1$$

The eigenfunctions of the Hamiltonian H depend on at least three indices, (k, ℓ, m); $\varphi_{k,\ell m}(r, \theta, \phi) = R_{k,\ell}(r)Y_{\ell m}(\theta, \phi)$ is a simultaneous eigenfunction of H, L^2, and L_z with respective eigenvalues $E_{k,\ell}, \hbar^2\ell(\ell+1)$, and $\hbar m$ where ℓ is called the azimuthal quantum number, and m, the magnetic quantum number. The radial part $R_{k,\ell}(r) = u_{k,\ell}(r)/r$ of the eigenfunction and the eigenvalue $E_{k,\ell}$ are independent of the magnetic quantum number. The angular part of the eigenfunction depends only on ℓ and m and not on k. This leads that the level $E_{k,\ell}$ is at least $(2\ell+1)$-fold degenerate. It is due to the fact that the Hamiltonian contains L^2 but not L_z, and m varies from $-\ell$ to $+\ell$ for a given ℓ.

(c) Total eigenfunctions and eigenvalues

$$\begin{aligned} \Psi_{total} &= Ae^{i\mathcal{P}\cdot\mathcal{R}/\hbar}\, R_{k,\ell}(r)Y_{\ell m}(\theta,\phi) \\ E_{total} &= E_{CM} + E_{rel} \\ &= \frac{\mathcal{P}^2}{2M} + \frac{p^2}{2\mu} = \frac{\hbar^2K^2}{2M} + \frac{\hbar^2k^2}{2\mu} \\ &\equiv \hbar\Omega + \hbar\omega \end{aligned}$$

The time-dependent wavefunctions are

$$\begin{aligned} \Psi_{total}(t) &= Ae^{i\mathcal{P}\cdot\mathcal{R}/\hbar}e^{i\Omega t} \\ &\qquad R_{k,\ell}(r)Y_{\ell m}(\theta,\phi)e^{i\omega t} \end{aligned}$$

3.4 Quantities commuting with angular momentum

We show that $\hat{p}^2, \hat{r}^2$, $\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}$, and any isotropic function $f(r^2)$ commute with every component of $\hat{\mathbf{L}}$.

If the statement is true for arbitrary unit vector $\hat{\mathbf{e}}$, it is true for all components of $\hat{\mathbf{L}}$. Then using the results of Section 2.3.4 gives

$$\begin{aligned} [\hat{p}^2, \mathbf{e}\cdot\hat{\mathbf{L}}] &= \hat{\mathbf{p}}\cdot[\hat{\mathbf{p}}, \mathbf{e}\cdot\hat{\mathbf{L}}] + [\hat{\mathbf{p}}, \mathbf{e}\cdot\hat{\mathbf{L}}]\cdot\hat{\mathbf{p}} \\ &= i\hbar(\hat{\mathbf{p}}\cdot\mathbf{e}\times\hat{\mathbf{p}} + \mathbf{e}\times\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}) = 0 \end{aligned}$$

Remember that the triple product with the same two vectors always vanishes.

$$\begin{aligned}
[\hat{r}^2, \mathbf{e}\cdot\hat{\mathbf{L}}] &= \hat{\mathbf{r}}\cdot[\hat{\mathbf{r}}, \mathbf{e}\cdot\hat{\mathbf{L}}] + [\hat{\mathbf{r}}, \mathbf{e}\cdot\hat{\mathbf{L}}]\cdot\hat{\mathbf{r}} \\
&= i\hbar(\hat{\mathbf{r}}\cdot\mathbf{e}\times\hat{\mathbf{r}} + \mathbf{e}\times\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}) = 0 \\
[\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}, \mathbf{e}\cdot\hat{\mathbf{L}}] &= \hat{\mathbf{r}}\cdot[\hat{\mathbf{p}}, \mathbf{e}\cdot\hat{\mathbf{L}}] + [\hat{\mathbf{r}}, \mathbf{e}\cdot\hat{\mathbf{L}}]\cdot\hat{\mathbf{p}} \\
&= i\hbar(\hat{\mathbf{r}}\cdot\mathbf{e}\times\hat{\mathbf{p}} + \mathbf{e}\times\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}) \\
&= i\hbar(-\mathbf{e}\cdot\hat{\mathbf{r}}\times\hat{\mathbf{p}} + \mathbf{e}\cdot\hat{\mathbf{r}}\times\hat{\mathbf{p}}) = 0
\end{aligned}$$

The rotation operator $\hat{R}_{\delta\phi}$ has no effect on any isotropic function $f(r^2)$.

$$\hat{R}_{\delta\phi} f(r^2) = f(r^2) \quad \Rightarrow \quad \frac{i\delta\phi\cdot\hat{\mathbf{L}}}{\hbar} f(r^2) = 0$$

since $\hat{R}_{\delta\phi} = (1 + i\delta\phi\cdot\hat{\mathbf{L}}/\hbar)$. This statement is true for all direction of the vector $\delta\phi$. We set $\delta\phi = \mathbf{e}$. It follows that any isotropic function is a null eigenstate of any component of angular momentum,

$$\mathbf{e}\cdot\hat{\mathbf{L}} f(r^2) = 0$$

If $g(\mathbf{r})$ is any function of $\mathbf{r}$, owing to the conclusion above,

$$\begin{aligned}
\mathbf{e}\cdot\hat{\mathbf{L}} f(r^2) g(\mathbf{r}) &= \{\mathbf{e}\cdot\hat{\mathbf{L}} f(r^2)\}\ g(\mathbf{r}) + f(r^2)\ \{\mathbf{e}\cdot\hat{\mathbf{L}} g(\mathbf{r})\} \\
&= f(r^2)\mathbf{e}\cdot\hat{\mathbf{L}} g(\mathbf{r})
\end{aligned}$$

$$\mathbf{e}\cdot\hat{\mathbf{L}} f(r^2) g(\mathbf{r}) - f(r^2)\mathbf{e}\cdot\hat{\mathbf{L}} g(\mathbf{r}) = [\mathbf{e}\cdot\hat{\mathbf{L}}, f(r^2)] g(\mathbf{r}) = 0$$

It follows that every component of $\hat{\mathbf{L}}$ commutes with any isotropic function $f(r^2)$.

3.5 Conservation of the total angular momentum

We show that the total angular momentum of the two-particle system under a central potential, $\mathbf{L_1} + \mathbf{L_2} = \mathbf{L} + \mathbf{L}_{CM}$, is conserved.

The Hamiltonian of the system in the coordinates relative to the center of mass may be written

$$\begin{aligned}
\hat{H}_{total} &= \hat{H}_{rel} + \hat{H}_{CM} \\
&= [\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + V(r)] + [\frac{\hat{\mathcal{P}_{\mathcal{R}}}^2}{2M} + \frac{\hat{L}_{CM}^2}{2M\mathcal{R}^2}]
\end{aligned}$$

Utilizing the fact that the CM and relative coordinates are independent of one another, and results of the previous subsection give

$$\begin{aligned}
[\hat{H}_{total}, \mathbf{L} + \mathbf{L}_{CM}] &= [\hat{H}, \mathbf{L}] + [\hat{H}_{CM}, \mathbf{L}_{CM}] \\
&= [(\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + V(r)), \mathbf{L}] \\
&\quad + [\frac{\hat{\mathcal{P}_{\mathcal{R}}}^2}{2M} + \frac{\hat{L}_{CM}^2}{2M\mathcal{R}^2}, \mathbf{L}_{CM}] \\
&= 0
\end{aligned}$$

It implies that the total angular momentum is quantum mechanically conserved.

4 Bound states - Shell model wave functions

4.1 Definition of the bound state

The bound state is defined as follows:

If a wave function φ represents a bound state, then

$$|\varphi| \to 0, \quad \text{as} \quad |x| \to \infty$$

for all t. Thus

$$\int_{-\infty}^{\infty} |\varphi|^2 dx < \infty, \qquad \text{(Square Integrable)}$$

(a) Arbitrary Phase Factor

Postulate III says that φ gives information about a system through

$$< C >= \int \varphi^* \hat{C} \varphi d\vec{r},$$

and normalization

$$1 = \int \varphi^* \varphi d\vec{r}.$$

They are invariant under the transformation $\varphi \to e^{i\alpha}\varphi$, where α is any real number!!

(b) Real function

Since the spectrum is non-degenerate, the bound states can be taken to be real by a suitable choice of phase factors.

(c) Expectation values of the linear momentum

$$< \hat{p} >= \frac{\hbar}{i} \int_{-\infty}^{\infty} \varphi^* \frac{\partial}{\partial x} \varphi = 0$$

since the integrand is real and $< \hat{p} >$ has to be real.

(d) Equality

The equality

$$\int_{-\infty}^{\infty} \varphi^* \varphi_{xx} dx \quad = \quad - \int_{-\infty}^{\infty} |\varphi_x|^2 dx$$

holds for the bound states, since

$$\int_{-\infty}^{\infty} \varphi^* \varphi_{xx} dx \quad = \quad [\varphi^* \varphi_x]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \varphi_x^* \varphi_x dx = - \int_{-\infty}^{\infty} |\varphi_x|^2 dx$$

where we use $\varphi^*(-\infty) = \varphi^*(\infty) = 0$.

4.2 Non-degeneracy of bound states

The Schrödinger radial equation may be written

$$[\hat{D}^2 - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2}(E-V)]u = 0$$

where $\hat{D} \equiv \frac{d}{dr}$ and $u = rR$. Let solutions to the preceding equation be written u_1 and u_2. Multiplying the equation for u_2 by u_1 and vice versa and subtracting the resulting equations gives

$$u_1\hat{D}^2u_2 - u_2\hat{D}^2u_1 = 0$$

or, equivalently,

$$\hat{D}[u_1\hat{D}u_2 - u_2\hat{D}u_1] = 0$$

Integrating both sides yields,

$$u_1\hat{D}u_2 - u_2\hat{D}u_1 = C$$

where C is a constant. For bound systems one may assume that either $u_1,\ u_2 \to 0$ or $\hat{D}u_1,\ \hat{D}u_2 \to 0$ as $r \to \infty$, which, in either case, gives $C = 0$. There results

$$\frac{d\ln u_2}{dr} = \frac{d\ln u_1}{dr} \quad \Rightarrow \quad u_2 = au_1$$

where a is a constant. Thus, u_1 and u_2 are not independent. It follows that the second-order differential radial equation for bound states has only one linearly independent solution for given ℓ and E values.

4.3 Deuteron in the spherical well

A more realistic estimate for the deuteron problem may be obtained using a three-dimensional spherical well with characteristics

$$V(r) = \begin{cases} -|V|, & r < a \quad \text{region I,} \\ 0, & r \geq a \quad \text{region II} \end{cases}$$

The range of nuclear force is approximately 2.3 fm, while the binding energy is 2.23 MeV. We may estimate the depth of the potential well.

We may write the eigenfunctions

$$\varphi(r,\theta,\phi) = R(r)Y_{\ell m}(\theta,\phi)$$

The ground state should not feel any repulsive angular momentum barrier, that is, $(\ell m) = (0,0)$, and thus

$$\varphi_g(r,\theta,\phi) = \frac{1}{\sqrt{4\pi}}R(r)$$

The radial component wavefunctions in the well domain, region I, are the spherical Bessel functions. The ground-state component is therefore

$$R_I(r) = Aj_0(kr) = A\frac{\sin kr}{kr}, \quad \text{or} \quad u_I(r) = A\sin kr$$

In region II the radial component ground state wavefunction is exponentially damped.

$$R_{II}(r) = B\frac{e^{-\kappa r}}{\kappa r}, \quad \text{or} \quad u_{II}(r) = Be^{-\kappa r}$$

Matching conditions of $u(r)$ at $r = a$ give

$$A\sin ka = Be^{-\kappa a}, \qquad Ak\cos ka = -B\kappa e^{-\kappa a}$$

We divide the two equations by each other and obtain the so-called the dispersion relation,

$$k\cot ka = -\kappa, \quad \text{or} \quad \eta = -\xi\cot\xi$$

where $\xi \equiv ka, \;\; \eta \equiv \kappa a$. We further have

$$\begin{aligned} \rho^2 &\equiv \frac{2\mu|V|a^2}{\hbar^2} = \frac{2\mu a^2}{\hbar^2}(\frac{\hbar^2\kappa^2}{2\mu} + \frac{\hbar^2k^2}{2\mu}) = \xi^2 + \eta^2 \\ |E| &= \frac{\hbar^2\kappa^2}{2\mu}, \quad |V| - |E| = \frac{\hbar^2k^2}{2\mu} \end{aligned}$$

where μ is the reduced mass of proton and neutron,

$$\mu = \frac{M_pM_n}{M_p + M_n} = \frac{938.8 \times 939.6}{938.8 + 939.6} = 469.6 \text{ MeV}/c^2$$

Thus we obtain

$$\begin{aligned} \rho^2 &= \frac{2\mu a^2|V|}{\hbar^2} = \frac{2 \times 469.6 \times (2.3)^2}{197.3^2}|V| = 0.128|V| \\ E_g &= \frac{\eta^2}{\rho^2}|V| = \frac{\eta^2}{0.128} = 2.23 \\ \eta &= 0.534 \end{aligned}$$

We also get

$$\begin{aligned} \xi\cot\xi = -\eta = -0.534 \quad &\Rightarrow \quad \xi = 1.852 \\ \xi^2 + \eta^2 = \rho^2 \quad &\Rightarrow \quad \rho^2 = 3.716 \end{aligned}$$

Finally, we obtain

$$|V| = \frac{\rho^2}{0.128} = \frac{3.716}{0.128} = 29.0 \text{ MeV}$$

Note that $\rho = 1.928$ is less than π, and there is only one bound state.

4.4 Spin-orbit interaction

4.4.1 Total angular momentum:

The total angular momentum, **J**, is defined as

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$$

for given values of the orbital angular momentum $\hat{L}$ and the spin $\hat{S}$.

(a) We first show that the four operators

$$\{\hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z\}$$

form a commuting set of observables. This representation is akin to the "uncoupled" representation.

Since $(\hat{L}, \hat{L}_z)$ and $(\hat{S}, \hat{S}_z)$ are independent

$$[\hat{L}^2, \hat{S}^2] = [\hat{L}^2, \hat{S}_z] = [\hat{L}_z, \hat{S}^2] = [\hat{L}_z, \hat{S}_z] = 0$$

The angular momentum commutation relations give

$$[\hat{L}^2, \hat{L}_z] = [\hat{S}^2, \hat{S}_z] = 0$$

Thus $\{\hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z\}$ form a commuting set of observables.

(b) We next show that the four operators

$$\{\hat{J}^2, \hat{J}_z, \hat{L}^2, \hat{S}^2\}$$

also form a commuting set of observables, called the $L - S$ representation or *Russell-Saunders* coupling scheme which compares to the "coupled" representation.

The total angular momentum, its components and its square can be written as

$$\begin{aligned}
\hat{\mathbf{J}} &= \hat{\mathbf{L}} + \hat{\mathbf{S}} \\
\hat{J}_x &= \hat{L}_x + \hat{S}_x \\
\hat{J}_y &= \hat{L}_y + \hat{S}_y \\
\hat{J}_z &= \hat{L}_z + \hat{S}_z \\
\hat{J}^2 &= \hat{L}^2 + \hat{S}^2 + 2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}
\end{aligned}$$

We thus have

$$\begin{aligned}
[\hat{J}^2, \hat{L}^2] &= [\hat{L}^2 + \hat{S}^2 + 2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}, \hat{L}^2] = 0 \\
[\hat{J}^2, \hat{S}^2] &= [\hat{L}^2 + \hat{S}^2 + 2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}, \hat{S}^2] = 0 \\
[\hat{J}^2, \hat{J}_z] &= 0 \\
[\hat{L}^2, \hat{J}_z] &= [\hat{L}^2, \hat{L}_x + \hat{S}_z] = 0 \\
[\hat{S}^2, \hat{J}_z] &= [\hat{S}^2, \hat{L}_x + \hat{S}_z] = 0 \\
[\hat{L}^2, \hat{S}^2] &= 0
\end{aligned}$$

Thus $\{\hat{J}^2, \hat{J}_z, \hat{L}^2, \hat{S}^2\}$ form a commuting set of observables. We note that $\hat{L}_z$ and $\hat{S}_z$ are not compatible with $\hat{J}^2$.

4.4.2 Non-compatibility between $\hat{J}^2$ and $\hat{L}_z$ ($\hat{S}_z$):

We show that
(a) $[\hat{J}^2, \hat{L}_z] = 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{L}} \times \hat{\mathbf{S}})$
(b) $[\hat{J}^2, \hat{S}_z] = 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{S}} \times \hat{\mathbf{L}})$

(a) Ignoring hats,

$$\begin{aligned}
[J^2, L_z] &= [L^2 + S^2 + 2\mathbf{L}\cdot\mathbf{S}, L_z] \\
&= 2[\mathbf{L}\cdot\mathbf{S}, \hat{L}_z] = 2[L_xS_x + L_yS_y + L_zS_z, \hat{L}_z] \\
&= 2i\hbar\ (-L_yS_x + L_xS_y) = 2i\hbar\ (\hat{\mathbf{L}} \times \hat{\mathbf{S}})_z \\
&= 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{L}} \times \hat{\mathbf{S}})
\end{aligned}$$

(b)

$$\begin{aligned}
[J^2, S_z] &= [L^2 + S^2 + 2\mathbf{L}\cdot\mathbf{S}, S_z] \\
&= 2[\mathbf{L}\cdot\mathbf{S}, \hat{S}_z] = 2[L_xS_x + L_yS_y + L_zS_z, \hat{S}_z] \\
&= 2i\hbar\ (-L_xS_y + L_yS_x) = 2i\hbar\ (\hat{\mathbf{S}} \times \hat{\mathbf{L}})_z \\
&= 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{S}} \times \hat{\mathbf{L}})
\end{aligned}$$

4.4.3 Conserved quantities under the spin-orbit interaction:

The total Hamiltonian with spin-orbit coupling can be written as

$$\begin{aligned}
\hat{H} &= \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V_0 f(r) + f_{SO}(r)\mathbf{L}\cdot\mathbf{S} \\
&= \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V_0 f(r) + f_{SO}(r)\frac{1}{2}[\hat{J}^2 - \hat{L}^2 - \hat{S}^2]
\end{aligned}$$

where $\mathbf{J} = \mathbf{L} + \mathbf{S}$. We show that $\mathbf{J}$ is conserved, but $\mathbf{L}$ and $\mathbf{S}$ are not.

All terms in the Hamiltonian commute with $\mathbf{J}$ as just seen, and thus $\mathbf{J}$ is conserved. However, we have, as seen in the previous subsection,

$$[\hat{J}^2, \hat{L}_z] = 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{L}} \times \hat{\mathbf{S}}), \quad [\hat{J}^2, \hat{S}_z] = 2i\hbar\ \mathbf{e_z} \cdot (\hat{\mathbf{S}} \times \hat{\mathbf{L}})$$

and thus the Hamiltonian does NOT commute with $\hat{L}_z$ and $\hat{S}_z$, and it follows that $\mathbf{L}$ and $\mathbf{S}$ are not conserved.

4.5 (Homework Set #2) Nuclear shell model - Generation of bound state wave functions

In the central field approximation it is assumed that each nucleon sees only the nuclear field generated by nucleons themselves and that this field is spherically symmetric, say,

$$V_j(r) \;=\; -V_0 f(r) + V_C(r) + \bar{\lambda}^2 \frac{V_{SO}}{r}(\vec{\sigma}\cdot\vec{\ell})\frac{df(r)}{dr}$$

where $\bar{\lambda} = \frac{\hbar}{m_\pi c}$ is the Compton wavelength of π-meson and $f(r)$ is of the Woods-Saxon form

$$f(r) \;=\; \frac{1}{1+\exp(\frac{r-R}{a})}$$

and V_C is the Coulomb potential. The quantum numbers of the state and corresponding wave-functions become, respectively,

$$\begin{aligned} \text{Quantum numbers} \;&:\; n, \ell, m_\ell, m_s \\ \varphi_{n\ell m_\ell m_s}(\mathbf{r}_i, \mathbf{S}_i) \;&=\; R_{n\ell}(r_i) Y_{\ell m_\ell}(\theta_i, \phi_i)\xi_z^{\pm}(i) \\ \xi_z^{\pm}(i) \;&=\; \alpha(i),\ \text{or}\ \beta(i) \end{aligned}$$

In the jj-coupling scheme,

$$\begin{aligned} \text{Quantum numbers} \;&:\; n, j, \ell, m_j \\ \varphi_{nj\ell m_j}(\mathbf{r}_i, \mathbf{S}_i) \;&=\; R_{n\ell}(r_i)[Y_{\ell m_\ell}(\theta_i, \phi_i)\xi_z^{\pm}(i)]_{jm_j} \end{aligned}$$

We can have a level structure similar to the atomic level structure. Furthermore, since

$$< jm_j|(\vec{\sigma}\cdot\vec{\ell})|jm_j > \;=\; \begin{cases} \ell & ;\ j = \ell + \frac{1}{2} \\ -(\ell+1) & ;\ j = \ell - \frac{1}{2} \end{cases}$$

the spin-orbit force is effectively repulsive for $j = \ell + \frac{1}{2}$, while attractive for $j = \ell - \frac{1}{2}$. Thus the level with the higher j value is lower for a given ℓ. An approximate level pattern for protons is given Fig. II-1.

1. Obtain the experimentally determined positions of the 3 single particles and 3 single hole states built on the ^{208}Pb core, relative to the ground states of ^{209}Bi, ^{207}Tl, ^{209}Pb and ^{207}Pb.

2. It is claimed that a Woods-Saxon potential with parameters V_0= 50.9 MeV, V_{SO} = 5.8 MeV, $r_0 = r_{SO}$ = 1.19 fm, and $a_0 = a_{SO}$ = 0.75 fm gives a pretty good description of the states of ^{209}Pb. Verify this using the program NEPTUNE (Appendix B).

3. Discuss behavior of wave functions obtained in the tail region, say around $R = 7 - 8$ fm.

4. Use the same potential to see how it works for the hole states of ^{207}Pb.

5. Use a potential of the same geometry, but input the experimental separation energies and search on the potential depth to get a good description of the single-proton ^{209}Bi states. What is the difference $V_p - V_n$ between this potential and the one of part(3)? If $V_p - V_n = 2V_1(N-Z)/A$, what value do you get for V_1?

5 Unbound states

5.1 General properties of unbound states

The unbound state is defined as follows:

Not obeys

$$|\psi| \to 0 \quad \text{as} \quad |x| \to \infty$$

but satisfies

$$\int_a^b |\psi|^2 dx < \infty \qquad |b-a| < \infty$$

Example: Scattering state, Momentum operator eigenstate. ($\varphi_k = \frac{1}{\sqrt{2\pi}} e^{ikx}$).

$\odot$ Normalization of Scattering State

Normalization in terms of the particle density ρ.

$$\begin{aligned} |\psi|^2 dx = \rho dx \quad &= dN \qquad && \text{(No. of particles in } dx\text{)} \\ \int_a^b |\psi|^2 dx &= N && \text{(No. of particles in } (b-a)\text{)} \end{aligned}$$

Example: 1-D beam of ρ particles/cm with $p = \hbar k_0$. The wavefunction would be

$$\psi = \sqrt{\rho} e^{i(k_0 x - \omega t)}$$

With definite momentum, $\Delta p = 0$. Because of uniform beam, $|\psi|^2 =$ const, $\Delta x = \infty$ (Uniformly probable). Thus the system satisfies the Uncertainty Relation.

5.2 Current density

The current density of particles moving in 1-D would be $\vec{j} = (J_x, 0, 0)$. The continuity equation becomes

$$\frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} = 0$$

From TDSE,

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\psi, \qquad \frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar}\hat{H}\psi^*$$

$$\begin{aligned} \frac{\partial}{\partial t}(\psi^*\psi) &= \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} = \psi^*(-\frac{i}{\hbar}\hat{H}\psi) + \psi(\frac{i}{\hbar}\hat{H}\psi^*) \\ &= \psi^*(\frac{i\hbar}{2m}\psi_{xx} - \frac{i}{\hbar}V\psi) + \psi(\frac{-i\hbar}{2m}\psi^*_{xx} + \frac{i}{\hbar}V\psi^*) \\ &= \frac{i\hbar}{2m}(\psi^*\psi_{xx} - \psi\psi^*_{xx}) \\ &= -\frac{\partial}{\partial x}[\frac{\hbar}{2mi}(\psi^*\psi_x - \psi\psi^*_x)] \\ \frac{\partial}{\partial t}(\psi^*\psi) &+ \frac{\partial}{\partial x}[\frac{\hbar}{2mi}(\psi^*\psi_x - \psi\psi^*_x)] = 0 \end{aligned}$$

Thus we obtain

$$\rho = \psi\psi^*, \quad J_x = \frac{\hbar}{2mi}(\psi^*\psi_x - \psi\psi_x^*) \qquad (\#/s)$$

For the the 3-D wavefunctions,

$$\begin{aligned} \rho = \psi\psi^*, \quad \vec{j} &= \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) \qquad (\#/m^2 s) \\ &= \frac{1}{2m}(\psi^*\hat{\vec{p}}\psi - \psi\hat{\vec{p}}\psi^*) \\ &= \frac{1}{2m}[\psi^*\hat{\vec{p}}\psi - (\psi^*\hat{\vec{p}}\psi)^*] \end{aligned}$$

where $\hat{\vec{p}}$ is the momentum operator and we use

$$(\psi^*\hat{\vec{p}}\psi)^* = \psi(\hat{\vec{p}})^*\psi^* = \psi\hat{\vec{p}}\psi^*$$

For a wave packet $\psi(x,t)$, the flux becomes

$$\int_{-\infty}^{\infty} J_x dx = \frac{< p >}{m}$$

since

$$J_x = \frac{1}{2m}[\psi^*\hat{p}_x\psi - (\psi^*\hat{p}_x\psi)^*]$$

Integrating over the whole x-axis yields

$$\begin{aligned} \int_{-\infty}^{\infty} J_x dx &= \int_{-\infty}^{\infty} \frac{1}{2m}[\psi^*\hat{p}_x\psi - (\psi^*\hat{p}_x\psi)^*]dx \\ &= \frac{1}{2m}(< \hat{p}_x > + < \hat{p}_x >^*) \\ &= \frac{< \hat{p}_x >}{m} =< v_x > \end{aligned}$$

5.3 Complex potential

Let a complex potential be

$$V(x) = V_r(x) + iV_c(x)$$

The TDSE becomes

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\psi, \qquad \frac{\partial\psi^*}{\partial t} = \frac{i}{\hbar}\hat{H}^*\psi^*$$

$$\begin{aligned} \frac{\partial}{\partial t}(\psi^*\psi) &= \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t} = \psi^*(-\frac{i}{\hbar}\hat{H}\psi) + \psi(\frac{i}{\hbar}\hat{H}\psi^*) \\ &= \psi^*(\frac{i\hbar}{2m}\psi_{xx} - \frac{i}{\hbar}(V_r + iV_c)\psi) \ + \ \psi(\frac{-i\hbar}{2m}\psi_{xx}^* + \frac{i}{\hbar}(V_r - iV_c)\psi^*) \\ &= \frac{i\hbar}{2m}(\psi^*\psi_{xx} - \psi\psi_{xx}^*) + \frac{2V_c}{\hbar}\psi\psi^* \end{aligned}$$

Finally,

$$\frac{\partial}{\partial t}(\psi^*\psi) + \frac{\partial}{\partial x}[\frac{\hbar}{2mi}(\psi^*\psi_x - \psi\psi_x^*)] = \frac{2V_c}{\hbar}\psi\psi^*$$

Using $\rho = \psi\psi^*, J_x = \frac{\hbar}{2mi}(\psi^*\psi_x - \psi\psi_x^*)$, we have

$$\frac{\partial\rho}{\partial t} + \frac{\partial J_x}{\partial x} = \frac{2V_c}{\hbar}\rho$$

It obviously contradicts the continuity equation because of the source term $2V_c\rho/\hbar$.

5.4 Free particle wave functions - Spherical Bessel functions

5.4.1 Radial wavefunction for a free particle - Spherical Bessel functions

Let us study the radial wavefunction and total wavefunction for a free particle in spherical coordinates. TISE becomes

$$\hat{H}\varphi_{k,\ell m} = (\frac{\hat{p}_r^2}{2m} + \frac{\hat{\mathbf{L}}^2}{2mr^2})\varphi_{k,\ell m} = E_{k,\ell m}\varphi_{k,\ell m}$$

We set

$$\varphi_{k,\ell m}(r,\theta,\phi) = R_{k\ell}(r)Y_{\ell m}(\theta,\phi)$$

Then $R_{k\ell}(r)$ satisfies

$$[-(\frac{1}{r}\frac{d^2}{dr^2}r) + \frac{\ell(\ell+1)}{r^2}]R_{k\ell}(r) = \frac{2mE}{\hbar^2}R_{k\ell}(r) = k^2R_{k\ell}(r)$$
$$\frac{d^2}{dx^2}R_\ell(x) + \frac{2}{x}\frac{dR_\ell(x)}{dx} + [1 - \frac{\ell(\ell+1)}{x^2}]R_\ell(x) = 0$$

where we set $x \equiv kr$. This equation is nothing but the *Spherical Bessel Differential Equation*, whose solutions are known as the regular spherical Bessel function, $j_\ell(r)$, ($j_\ell(r=0) = 0$), and the irregular spherical Neumann function, $n_\ell(r)$, ($n_\ell(0) = \infty$). The first few values of these functions are

ℓ	$j_\ell(r)$	$n_\ell(r)$
0	$\frac{\sin x}{x}$,	$-\frac{\cos x}{x}$
1	$\frac{\sin x}{x^2} - \frac{\cos x}{x}$,	$-\frac{\cos x}{x^2} - \frac{\sin x}{x}$
2	$(\frac{3}{x^3} - \frac{1}{x})\sin x - \frac{3}{x^2}\cos x$,	$-(\frac{3}{x^3} - \frac{1}{x})\cos x - \frac{3}{x^2}\sin x$
...		
n	$(-)^n x^n(\frac{d}{xdx})^n(\frac{\sin x}{x})$,	$-(-)^n x^n(\frac{d}{xdx})^n(\frac{\cos x}{x})$
...		

Finally we have the eigenstates and eigenenergies of the free particle Hamiltonian in spherical coordinates are

$$\varphi_{k\ell m}(r,\theta,\phi) = j_\ell(kr)Y_{\ell m}(\theta,\phi)$$
$$E_k = \frac{\hbar^2k^2}{2m}$$

The orthonormality is given as

$$\begin{aligned} <\ell mk|\ell_0 m_0 k_0> &= \int_{4\pi} d\Omega Y^*_{\ell m}Y_{\ell_0 m_0}\int_0^\infty j_\ell(kr)j_{\ell_0}(k_0 r)r^2dr \\ &= \delta_{\ell\ell_0}\delta_{mm_0}\int_0^\infty j_\ell(kr)j_\ell(k_0 r)r^2dr \\ &= \delta_{\ell\ell_0}\delta_{mm_0}\frac{\pi}{2k^2}\delta(k-k_0) \end{aligned}$$

The coordinate representations of the ket vector $|\ell mk>$ and $|\mathbf{k}>$ are given by

$$\begin{aligned} <r\theta\phi|\ell mk> &= j_\ell(kr)Y_{\ell m}(\theta,\phi) \\ <\mathbf{r}|\mathbf{k}> &= \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}} \end{aligned}$$

5.4.2 Generating function of the spherical Bessel functions

The generating functions for spherical Bessel and Neumann functions are given as,

$$\begin{aligned}\frac{1}{x}\cos\sqrt{x^2-2xs} &= \sum_{\ell=0}^{\infty}\frac{s^\ell}{\ell!}j_{\ell-1}(x)\\ \frac{1}{x}\sin\sqrt{x^2+2xs} &= \sum_{\ell=0}^{\infty}\frac{(-s)^\ell}{\ell!}n_{\ell-1}(x)\end{aligned}$$

From these generating functions, we can obtain $j_\ell(\ell=-1,0,1,...)$

$$\begin{aligned}g(s) &= \frac{1}{x}\cos\sqrt{x^2-2xs}\\ g(s)|_{s=0} &= \frac{1}{x}\cos x = j_{-1}(x) = -n_0(x)\\ g'(s)|_{s=0} &= -\frac{1}{x}\sin\sqrt{x^2-2xs}\frac{-2x}{2\sqrt{x^2-2xs}}|_{s=0}\\ &= \frac{1}{x}\sin x = j_0(x)\\ g''(s)|_{s=0} &= \sin\sqrt{x^2-2xs}\frac{2x}{2(\sqrt{x^2-2xs})^3}|_{s=0}+\cos\sqrt{x^2-2xs}\frac{-2x}{2(\sqrt{x^2-2xs})^2}|_{s=0}\\ &= \frac{\sin x}{x^2}-\frac{\cos x}{x} = j_1(x)\end{aligned}$$

and $n_\ell(\ell=-1,0,1,...)$

$$\begin{aligned}g(s) &= \frac{1}{x}\sin\sqrt{x^2+2xs}\\ g(s)|_{s=0} &= \frac{1}{x}\sin x = n_{-1}(x) = j_0(x)\\ g'(s)|_{s=0} &= \frac{1}{x}\cos\sqrt{x^2+2xs}\frac{2x}{2\sqrt{x^2+2xs}}|_{s=0}\\ &= \frac{1}{x}\cos x = -n_0(x)\\ g''(s)|_{s=0} &= \cos\sqrt{x^2+2xs}\frac{-2x}{2(\sqrt{x^2+2xs})^3}|_{s=0}-\sin\sqrt{x^2+2xs}\frac{2x}{2(\sqrt{x^2+2xs})^2}|_{s=0}\\ &= -\frac{\cos x}{x^2}-\frac{\sin x}{x} = n_1(x)\end{aligned}$$

5.4.3 Asymptotic values of the spherical Bessel functions

We establish the following properties of the spherical Bessel functions,

$$\begin{aligned}x\to 0 \qquad & j_\ell(x)\sim\frac{x^\ell}{(2\ell+1)!!},\\ x\to\infty \qquad & j_\ell(x)\sim\frac{1}{x}\sin(x-\ell\frac{\pi}{2})\end{aligned}$$

In order to obtain the behavior at the origin we first expand $\sin x/x$ in a power series in x,

$$\frac{\sin x}{x} = \sum_{n=0}^{\infty}(-)^n\frac{x^{2n}}{(2n+1)!}$$

and then apply the operator $(\frac{d}{xdx})^\ell$, which yields

$$\begin{aligned} j_\ell(x) &= (-)^\ell x^\ell (\frac{d}{xdx})^{\ell-1} \sum_{n=0}^{\infty} (-)^n \frac{2n x^{2n-1-1}}{(2n+1)!} \\ &= (-)^\ell x^\ell \sum_{n=0}^{\infty} (-)^n \frac{x^{2n-2\ell}}{(2n+1)!} 2n(2n-2)(2n-4)...[2n-2(\ell-1)] \end{aligned}$$

The first ℓ terms of the sum ($n = 0$ to $\ell - 1$) are zero, and the $(\ell+1)$th is written

$$\begin{aligned} j_\ell(x) &\sim (-)^\ell x^\ell (-)^\ell \frac{2\ell(2\ell-2)(2\ell-4)...2}{(2\ell+1)!} \\ &\sim \frac{x^\ell}{(2\ell+1)!!} \end{aligned}$$

Note that the eigenstates of the free particle Hamiltonian is proportional to r^ℓ in the neighborhood of the origin

$$\varphi_{k\ell m}(r,\theta,\phi) \sim \sqrt{\frac{2k^2}{\pi}} Y_{\ell m}(\theta,\phi) \frac{(kr)^\ell}{(2\ell+1)!!}$$

For the asymptotic behavior as $x \to \infty$, we again apply the operator $(\frac{d}{xdx})^\ell$ on $\sin x/x$ and then write $j_\ell(x)$ in the form,

$$j_\ell(x) = (-)^\ell x^\ell (\frac{d}{xdx})^{\ell-1} [\frac{\cos x}{x^2} - \frac{\sin x}{x^3}]$$

The second term inside the bracket is negligible compared to the first term when x approaches infinity. Moreover, when we apply $(\frac{d}{xdx})$ a second time, the dominant term still comes from the derivative of the cosine. Thus we see that

$$j_\ell(x) \sim (-)^\ell x^\ell \frac{1}{x^\ell} \frac{1}{x} (\frac{d}{dx})^\ell \sin x$$

Since we have

$$\begin{aligned} (\frac{d}{dx})^\ell \sin x &= (-)^\ell \sin(x - \ell\frac{\pi}{2}) \\ x \to \infty, \qquad j_\ell(x) &\sim \frac{1}{x} \sin(x - \ell\frac{\pi}{2}) \end{aligned}$$

5.4.4 (Homework Set #3) Generation of spherical Bessel functions

1. Generate the spherical Bessel functions ($\ell = 0, 1, 2, 3, 4$) for the free moving 10 MeV proton in the presence of ^{208}Pb (Neglect the Coulomb force.) by using the Program "MAINJL" (Appendix C).

2. Verify the asymptotic behaviors discussed in Section III-6.

3. Discuss the validity of the program "mainjl.f"

5.5 The Plane wave expansion in spherical harmonics

We prove that the expansion of a plane wave in spherical harmonics,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} j_{\ell}(kr)[Y_{\ell m}(\alpha,\beta)]^* Y_{\ell m}(\theta,\phi)$$

where (r,θ,ϕ) and (k,α,β) are the spherical coordinates of $\mathbf{r}$ and $\mathbf{k}$, respectively.

We here first assume that the vector $\mathbf{k}$ chosen is collinear with z-axis, i.e., $\mathbf{k} = k\hat{k}$. We then want to expand the function

$$e^{ikz} = e^{ikr\cos\theta}$$

Since this function is independent of the angle ϕ, it is a linear combination of only those basis functions with $m = 0$, $Y_{\ell 0}(\theta)$.

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} a_{\ell} j_{\ell}(kr) Y_{\ell 0}(\theta)$$

The coefficients $a_\ell j_\ell(kr)$ can be expressed as, by using the ladder operators ($\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$),

$$\begin{aligned} a_{\ell} j_{\ell}(kr) &= \int d\Omega Y_{\ell 0}^*(\theta) e^{ikr\cos\theta} \\ &= \frac{1}{\sqrt{(2\ell)!}} \int d\Omega [(\frac{\hat{L}_-}{\hbar})^{\ell} Y_{\ell\ell}(\theta,\phi)]^* e^{ikr\cos\theta} \\ &= \frac{1}{\sqrt{(2\ell)!}} \int d\Omega Y_{\ell\ell}^*(\theta,\phi) [(\frac{\hat{L}_+}{\hbar})^{\ell} e^{ikr\cos\theta}] \end{aligned}$$

since $\hat{L}_+$ is the adjoint operator of $\hat{L}_-$. We now have

$$\begin{aligned} (\frac{\hat{L}_+}{\hbar})^{\ell} e^{ikr\cos\theta} &= (-)^{\ell} e^{i\ell\phi} (\sin\theta)^{\ell} \frac{d^{\ell}}{d(\cos\theta)^{\ell}} e^{ikr\cos\theta} \\ &= (-)^{\ell} e^{i\ell\phi} (\sin\theta)^{\ell} (ikr)^{\ell} e^{ikr\cos\theta} \end{aligned}$$

Using the normalized $Y_{\ell\ell}$ gives

$$\begin{aligned} Y_{\ell\ell} &= \frac{(-)^{\ell}}{2^{\ell}\ell!} \sqrt{\frac{(2\ell+1)!}{4\pi}} \sin^{\ell}\theta e^{i\ell\phi} \\ a_{\ell} j_{\ell}(kr) &= \frac{2^{\ell}\ell!}{\sqrt{(2\ell)!}} \sqrt{\frac{4\pi}{(2\ell+1)!}} (ikr)^{\ell} \\ &\qquad \int d\Omega |Y_{\ell\ell}(\theta,\phi)|^2 e^{ikr\cos\theta} \end{aligned}$$

In order to evaluate a_ℓ, it is sufficient to choose a particular value of kr, for which we know the value of $j_\ell(kr)$, for example, kr to approach zero. We thus obtain

$$\begin{aligned} a_{\ell} \frac{1}{(2\ell+1)!!} &= \frac{2^{\ell}\ell!}{\sqrt{(2\ell)!}} \sqrt{\frac{4\pi}{(2\ell+1)!}} i^{\ell} \int d\Omega |Y_{\ell\ell}(\theta,\phi)|^2 \\ a_{\ell} &= i^{\ell} \sqrt{4\pi(2\ell+1)} \end{aligned}$$

since $Y_{\ell\ell}$ is normalized to 1. We have

$$\begin{aligned} e^{ikr\cos\theta} &= \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)} j_\ell(kr) Y_{\ell 0}(\theta) \\ &= \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta) \end{aligned}$$

We now utilize the addition theorem for spherical harmonics for $P_\ell(\cos\theta)$,

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} [Y_{\ell m}(\alpha,\beta)]^* Y_{\ell m}(\theta,\phi)$$

where γ is the angle between two vectors. [See C. Cohen-Tannoudji, B. Diu, and F. Laloë, "Quantum Mechanics", 1977, Complement A_{VI} γ, for the proof.] where θ is the angle between $\mathbf{k}$ and $\mathbf{r}$. We finally obtain the expansion of a plane wave in spherical harmonics,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr) [Y_{\ell m}(\alpha,\beta)]^* Y_{\ell m}(\theta,\phi)$$

5.6 Coulomb wave function

5.6.1 Radial wave function in the Coulomb field

The Schrödinger equation for the Coulomb field can be written as

$$[-\frac{\hbar^2}{2\mu}(\frac{1}{r}\frac{d^2}{dr^2}r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + \frac{Z_1 Z_2 e^2}{r}] R_\ell(r) = E R_\ell(r)$$

The two charges are $Z_1 e$ and $Z_2 e$, μ is the reduced mass of the system in amu, and E is the center-of-mass energy in MeV. We now set

$$R_\ell(r) \equiv \frac{u_\ell(r)}{r}$$

then, $u(r)$ satisfies

$$[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + \frac{Z_1 Z_2 e^2}{r}] u_\ell(r) = E u_\ell(r)$$

We further define

$$\begin{aligned} \rho &\equiv kr = \frac{\sqrt{2\mu E}}{\hbar} r = 0.218741\sqrt{\mu E} r, \quad k \text{ is in fm}^{-1} \\ \eta &\equiv \frac{\mu Z_1 Z_2 e^2}{\hbar^2 k} = \frac{Z_1 Z_2 e^2}{\hbar v} = 0.157483 Z_1 Z_2 \sqrt{\mu/E} \end{aligned}$$

where k is the wave number. Then, the second order differential equation becomes

$$\frac{d^2 u_\ell(\rho)}{d\rho^2} + [1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}] u_\ell(\rho) = 0$$

The regular, $F_\ell(\eta,\rho)$, and irregular, $G_\ell(\eta,\rho)$, solutions of the above equation can be found in the most of the quantum mechanics books, *e.g.*, Merzbacher, Chap 11-8, and Schiff, Chap. 5-21. These functions have boundary conditions

$$\begin{aligned} F_\ell(\eta,0) &= 0, \quad F_\ell(\eta,\infty) \longrightarrow \sin\theta_\ell \\ G_\ell(\eta,0) &= \infty, \quad G_\ell(\eta,\infty) \longrightarrow \cos\theta_\ell \\ \theta_\ell &= \rho - \eta \ln(2\rho) - \frac{1}{2}\ell\pi + \sigma_\ell \\ \sigma_\ell &= \arg\Gamma(\ell+1+i\eta) \end{aligned}$$

where σ_ℓ is the Coulomb phase shift.

The solutions for successive ℓ values are connected by the following recurrence relations, with $u_\ell = F_\ell$ or G_ℓ.

$$\begin{aligned} R_\ell u_{\ell-1} &= \frac{d}{d\rho}u_\ell + S_\ell u_\ell \\ \frac{d}{d\rho}u_{\ell-1} &= S_\ell u_{\ell-1} - R_\ell u_\ell \\ R_{\ell+1}u_{\ell+1} &= T_\ell u_\ell - R_\ell u_{\ell-1} \end{aligned}$$

where the coefficients are given for $\ell \geq 1$ by

$$\begin{aligned} R_\ell &= \frac{\sqrt{\ell^2+\eta^2}}{\ell}, \qquad S_\ell = \frac{\ell}{\rho} + \frac{\eta}{\ell} \\ T_\ell &= \frac{(2\ell+1)[\ell(\ell+1)/\rho + \eta]}{\ell(\ell+1)} \end{aligned}$$

Further necessary relations are the Wronskian

$$\begin{aligned} W &= F'_\ell G_\ell - F_\ell G'_\ell = 1 \\ W_\ell &= F_\ell G_{\ell+1} - F_{\ell+1} G_\ell = 1/R_{\ell+1} \end{aligned}$$

5.6.2 (Homework Set #4) Generation of Coulomb wave functions

In 1974, the Manchester group (A. R. Barnett, D. H. Feng, J. W. Steed and L. J. B. Goldfarb, "Coulomb wave functions for all real η and ρ", Comp. Phys. Comm. **8** (1974) 377-395.) made a program for the Coulomb wave functions by using the continued fraction method, called here FLGLCH.

This subroutine is applicable for all values of

$$\rho \geq \rho_T = \eta + \sqrt{\eta + [\eta^2 + \ell(\ell+1)]},$$

where ρ_T is the corresponding ρ to the turning point, without restriction. A somewhat modified method is used for values of $\rho < \rho_T$, but not useful $\rho < 0.2\rho_T$.

1. Generate the Coulomb wave functions ($\ell = 0, 1, 2, 3, 4$) for the 10 MeV proton in the presence of ^{208}Pb by using the Program "MAINFLGL" (Appendix D).

2. Verify the asymptotic behaviors discussed in Section III-9.

3. Discuss the validity of the program "mainflgl.f"

4. Take a partial wave, say $\ell = 1$, compare $krj_\ell(kr)$ with $F(kr)$ at a region around 20fm and discuss the Coulomb phase shift.

6 Addition of angular momenta

6.1 Uncoupled representation of the two-component system

Consider two systems that are rotating about a common origin independently. Each system has two good angular momentum quantum numbers, say $(j_1 m_1)$ and $(j_2 m_2)$. We prove that a set of eigenvalues $(j_1 m_1 j_2 m_2)$ are good quantum numbers in the uncoupled representation.

We first show that the set of four operators $(\hat{J}_1^2, \hat{J}_{1z}, \hat{J}_2^2, \hat{J}_{2z})$ are a set of completely, mutually commutating operators so that their eigenvalues may be simultaneously specified in a eigenstate $|j_1 m_1 j_2 m_2>$, that is,

$$\begin{aligned} [J_1^2, J_{1z}] &= [J_2^2, J_{2z}] = 0 \\ [J_1^2, J_2^2] &= [J_1^2, J_{2z}] = [J_{1z}, J_2^2] = [J_{1z}, J_{2z}] = 0 \end{aligned}$$

The former equations are from the definition of angular momentum eigenstates, while the latter ones from the fact that the coordinates 1 and 2 are independent each other. The eigenvalue equations can be written

$$\begin{pmatrix} \hat{J}_1^2 \\ \hat{J}_{1z} \\ \hat{J}_2^2 \\ \hat{J}_{2z} \end{pmatrix} |j_1 m_1 j_2 m_2> = \begin{pmatrix} j_1(j_1+1)\hbar^2 \\ m_1\hbar \\ j_2(j_2+1)\hbar^2 \\ m_2\hbar \end{pmatrix} |j_1 m_1 j_2 m_2>$$

Note that there are $(2j_1+1)(2j_2+1)$ linearly independent eigenstates for a given $(j_1 j_2)$ set.

6.2 Coupled representation of the two-component system

Consider two systems that are rotating about a common origin independently. Each system has two good angular momentum quantum numbers, say $(j_1 m_1)$ and $(j_2 m_2)$. Let $\hat{\mathbf{J}}_1$ and $\hat{\mathbf{J}}_2$ be the respective angular momentum operators. The total system has angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$ and its z-component $\hat{\mathbf{J}}_z = \hat{\mathbf{J}}_{1z} + \hat{\mathbf{J}}_{2z}$ of which quantum numbers are j and m, respectively. We prove that a set of eigenvalues $(j m j_1 j_2)$ are good quantum numbers in the coupled representation.

We first show that

$$\begin{aligned} \hat{J}^2 &= (\hat{J}_1 + \hat{J}_2)^2 = \hat{J}_1^2 + \hat{J}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2 \\ [\hat{J}^2, \hat{J}_z] &= [\hat{J}_1^2 + \hat{J}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2, \hat{J}_{1z} + \hat{J}_{2z}] \\ &= 2[\hat{J}_{1x}\hat{J}_{2x} + \hat{J}_{1y}\hat{J}_{2y} + \hat{J}_{1z}\hat{J}_{2z}, \hat{J}_{1z}] + 2[\hat{J}_{1x}\hat{J}_{2x} + \hat{J}_{1y}\hat{J}_{2y} + \hat{J}_{1z}\hat{J}_{2z}, \hat{J}_{2z}] \\ &= 2\hbar(-\hat{J}_{1y}\hat{J}_{2x} + \hat{J}_{1x}\hat{J}_{2y} - \hat{J}_{1x}\hat{J}_{2y} + \hat{J}_{1y}\hat{J}_{2x}) \\ &= 0 \\ [\hat{J}^2, \hat{J}_1^2] &= [\hat{J}_1^2 + \hat{J}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2, \hat{J}_1^2] \\ &= 2[\hat{\mathbf{J}}_1, \hat{J}_1^2] \cdot \hat{\mathbf{J}}_2 = 0 \\ [\hat{J}^2, \hat{J}_2^2] &= 0 \end{aligned}$$

$$\begin{aligned} [\hat{J}_z, \hat{J}_1^2] &= [\hat{J}_{1z} + \hat{J}_{2z}, \hat{J}_1^2] = [\hat{J}_{1z}, \hat{J}_1^2] = 0 \\ [\hat{J}_z, \hat{J}_2^2] &= [\hat{J}_{1z} + \hat{J}_{2z}, \hat{J}_2^2] = [\hat{J}_{2z}, \hat{J}_2^2] = 0 \\ [\hat{J}_1^2, \hat{J}_2^2] &= = 0 \end{aligned}$$

The set of four operators $(\hat{J}^2, \hat{J}_z, \hat{J}_1^2, \hat{J}_2^2)$ are a set of completely commutating operators so that their eigenvalues may be simultaneously specified in an eigenstate $|j m j_1 j_2>$ in the coupled

representation. The eigenvalue equations can be written

$$\begin{pmatrix} \hat{J}^2 \\ \hat{J}_z \\ \hat{J}_1^2 \\ \hat{J}_2^2 \end{pmatrix} |jmj_1j_2> = \begin{pmatrix} j(j+1)\hbar^2 \\ m\hbar \\ j_1(j_1+1)\hbar^2 \\ j_2(j_2+1)\hbar^2 \end{pmatrix} |jmj_1j_2>$$

There are $(2j_1+1)(2j_2+1)$ linearly independent eigenstates in the uncoupled representation. A change into the coupled representation should maintain the dimensionality of the space. It gives a limitation of values of j. Since $J_z = J_{1z} + J_{2z}$, the maximum value m can have is

$$m_{max} = m_{1_{max}} + m_{2_{max}}, \quad \Rightarrow \quad m_{max} = j_1 + j_2$$

It is clear that the maximum value of j is equal to m_{max}.

$$j_{max} = j_1 + j_2$$

We now obtain j_{min} such that the total number of states are $(2j_1+1)(2j_2+1)$. The number of independent eigenstates with a given j is $2j+1$. Thus the value of j_{min} we seek satisfies the equation

$$\sum_{j=j_{min}}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1)$$

It gives $j_{min} = |j_1 - j_2|$. It is then easy to prove the sum, if we set $j = j_1 - j_2 + i$, (assume $j_1 \geq j_2$)

$$\begin{aligned} \sum_{j=j_1-j_2}^{j_1+j_2} 2j+1 &= \sum_{i=0}^{2j_2} [2(j_1 - j_2 + i) + 1] \\ &= [2(j_1 - j_2) + 1](2j_2 + 1) + 2\frac{2j_2(2j_2+1)}{2} \\ &= (2j_1+1)(2j_2+1) \end{aligned}$$

We thus find that the possible values of j are

$$j = |j_1 - j_2|, |j_1 - j_2| + 1, ..., j_1 + j_2 - 1, j_1 + j_2$$

For example, for $j_1 = 5$, and $j_2 = 2$, the possible values of j and the number of states in the uncoupled representation (N_u), and in the coupled representation (N_c) are

$$\begin{aligned} j &= 3, 4, 5, 6, 7 \\ N_u &= (2 \times 5 + 1) \times (2 \times 2 + 1) = 55 \\ N_c &= 7 + 9 + 11 + 13 + 15 = 55 \end{aligned}$$

6.3 Clebsch-Gordan coefficients

The eigenstates in the coupled representation can be expanded in terms of the eigenstates in the uncoupled representation, that is,

$$\begin{aligned} |jmj_1j_2> &= \sum_{m_1}\sum_{m_2} |j_1m_1j_2m_2>< j_1m_1j_2m_2|jmj_1j_2> \\ &\equiv \sum_{m_1}\sum_{m_2} C_{m_1m_2}|j_1m_1j_2m_2> \\ C_{m_1m_2} &\equiv < j_1m_1j_2m_2|jmj_1j_2> \\ &\equiv < j_1m_1j_2m_2|jm> \quad \text{(short-hand)} \end{aligned}$$

where $m = m_1 + m_2$, and $C_{m_1m_2}$ is called the Clebsch-Gordan (C-G) coefficients. The square of the C-G coefficient is the probability that at fixed J and J_z measurement finds one particle with $J_{1z} = m_1\hbar$ and the other $J_{2z} = m_2\hbar$.

Example 1. Two electrons in s-orbit ($j_1 = j_2 = 1/2$)

There are 4 independent states in both representations.
In the uncoupled representation ($|j_1m_1j_2m_2>$),

$$\psi_1 = |\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}>, \quad \psi_2 = |\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}>, \quad \psi_3 = |\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}>, \quad \psi_4 = |\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{-1}{2}>$$

In the coupled representation ($|jmj_1j_2>$),

$$\varphi_1 = |11\frac{1}{2}\frac{1}{2}>, \quad \varphi_2 = |10\frac{1}{2}\frac{1}{2}>, \quad \varphi_3 = |1,-1\frac{1}{2}\frac{1}{2}>, \quad \varphi_4 = |00\frac{1}{2}\frac{1}{2}>$$

We expand coupled states in terms of uncoupled states

$$\begin{aligned} \varphi_1 &= C^{(1)}_{1/2,1/2}\psi_1 + C^{(1)}_{1/2,-1/2}\psi_2 + C^{(1)}_{-1/2,1/2}\psi_3 + C^{(1)}_{-1/2,-1/2}\psi_4 \\ \varphi_2 &= C^{(2)}_{1/2,1/2}\psi_1 + C^{(2)}_{1/2,-1/2}\psi_2 + C^{(2)}_{-1/2,1/2}\psi_3 + C^{(2)}_{-1/2,-1/2}\psi_4 \\ \varphi_3 &= C^{(3)}_{1/2,1/2}\psi_1 + C^{(3)}_{1/2,-1/2}\psi_2 + C^{(3)}_{-1/2,1/2}\psi_3 + C^{(3)}_{-1/2,-1/2}\psi_4 \\ \varphi_4 &= C^{(4)}_{1/2,1/2}\psi_1 + C^{(4)}_{1/2,-1/2}\psi_2 + C^{(4)}_{-1/2,1/2}\psi_3 + C^{(4)}_{-1/2,-1/2}\psi_4 \end{aligned}$$

Applying a condition $m = m_1 + m_2$ gives

$$\begin{aligned} 1 = m_1 + m_2 \;\Rightarrow\quad & C^{(1)}_{1/2,-1/2} = 0,\ C^{(1)}_{-1/2,1/2} = 0,\ C^{(1)}_{-1/2,-1/2} = 0, \\ 0 = m_1 + m_2 \;\Rightarrow\quad & C^{(2)}_{1/2,1/2} = 0,\ C^{(2)}_{-1/2,-1/2} = 0, \\ -1 = m_1 + m_2 \Rightarrow\quad & C^{(3)}_{1/2,1/2} = 0,\ C^{(3)}_{1/2,-1/2} = 0,\ C^{(3)}_{-1/2,1/2} = 0 \\ 0 = m_1 + m_2 \;\Rightarrow\quad & C^{(4)}_{1/2,1/2} = 0,\ C^{(4)}_{-1/2,-1/2} = 0, \end{aligned}$$

Thus the expansions simply become

$$\begin{aligned} \varphi_1 &= C^{(1)}_{1/2,1/2}\psi_1 \\ \varphi_2 &= C^{(2)}_{1/2,-1/2}\psi_2 + C^{(2)}_{-1/2,1/2}\psi_3 \\ \varphi_3 &= C^{(3)}_{-1/2,-1/2}\psi_4 \\ \varphi_4 &= C^{(4)}_{1/2,-1/2}\psi_2 + C^{(4)}_{-1/2,1/2}\psi_3 \end{aligned}$$

The normalization of φ's gives

$$\begin{aligned} C^{(1)}_{1/2,1/2} &= <\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}|11>=1 \\ C^{(3)}_{-1/2,-1/2} &= <\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{-1}{2}|1,-1>=1 \end{aligned}$$

$$(C^{(2)}_{1/2,-1/2})^2+(C^{(2)}_{-1/2,1/2})^2=1, \quad (C^{(4)}_{1/2,-1/2})^2+(C^{(4)}_{-1/2,1/2})^2=1$$

To obtain $C^{(2)}_{1/2,-1/2}$ and $C^{(2)}_{-1/2,1/2}$, we use the ladder operator

$$\hat{J}_- = \hat{J}_{1-}+\hat{J}_{2-}$$

and operate this operator on

$$\varphi_1 = \psi_1 \text{ or } |11>=|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}> .$$

By using relations

$$\begin{aligned} \hat{L}_+|\ell m> &= \hbar[(\ell-m)(\ell+m+1)]^{1/2}|\ell,m+1> \\ \hat{L}_-|\ell m> &= \hbar[(\ell+m)(\ell-m+1)]^{1/2}|\ell,m-1> \end{aligned}$$

we have

$$\begin{aligned} \hat{J}_-|11>&=\sqrt{2}\hbar|10> \\ \hat{J}_-|\frac{1}{2}\frac{1}{2}>&=\hbar|\frac{1}{2}\frac{-1}{2}> \end{aligned}$$

that is,

$$\begin{aligned} \sqrt{2}\hbar|10> &= \hbar(|\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}>+|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}>) \\ \varphi_2 &= \frac{1}{\sqrt{2}}(\psi_2+\psi_3) \end{aligned}$$

We thus obtain

$$\begin{aligned} C^{(2)}_{1/2,-1/2} &= <\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}|10>=\frac{1}{\sqrt{2}} \\ C^{(2)}_{-1/2,1/2} &= <\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}|10>=\frac{1}{\sqrt{2}} \end{aligned}$$

Now we evaluate $C^{(4)}_{1/2,-1/2}$ and $C^{(4)}_{-1/2,1/2}$. The φ_4 with the total $J=0$ is the antisymmetric state under the exchange of two particles, while φ_1, φ_2 and φ_3 with the total $J=1$ are the symmetric states. Thus

$$\begin{aligned} \varphi_4 &= \frac{1}{\sqrt{2}}(\psi_2-\psi_3) \\ &= C^{(4)}_{1/2,-1/2}\psi_2+C^{(4)}_{-1/2,1/2}\psi_3 \end{aligned}$$

It gives

$$\begin{aligned} C^{(4)}_{1/2,-1/2} &= <\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}|00>=\frac{1}{\sqrt{2}} \\ C^{(4)}_{-1/2,1/2} &= <\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}|00>=-\frac{1}{\sqrt{2}} \end{aligned}$$

We summarize the C-G coefficients for the coupling of $j_1 \times j_2 = \frac{1}{2} \times \frac{1}{2}$

$\|jm>$	$\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}>$	$\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}>$	$\|\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}>$	$\|\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{-1}{2}>$
$\|11>$	1	0	0	0
$\|10>$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0
$\|1,-1>$	0	0	0	1
$\|00>$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0

In fact, there is a closed general formula to obtain the C-G coefficients (See the next subsection and D. M. Brink and C. R. Satchler, "Angular Momentum", 1968, Oxford). One can also find the values of C-G coefficients in the books related to the angular momentum. (For example, D. A. Varshalovich *et al.*, "Quantum Theory of Angular Momentum", 1988, World Scientific).

The coupled states can thus be written in terms of the uncoupled states for this system

$$\begin{aligned}
|11> &= |\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}> \\
|10> &= \frac{1}{\sqrt{2}}(|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}> + |\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}>) \\
|1,-1> &= |\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{-1}{2}> \\
|00> &= \frac{1}{\sqrt{2}}(|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{-1}{2}> - |\frac{1}{2}\frac{-1}{2}\frac{1}{2}\frac{1}{2}>)
\end{aligned}$$

Note that they are orthonormal. For example,

$$\begin{aligned}
<10|10> &= (\frac{1}{\sqrt{2}})^2 + (\frac{\sqrt{1}}{\sqrt{2}})^2 = 1 \\
<00|00> &= (\frac{1}{\sqrt{2}})^2 + (\frac{-1}{\sqrt{2}})^2 = 1 \\
<10|00> &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} + \frac{\sqrt{1}}{\sqrt{2}}\frac{-1}{\sqrt{2}} = 0
\end{aligned}$$

Example 2. Two electrons (neglecting spin) in p-orbit ($j_1 = j_2 = 1$)

There are 9 independent states in both representations. In the uncoupled representation ($|j_1 m_1 j_2 m_2>$),

$$\begin{aligned}
\psi_1 = |1111>, \quad \psi_2 = |1110>, \quad \psi_3 = |111,-1>, \\
\psi_4 = |1011>, \quad \psi_5 = |1010>, \quad \psi_6 = |101,-1>, \\
\psi_7 = |1,-111>, \quad \psi_8 = |1,-110>, \quad \psi_9 = |1,-11,-1>,
\end{aligned}$$

In the coupled representation ($|jmj_1 j_2>$),

$$\begin{aligned}
&\varphi_1 = |2211>, \quad \varphi_2 = |2111>, \quad \varphi_3 = 2011>, \\
&\varphi_4 = |2,-111>, \quad \varphi_5 = |2,-211>, \\
&\varphi_6 = |1111>, \quad \varphi_7 = |1011>, \quad \varphi_8 = |1,-111>, \\
&\varphi_9 = |0011>,
\end{aligned}$$

The C-G coefficients are

	ψ_1	ψ_2	ψ_3	ψ_4	ψ_5	ψ_6	ψ_7	ψ_8	ψ_9
φ_1	1	0	0	0	0	0	0	0	0
φ_2	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	0
φ_3	0	0	$\frac{1}{\sqrt{6}}$	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	$\frac{1}{\sqrt{6}}$	0	0
φ_4	0	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
φ_5	0	0	0	0	0	0	0	0	1
φ_6	0	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	0
φ_7	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0
φ_8	0	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
φ_9	0	0	$\frac{1}{\sqrt{3}}$	0	$-\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0

The coupled states (in $|jm>\equiv|jmj_1j_2>$ notation) can thus be written in terms of the uncoupled states for this system

$$
\begin{aligned}
|22> &= |1111> \\
|21> &= \frac{1}{\sqrt{2}}|1110> + \frac{1}{\sqrt{2}}|1011> \\
|20> &= \frac{1}{\sqrt{6}}|111,-1> + \frac{\sqrt{2}}{\sqrt{3}}|1010> + \frac{1}{\sqrt{6}}|1,-111> \\
|2,-1> &= \frac{1}{\sqrt{2}}|101,-1> + \frac{1}{\sqrt{2}}|1,-110> \\
|2,-2> &= |1,-11,-1> \\
|11> &= \frac{1}{\sqrt{2}}|1110> - \frac{1}{\sqrt{2}}|1011> \\
|10> &= \frac{1}{\sqrt{2}}|111,-1> - \frac{1}{\sqrt{2}}|1,-111> \\
|1,-1> &= \frac{1}{\sqrt{2}}|101,-1> - \frac{1}{\sqrt{2}}|1,-110> \\
|00> &= \frac{1}{\sqrt{3}}|111,-1> - \frac{1}{\sqrt{3}}|1010> + \frac{1}{\sqrt{3}}|1,-111>
\end{aligned}
$$

Note that they are orthonormal. For example,

$$
\begin{aligned}
<20|20> &= (\frac{1}{\sqrt{6}})^2 + (\frac{\sqrt{2}}{\sqrt{3}})^2 + (\frac{1}{\sqrt{6}})^2 = 1 \\
<10|10> &= (\frac{1}{\sqrt{2}})^2 + (\frac{-1}{\sqrt{2}})^2 = 1 \\
<00|00> &= (\frac{1}{\sqrt{3}})^2 + (\frac{-1}{\sqrt{3}})^2 + (\frac{1}{\sqrt{3}})^2 = 1 \\
<20|10> &= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}}\frac{-1}{\sqrt{2}} = 0 \\
<20|00> &= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{3}} + \frac{\sqrt{2}}{\sqrt{3}}\frac{-1}{\sqrt{3}} + \frac{1}{\sqrt{6}}\frac{1}{\sqrt{3}} = 0 \\
<10|00> &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{3}} + \frac{-1}{\sqrt{2}}\frac{1}{\sqrt{3}} = 0
\end{aligned}
$$

6.4 Properties of Clebsch-Gordan coefficients

1) Orthonormality

$$\sum_{m_1 m_2} (j_1 m_1 j_2 m_2|jm)(j_1 m_1 j_2 m_2|j'm') = \delta(j,j')\delta(m,m')$$
$$\sum_{jm} (j_1 m_1 j_2 m_2|jm)(j_1 m_1' j_2 m_2'|jm) = \delta(m_1,m_1')\delta(m_2,m_2')$$

2) Symmetries

$$\begin{aligned}
(j_1 m_1 j_2 m_2|jm) &= (-)^{j_1+j_2-j}(j_2 m_2 j_1 m_1|jm) \\
&= (-)^{j_1+j_2-j}(j_1,-m_1 j_2,-m_2|j,-m) \\
&= (j_2,-m_2 j_1,-m_1|j,-m) \\
&= (-)^{j_1-m_1}\frac{\hat{j}}{\hat{j}_2}(j_1,m_1 j,-m|j_2,-m_2) \\
&= (-)^{j_1-m_1}\frac{\hat{j}}{\hat{j}_2}(jmj_1,-m_1|j_2 m_2) \\
&= (-)^{j_2+m_2}\frac{\hat{j}}{\hat{j}_1}(j,-mj_2 m_2|j_1,-m_1)
\end{aligned}$$

3) Analytic expression

$$\begin{aligned}
(j_1 m_1 j_2 m_2|jm_j) &= \delta_{m,m_1+m_2}\sqrt{\frac{(2j+1)(j+j_1-j_2)!(j-j_1+j_2)!(j_1+j_2-j)!}{(j_1+j_2+j+1)!}} \\
&\times \sqrt{(j+m)!(j-m)!(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!} \\
&\times \sum_k \Big[\frac{(-)^k}{k!(j_1+j_2-j-k)!(j_1-m_1-k)!(j_2+m_2-k)!} \\
&\qquad \times \frac{1}{(j-j_2+m_1+k)!(j-j_1-m_2+k)!}\Big]
\end{aligned}$$

3) Special Values

$$\begin{aligned}
(j_1 0 j_2 0|j0) &= (-)^{g+j}\hat{j} \\
&\times \sqrt{\frac{(j_1+j_2-j)!(j+j_1-j_2)!(j+j_2-j_1)!}{(2g+1)!}} \\
&\times \frac{g!}{(g-j)!(g-j_1)!(g-j_2)!} \\
&\qquad \text{for } j+j_1+j_2 = 2g = \text{ even} \\
&= 0 \qquad \text{for } j+j_1+j_2 = 2g = \text{ odd}
\end{aligned}$$

$$(j_1 m_1 00|jm) = \delta(j_1,j)\delta(m_1,m)$$

6.5 Addition of three or more angular momenta

The general rule for finding the possible values in addition of three or more angular momenta.

Let N angular momenta denote $\ell_1, \ell_2, ..., \ell_N$. These values are ordered so that

$$\ell_1 \leq \ell_2 \leq ... \leq \ell_N$$

Define

$$\Sigma \equiv \sum_{i=1}^{N-1} \ell_i$$

$$\text{If } \ell_N - \Sigma \begin{cases} > 0, & \ell_{min} = \ell - \Sigma \\ \leq 0, & \ell_{min} = 0 \end{cases}$$

$$\ell_{max} = \sum_{i=1}^{N} \ell_i$$

The possible values of ℓ are

$$\ell = |\ell_{max}|, |\ell_{max} - 1|, ..., |\ell_{min}|$$

This is a good rule for identifying the all possible ℓ's. However in order to count the total number of states in the coupled representation one usually adopt the sequential addition method.

In the sequential addition method, we combine ℓ_1 and ℓ_2 to reach A, then

$$A = \ell_1 + \ell_2, \ell_1 + \ell_2 - 1, ..., |\ell_1 - \ell_2|$$

the total number of states becomes

$$\begin{aligned} N_2 &= \sum_{A=|\ell_1-\ell_2|}^{\ell_2+\ell_1} (2A+1) \\ &= (2\ell_1+1)(2\ell_2+1) \end{aligned}$$

The next step is that A couples to ℓ_3 to form B,

$$B = \ell_3 + A, \ell_3 + A, ..., |\ell_3 - A|$$

and the total number of states becomes

$$\begin{aligned} N_3 &= \sum_{A=|\ell_1-\ell_2|}^{\ell_2+\ell_1} \sum_{B=|A-\ell_3|}^{A+\ell_3} (2B+1) \\ &= \sum_{A=|\ell_1-\ell_2|}^{\ell_2+\ell_1} (2A+1)(2\ell_3+1) \\ &= (2\ell_1+1)(2\ell_2+1)(2\ell_3+1) \end{aligned}$$

We just keep continuing in this manner until all individual angular momentum ℓ values are accounted for. The final sequence gives all possible values of ℓ.

We may have the total number of states in the sequential addition method as

# of **L**	# of states
1	$(2\ell_1+1)$
2	$(2\ell_1+1)(2\ell_2+1)$
3	$(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)$
...	...
N	$(2\ell_1+1)(2\ell_2+1)...(2\ell_N+1)$

Example 1. Three d ($\ell = 2$) electrons

We set $\ell_1 = \ell_2 = \ell_3 = 2$ in unit of $\hbar$.
Since $\Sigma = 2+2 = 4 > 2$, $\ell_{min} = 0$. We also have $\ell_{max} = 2+2+2 = 6$. The possible ℓ values are

$$\ell = 6, 5, 4, 3, 2, 1, 0$$

In the sequential method,

$\ell' = \ell_1 + \ell_2$	$\ell'' = \ell' + \ell_3$	#
0	2	5
1	1, 2, 3	15
2	0, 1, 2, 3, 4	25
3	1, 2, 3, 4, 5	35
4	2, 3, 4, 5, 6	45
Total		125

The possible ℓ values are again $\ell = 6, 5, 4, 3, 2, 1, 0$, and the total number of states are 125 in agreement with $5 \times 5 \times 5 = 125$.

Example 2. Four p ($\ell = 1$) electrons

We set $\ell_1 = \ell_2 = \ell_3 = \ell_4 = 1$ in unit of $\hbar$.
Since $\Sigma = 1+1+1 = 3 > 1$, $\ell_{min} = 0$. We also have $\ell_{max} = 1+1+1+1 = 4$ The possible ℓ values are

$$\ell = 4, 3, 2, 1, 0$$

In the sequential method,

$\ell' = \ell_1 + \ell_2$	$\ell'' = \ell' + \ell_3$
0	1
1	0, 1, 2
2	1, 2, 3

$\ell'' = \ell' + \ell_3$	# of ℓ''	$\ell = \ell'' + \ell_4$	# of ℓ	Total #
0	1	1	3	3
1	3	0, 1, 2	9	27
2	2	1, 2, 3	15	30
3	1	2, 3, 4	21	21
Total				81

The possible ℓ values are again $\ell = 4, 3, 2, 1, 0$, and the total number of states are 81 in agreement with $3 \times 3 \times 3 \times 3 = 81$.

Example 3. Total Angular Momentum of the Two Fermions

The total angular momentum operator of two fermions can be written

$$\hat{\mathbf{J}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 + \hat{\mathbf{L}}$$

where $\hat{\mathbf{L}}$ is the orbital angular momentum of the two-particle system. With $s_1 = n_1/2$, and $s_2 = n_2/2$, where n_1 and n_2 are odd integers, we find the total spin numbers

$$s = (\frac{n_1}{2} + \frac{n_1}{2}), ..., |\frac{n_1}{2} - \frac{n_2}{2}|$$

which are all integers. The total angular momentum j is then given by

$$j = \ell + s, ..., |\ell - s|$$

which are all integers.

6.6 Racah coefficients: Coupling of 3 angular momenta

1. Definition

$$j_1 + j_2 = J_{12}, \quad j_2 + j_3 = J_{23} \quad J_{12} + j_3 = j_1 + J_{23} = J$$

$$\begin{aligned} < j_1 j_2 (J_{12}) j_3 JM | j_1, j_2 j_3 (J_{23}) JM > &= \hat{J}_{12}\hat{J}_{23} W(j_1 j_2 J j_3; j_{12} J_{23}) \\ &= \sum_{m_1 m_2 m_3} (j_1 m_1 j_2 m_2 | J_{12} M_{12})(J_{12} M_{12} j_3 m_3 | JM) \\ &\quad \times (j_2 m_2 j_3 m_3 | J_{23} M_{23})(j_1 m_1 J_{23} M_{23} | JM) \end{aligned}$$

In $W(abcd; ef)$, $(abe)(cde)(acf)(bdf)$ must satisfy the triangular relation ($|a - b| \leq c \leq a + b$).

2. Symmetries

$$\begin{aligned} W(abcd; ef) &= W(badc; ef) = W(cdab; ef) \\ &= W(acbd; fe) \\ &= (-)^{e+f-a-d} W(ebcf; ad) \\ &= (-)^{e+f-b-c} W(aefd; bc) \end{aligned}$$

3. Orthogonality

$$\sum_e \hat{e}^2 W(abcd; ef) W(abcd; ef') = \delta(f, f')/\hat{f}^2$$

$$\sum_c \hat{c}^2 W(abcd; ef) W(ab'cd; ef) = \delta(b, b')/\hat{b}^2$$

$$\sum_d \hat{d}^2 W(abcd; ef) W(a'bcd; ef') = \delta(a, a')/\hat{a}^2$$

4. Equality

$$\begin{aligned} \sum_e (-)^{a+b-e} \hat{e}^2 W(abcd; ef) W(bacd; ef') &= W(aff'b; cd) \\ \sum_\lambda \hat{\lambda}^2 W(a'\lambda be; ac') W(c\lambda de'; c'e) W(a'\lambda fc; ac') &= W(abcd; ef) W(a'bc'd; e'f) \\ \sum_\beta (a\alpha b\beta | e\epsilon)(e\epsilon d\delta | c\gamma)(b\beta d\delta | f\varphi) &= \hat{e}\hat{f}(a\alpha f\varphi | c\gamma) W(abcd; ef) \\ \sum_f \hat{e}\hat{f}(a\alpha f\varphi | c\gamma)(b\beta d\delta | f\varphi) W(abcd; ef) &= (a\alpha b\beta | e\epsilon)(e\epsilon d\delta | c\gamma) \\ \sum_e \hat{e}\hat{f}(a\alpha b\beta | e\epsilon)(e\epsilon d\delta | c\gamma) W(abcd; ef) &= (a\alpha f\varphi | c\gamma)(c\gamma d\delta | f\varphi) \end{aligned}$$

5) Special values

$$\begin{aligned} W(0bcd; bc) &= \hat{b}^{-1}\hat{c}^{-1} \\ W(aa'cc'; 0f) &= (-)^{a+c-f} \hat{a}^{-1}\hat{c}^{-1} \delta(a, a')\delta(c, c') \end{aligned}$$

6.7 X (Fano) coefficients and 9-j (Wigner) symbols: Coupling of 4 angular momenta

1) Definition

$$j_1 + j_2 = J_{12},\ j_3 + j_4 = J_{34},\ j_1 + j_3 = J_{13},\ j_2 + j_4 = J_{24},$$
$$J_{12} + J_{34} = J_{13} + J_{24} = J$$

$$\begin{aligned} < j_1 j_2 (J_{12}) j_3 j_4 (J_{34}) JM | j_1 j_3 (J_{13}) j_2 j_4 (J_{24}) JM > &= X(j_1 j_2 J_{12}, j_3 j_4 J_{34}; J_{13} J_{24} J) \\ &= \hat{J}_{12}\hat{J}_{34}\hat{J}_{13}\hat{J}_{24} U \begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ j_{13} & j_{24} & J \end{pmatrix} \end{aligned}$$

2) Relation with Racah coefficients

$$\begin{aligned} U \begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} &= (-)^{\sigma} \sum_{\lambda} \hat{\lambda}^2 W(bcef; \lambda a) W(bcf'e'; \lambda d) W(efe'f'; \lambda g) \\ \sigma &= a + b + c + d + e + e' + f + f' + g = \text{ integer} \end{aligned}$$

3) Symmetries

$$\begin{aligned} U \begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} &= U \begin{pmatrix} a & c & f \\ b & d & f' \\ e & e' & g \end{pmatrix} \quad \text{(transposition)} \\ &= (-)^{\sigma} U \begin{pmatrix} c & d & e' \\ a & b & e \\ f & f' & g \end{pmatrix} \\ &= (-)^{\sigma} U \begin{pmatrix} f & f' & g \\ c & d & e' \\ a & b & e \end{pmatrix} \end{aligned}$$

4) Special values

$$\begin{aligned} U \begin{pmatrix} a & b & e \\ a & b & e \\ f & f' & g \end{pmatrix} &= 0 \quad (f + f' + g = \text{ odd}) \\ U \begin{pmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{pmatrix} &= (-)^{e+f-a-d} \hat{e}^{-1} \hat{f}^{-1} W(abcd; ef) \end{aligned}$$

6.8 (Homework Set #5) Calculation of the vector coupling coefficients

1. Obtain Clebsch-Gordan coefficients for $\ell_1, \ell_2, \ell_3 = \hat{\ell}_1 + \hat{\ell}_2 = 3$ with all-zero m's by using the Program "MAINVC" (Appendix E). Plot your values in the 3-dimensional space; x-axis = ℓ_1, y-axis = ℓ_2, and z-axis = "obtained values". Make sure that properties of the Clebsch-Gordan coefficients, presented in subsection 5.4, and discuss your results.

2. Obtain Clebsch-Gordan coefficients for $\ell_1 = 1, \ell_2 = 2, \ell_3 = \hat{\ell}_1 + \hat{\ell}_2 = 3$ with different m's by using the Program "MAINVC" (Appendix E). Plot your values in the 3-dimensional space; x-axis = m_1, y-axis = m_2, and z-axis = obtained value. Make sure that properties of the Clebsch-Gordan coefficients, presented in 5.4, and discuss your results.

3. Obtain Racah coefficients for the three p ($\ell = 1$)-electron system by using the Program "MAINVC" (Appendix E). Make sure that properties of the Racah coefficients, presented in 5.6, and discuss your results.

4. Obtain 9-j coefficients for the four p ($\ell = 1$)-electron system by using the Program "MAINVC" (Appendix E). Make sure that properties of the 9-j coefficients, presented in 5.7, and discuss your results.

A Spherical Harmonics - MAINYLM

A.1 Generation of the spherical harmonics

The subroutine "ylmcal.f" calculates a part of spherical harmonics, $Y_{\ell m}(\mu)$,

$$[\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}]^{1/2}P_{\ell m}(\mu), \quad \mu=\cos\theta$$

by utilizing the recurrence relations of the Legendre functions, $P_{\ell m}(\mu)$,

$$(2\ell+1)\mu P_{\ell m} = (\ell-m+1)P_{\ell+1,m} + (\ell+m)P_{\ell-1,m}$$
$$(2\ell+1)(1-\mu^2)^{1/2}P_{\ell m} = P_{\ell-1,m+1} - P_{\ell+1,m+1}.$$

A.2 Input data of the program "mainylm.f"

Line 1: READ(7,10) AMIN, ASTEP
FORMAT(10F7.3)

AMIN	Minimum angle of θ
ASTEP	Angle steps

Line 2: READ(7,11) MUANG,NMAX,LLL,MMM
FORMAT(10I5)

MUANG =0	Angles in Line 1 are in $\cos\theta$
MUANG=1	Angles in Line 1 are in θ
NMAX	Number of angles
LLL	Maximum value of ℓ
MMM	Maximum value of m

B Nuclear shell model wave function - NEPTUNE

B.1 Generation of the nuclear shell model wave function

The program "NEPTUNE" calculates the bound state wave function. It consists of a main program, also called NEPTUNE, and subroutines BSAXON and UNCPST.

The main program reads in 7 data cards, containing control characters, the quantum numbers of the bound state, mass and charge of the orbiting particle, mass and charge of the nucleus, binding energy of the particle in the nucleus, accuracy parameters for the program's automatic search feature, and the parameters of the Woods-Saxon potential in which the particle moves. It outputs this data, and calls BSAXON.

BSAXON sets up the initial constants needed for numerical integration of the bound state Schrödinger equation and for automatic search on well depth of binding energy, and calls UNCPST.

BSAXON first calculates up the total potential, consisting of a real Woods-Saxon central potential plus a Thomas-type derivative Woods-Saxon spin-orbit potential and a Coulomb potential if the orbiting particle is charged.

UNCPST computes the radial wave function using the Störmer method to solve the radial Schrödinger equation. It tests input quantum numbers, well depth, and binding energy for consistency and ability to satisfy boundary conditions at this point, iterates either well depth or binding energy, and solve the Schrödinger equation again. This process is repeated until a solution is found satisfying the boundary conditions.

The Schrödinger equation solved is

$$[-\frac{\hbar^2}{2\mu}(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}) + \epsilon + V_j]u_{j\ell}(r) = 0$$

where $u_{j\ell}(r)$ is the radial state function times r, ϵ is the binding energy, j and ℓ are the total and orbital angular momentum quantum numbers, and $V_j(r)$ is the total potential energy function. $u_{j\ell}(r)$ is subject to the boundary condition $u_{j\ell}(0) = 0$. The potential $V_j(r)$ is of standard form,

$$\begin{aligned} V_j(r) &= \frac{-V_0}{1+\exp(\frac{r-R_0}{a_0})} + V_C(r) \\ &\quad +(\frac{\hbar}{m_\pi c})^2 \frac{V_{SO}}{r}(\vec{\sigma}\cdot\vec{\ell})\frac{d}{dr}[\frac{1}{1+\exp(\frac{r-R_{SO}}{a_{SO}})}] \end{aligned}$$

where

$$V_C(r) = \begin{cases} \frac{Ze^2}{2R_C}[3-(\frac{r}{R_C})^2] & r < R_C \\ \frac{Ze^2}{r} & r > R_C \end{cases}$$

$$< jm_j|(\vec{\sigma}\cdot\vec{\ell})|jm_j > = \begin{cases} \ell & j = \ell + \frac{1}{2} \\ -(\ell+1) & j = \ell - \frac{1}{2} \end{cases}$$

with $R_0 = r_0 A^{1/3}$, $R_C = r_C A^{1/3}$, and $R_{SO} = r_{SO} A^{1/3}$

The region of integration is divided into two parts at a distance of $R_m \approx r_0 A^{1/3}$, the *half-radius* of the central potential. The solution started from the origin is carried two points past R_m. A second solution is started at a large distance (generally 2 or 3 fermis beyond the greatest distance at which the function is needed) and carried inward two points inside R_m. Its logarithmic derivative at R_m is compared to the logarithmic derivative of the inner solution.

Let α_0 be the value of some parameter α (well-depth or binding energy), such that the logarithmic derivatives are the same to within some desired accuracy. The value actually used for α may be

$\alpha_1 = \alpha_0 + \Delta\alpha$. But the condition that the logarithmic derivatives agree can be put in the form $f(\alpha_0) = 0$. Thus

$$f(\alpha_0) = f(\alpha_1 - \Delta\alpha) = f(\alpha_1) - \frac{\partial f}{\partial \alpha}|_{\alpha_1} \Delta\alpha = 0,$$

or

$$\Delta\alpha = f(\alpha_1)/[\frac{\partial f}{\partial \alpha}|_{\alpha_1}]$$

This condition is used to iterate well depth or binding energy until $\Delta\alpha/\alpha$ is sufficiently small ($|\Delta\alpha/\alpha| \approx$ ACURCY). In practice, in NEPTUNE,

$$\frac{\partial f}{\partial \alpha}|_{\alpha_1} = [f(1.01\alpha_1) - f(0.99\alpha_1)]/(0.02\alpha_1)$$

is used to evaluate the derivative.

B.2 Meaning of key quantities.

XMES1 and XMES2 (recommended values are 0.0125 and 0.1 fm, respectively) are the minimum and maximum mesh sizes used in the Störmer method.

NXRM and NXCPL2 are defined by R_m = XMES2 *NXRM, R_c = XMES2*NXCPL2. Here R_c is the largest distance at which the state function is desired to be evaluated and R_m is the point at which the inner and outer solutions are matched. A third radius, R_a = XMES2*NXRA is used to extend the range of the inward integration that produces the outer solution, to ensure that it has the correct asymptotic form. Generally it is sufficient for R_a is to be 2 to 3 fermis greater than R_c.

NODER is the desired number of nodes. The actual number of nodes is counted in UNCPLB and stored in KEXCOM(42). If the two quantities differ, the quantity being searched is changed by 10 % in a direction determined to reduce the disagreement, and the calculation is repeated until the two agree or the number of iterations (Input data) is exceeded.

B.3 Input data of the program NEPTUNE

Line 1: READ(7,10) KTRL(1) - (14)
FORMAT(14I5)

KTRL(2)=0 causes the binding energy be searched for a given potential
KTRL(2)=1 causes the potential depth be searched for a given binding energy

Line 2: READ(7,10) KEXCOM(1) - (14)
FORMAT(14I5)

KEXCOM are all zero, unless one wants to input NXCPL2, NXRA
KEXCOM(2) = NXCPL2
KEXCOM(4) = NXRA-NXCPL2

Line 3: READ(7,10) KTLOUT(1) - (14)
FORMAT(14I5)

KTLOUT gives intermediate output, useful in case of suspicion
of numerical errors in the program.
KTLOUT(1) =1, Output of calculations
KTLOUT(2) =1, Detailed output (Potential etc.)

Line 4: READ(7,11) EXTCOM(1) - (14)
FORMAT(10F7.3)

EXTCOM(1) = XMES2 =0.10
EXTCOM(2) = XMES1 =0.0125
EXTCOM(3) = Desired normalization =1.0

Line 5: READ(7,10) ITBEMX,JBTRTW,LBTR,NODER
FORMAT(14I5)

ITBEMX	# of iterations
JBTRTW	$2j$
LBTR	ℓ
NODER	n, the desired # of nodes, not counting the zero at the origin.

Line 6: READ(7,11) TMAS,PMAS,ZZT,ZZP,
ACURCY, PERCNT, EGES
FORMAT(10F7.3)

TMAS	M_T, mass of the core nucleus.
PMAS	M_P, mass of the orbiting nucleus.
ZZT	Z_T, charge of the core nucleus.
ZZP	Z_P, charge of the orbiting nucleus.
ACURCY	"Accuracy" is the criterion for matching of interior and exterior solution. 0.003 is recommended.
PERCNT	"Percent" is the maximum allowed value of $\|\Delta\alpha/\alpha_1\|$ as discussed earlier. 0.2 is recommended. Should not exceed 1.0.
EGES	$\epsilon > 0$, the binding energy.

Line 7: READ(7,11) VSX,VSOR,DFNR,DFNSO,
RZR,RZSO,RZC,
FORMAT(10F7.3)

VSX	V_0, Potential depth parameter of the central potential.
VSOR	V_{SO}, Potential depth parameter of the spin-orbit potential.
DFNR	a_0, Diffuseness parameter of the central potential.
DFNSO	a_{SO}, Diffuseness parameter of the spin-orbit potential.
RZR	V_0, Radius parameter of the central potential.
RZSO	r_{SO}, Radius parameter of the spin-orbit potential.
RZC	r_C, Radius parameter of the Coulomb potential.

C Spherical Bessel functions - MAINJL

C.1 Generation of the spherical Bessel functions

The subroutine bessel.f generates the spherical bessel function by using the recurrence relations,

$$\begin{aligned} \frac{n+1}{z} j_n(z) + \frac{dj_n(z)}{dz} &= j_{n-1}(z) \\ \frac{n}{z} j_n(z) - \frac{dj_n(z)}{dz} &= j_{n+1}(z) \end{aligned}$$

C.2 Input data of the program "mainjl.f"

Line 1: READ(7,10) TMAS,ZZT,PMAS,ZZP,
ELAB
FORMAT(10F7.3)

TMAS	M_T, mass of the target.
ZZT	Z_T, charge of the target.
PMAS	M_P, mass of the projectile.
ZZP	Z_P, charge of the projectile.
ELAB	incident energy in the lab.

Line 2: READ(7,10) XMIN, XSTEP
FORMAT(10F7.3)

XMIN	Minimum radial distance
XSTEP	radial distance step

Line 3: READ(7,11) NMAX,MAXL
FORMAT(10I5)

NMAX	Number of radial points
MAXL	Maximum value of ℓ

D Coulomb wave functions - MAINFLGL

D.1 Generation of Coulomb Wave Functions

In 1974, the Manchester group (A. R. Barnett, D. H. Feng, J. W. Steed and L. J. B. Goldfarb, "Coulomb wave functions for all real η and ρ", Comp. Phys. Comm. **8** (1974) 377-395.) made a program for the Coulomb wave functions by using the continued fraction method, called here FLGLCH.

This subroutine is applicable for all values of

$$\rho \geq \rho_T = \eta + \sqrt{\eta + [\eta^2 + \ell(\ell+1)]},$$

where ρ_T is the corresponding ρ to the turning point, without restriction. A somewhat modified method is used for values of $\rho < \rho_T$, but not useful $\rho < 0.2\rho_T$.

D.2 Input data of the program "mainflgl.f"

Line 1: READ(7,10) TMAS,ZZT,PMAS,ZZP,
ELAB
FORMAT(10F7.3)

TMAS	M_T, mass of the target.
ZZT	Z_T, charge of the target.
PMAS	M_P, mass of the projectile.
ZZP	Z_P, charge of the projectile.
ELAB	incident energy in the lab.

Line 2: READ(7,10) XMIN, XSTEP
FORMAT(10F7.3)

XMIN	Minimum radial distance
XSTEP	radial distance step

Line 3: READ(7,11) NMAX,MAXL
FORMAT(10I5)

NMAX	Number of radial points
MAXL	Maximum value of ℓ

E Vector coupling coefficients - MAINVC

E.1 Input data of the program "mainvc.f"

Line 1: READ(7,10) KTRL,NCAL
FORMAT(10I5)

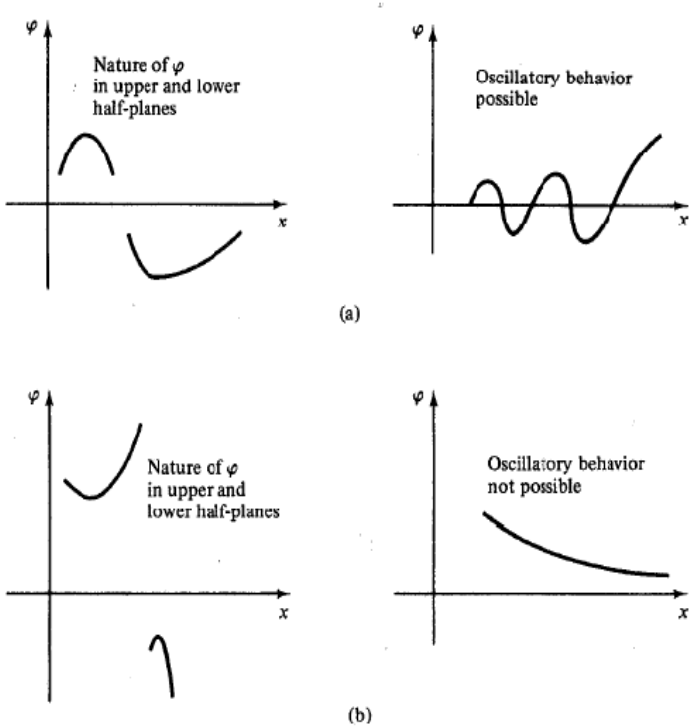
KTRL	=1, Clebsch-Gordan Coefficients with all-zero m's
	=2, Clebsch-Gordan Coefficients with non-zero m's
	=3, Racah Coefficients
	=4, 9-j Coefficients
NCAL	Number of coefficients calculated

Line 2: READ(7,11) Reads as follows.
FORMAT(10F7.3)

CLEBZ	IA,IB,IC
CLEB	IA,IB,IC,ID,IE,IFF
	(IA,ID,IB,IE |IC,IFF)
RAC7	IA,IB,IC,ID,IE,IFF
	W(IA,IB,IC,ID;IE,IFF)
NINEJ	(L9(N),N=1,9)
	$U \begin{pmatrix} L9(1) & L9(2) & L9(5) \\ L9(3) & L9(4) & L9(6) \\ L9(7) & L9(8) & L9(9) \end{pmatrix}$

***L9 is TWICE of angular momentum.

1. QM_fig


φ
Nature of φ
in upper and lower
half-planes
x
φ
Oscillatory behavior
possible
x
(a)
φ
Nature of φ
in upper and
lower half-planes
x
φ
Oscillatory behavior
not possible
x
(b)