MA3442: Quantum Mechanics II

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Chapter 1

3D Potentials

1.1 Introduction

In 3D,

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}),$$

or, in spherical coordinates:

$$H = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

The orbital angular momentum operator, $\vec{L}$, is:

$$\vec{L} = \vec{r}\times\vec{p} = \frac{\hbar}{i}(\vec{r}\times\vec{\nabla}).$$

Using:

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}, \quad \text{and}$$

$$\frac{L^2}{\hbar^2} = -\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta},$$

H can be written as:

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r,\theta,\phi),$$

where $p_r = \frac{\hbar}{i}(\frac{1}{r} + \frac{\partial}{\partial r})$.

1.2 Notes

1.

$$\begin{aligned}\frac{p_r^2}{\hbar^2} &= -\left(\frac{1}{r}+\frac{\partial}{\partial r}\right)\left(\frac{1}{r}+\frac{\partial}{\partial r}\right)\\ &= -\frac{1}{r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{\partial^2}{\partial r^2}\\ &= -\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}.\end{aligned}$$

2.

$$\int d^3r\, \psi^* p_r \psi = \int d\Omega \int_0^\infty r^2\, dr\, \psi^* p_r \psi$$
$$= \int d\Omega \int_0^\infty r^2\, dr\, (p_r\psi)^* \psi, \text{ for suitable boundary conditions.}$$

Therefore, while $\frac{\hbar}{i}\frac{\partial}{\partial r}$ is not Hermitian, p_r *is* Hermitian.

3. H takes the same form as the classical Hamiltonian:

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(\vec{r}),$$

where $p_r = m\dot{r}$ and $L = mr^2\dot{\theta}$.

1.3 Central potentials

Suppose $V(\vec{r})$ is central, i.e. $V(\vec{r}) = V(r)$. Then:

$$[L^2, H] = [L_z, H] = [L_z, L^2] = 0.$$

Thus, we can choose simultaneous eigenstates $\psi_{E\ell m}$ of L^2, L_z and H such that:

$$H\psi_{E\ell m} = E\psi_{E\ell m}, \quad L^2\psi_{E\ell m} = \hbar^2\ell(\ell+1)\psi_{E\ell m}, \quad L_z\psi_{E\ell m} = m\hbar\psi_{E\ell m}.$$

Factoring the $\hbar$ out of L^2 and L_z, and renaming, gives:

$$H = \frac{p_r^2}{2m} + \frac{\hbar^2 L^2}{2mr^2} + V(r).$$

Since $V(r)$ is spherically symmetric, we can separate r from θ and ϕ in our expression for ψ. We let $\psi_{E\ell m}(\vec{r}) = R_{E\ell}(r)Y_{\ell m}(\theta,\phi)$ where the spherical harmonics $Y_{\ell m}$ satisfy:

$$L^2 Y_{\ell m} = \ell(\ell+1)Y_{\ell m}$$
$$L_z Y_{\ell m} = mY_{\ell m},$$

where $\ell = 0, 1, 2, \ldots$ and $m = -\ell, -\ell+1, \ldots, \ell$.

Note: The quantum numbers for ℓ and m are a consequence of the algebra of angular momentum, i.e. $[L_x, L_y] = L_z$ (+ cyc.). See later.

The Schrödinger equation for the radial eigenfunction $R_{E\ell}$ reads:

$$\left(\frac{p_r^2}{2m} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right) R_{E\ell}(r) = ER_{E\ell}(r), \text{ or:}$$

$$\left[\frac{\hbar^2}{2m}\left(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\ell(\ell+1)}{r^2}\right) + V(r)\right] R_{E\ell}(r) = ER_{E\ell}(r).$$

Since $Y_{\ell m}$s satisfy:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, \sin\theta Y^*_{l'm'}(\theta,\phi) Y_{\ell m}(\theta,\phi) = \delta_{l\,l'}\delta_{m\,m'}$$

the bound-state normalisation condition:

$$\int d^3r \, |\psi_{E\ell m}(\vec{r})|^2 = 1$$

reduces to:

$$\int_0^{\infty} r^2 |R_{E\ell}(r)|^2 \, dr = 1.$$

If E lies in the continuum part of H's spectrum, then set

$$\int_0^{\infty} r^2 R^*_{E'\ell}(r) R_{E\ell}(r) \, dr = \delta(E - E').$$

Let $R_{E\ell}(r) = \frac{U_{E\ell}(r)}{r}$. Then $U_{E\ell}$ satisfies:

$$\left[\frac{\hbar^2}{2m^2}\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}\right) + V(r)\right] U_{E\ell}(r) = E U_{E\ell}(r).$$

Note: This is equivalent to the Schrödinger equation in 1D, with $x = r > 0$, and effective potential given by $V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$.

The Hermiticity requirement:

$$\int d^3r \, \psi^*_{E'\ell'm'} H \psi_{E\ell m} = \int d^3r \, (H\psi_{E'\ell'm'})^* \psi_{E\ell m}$$

reduces to:

$$\int_0^{\infty} U^*_{E'\ell} \frac{d^2}{dr^2} U_{E\ell} \, dr = \int_0^{\infty} \left(\frac{d^2 U_{E'\ell}}{dr^2}\right)^* U_{E\ell} \, dr.$$

In other words,

$$\left(U^*_{E'\ell}\frac{dU_{E\ell}}{dr} - \frac{dU^*_{E'\ell}}{dr}U_{E\ell}\right)\Bigg|_0^{\infty} = 0.$$

A *sufficient* set of conditions for this is:

- $U_{E\ell}(0) = 0$
- $U'_{E\ell}(0) =$ finite
- $U_{E\ell}(\infty) = U'_{E\ell}(\infty) = 0$

Note: The Schrödinger equation for U and $R = U/r$ are 1D problems with $r \geqslant 0$. In 1D, none of the bound states of $V(r)$ are degenerate. Therefore, bound-state wavefunctions U and R may be assumed to be real.

1.4 The hydrogen atom

Consider the hydrogen atom with potential:

$$V(r) = -\frac{e^2}{r}.$$

Then,

$$\left[\frac{\hbar^2}{2m}\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}\right) - \frac{e^2}{r}\right] U_{E\ell}(r) = EU_{E\ell}(r).$$

The effective potential is $\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - \frac{e^2}{r}$, which has a bound-state spectrum for $E < 0$. Hence, we assume $E < 0$ and look for bound states.

Let:

$$r = \frac{n\hbar^2}{2me^2}\rho,$$
$$E = -\frac{1}{n^2}\frac{me^4}{2\hbar^2},$$

where n and ρ are dimensionless.

This gives:

$$\left(\frac{d^2}{dr^2} + \frac{n}{\rho} - \frac{1}{4} - \frac{\ell(\ell+1)}{\rho^2}\right) U_{E\ell}(\rho) = 0.$$

For $\rho \to 0$, $U''_{E\ell} \sim \frac{\ell(\ell+1)}{\rho^2} U_{E\ell}$. Therefore, $U_{E\ell} \sim A\rho^{\ell+1} + B\rho^{-\ell}$. Hence, we seek a solution that behaves like ρ^{l+1} as $\rho \to 0$.

For $\rho \to \infty$, $U''_{E\ell} \sim \frac{1}{4}U_{E\ell}$, so $U_{E\ell} \sim e^{\pm\rho/2}$. So we seek a solution that behaves like $e^{-\rho/2}$ as $\rho \to \infty$ because we need it to be normalisable.

Hence, we make the substitution $U_{E\ell}(\rho) = \rho^{l+1}e^{-\rho/2}w(\rho)$. Then,

$$\rho w'' + (2\ell + 2 - \rho)w' + (n - \ell - 1)w = 0 \tag{1.1}$$

We seek a solution of (1.1) which is finite at $\rho = 0$ and which satisfies

$$\int_0^\infty U_{E\ell}^2 < \infty$$

Solutions are of the form:

$$w(\rho) = \rho^\alpha \sum_{j=0}^{\infty} a_j \rho^j.$$

Substituting this into (1.1) gives:

$$\sum_{j=0}^{\infty}(\alpha + j)(\alpha + j + 1 + 2\ell)a_j\rho^{j+\alpha-1} = \sum_{j=1}^{\infty}(\alpha + j + \ell - n)a_{j-1}\rho^{j+\alpha-1}$$

Equating the summands with $j = 0$:

$$\alpha(\alpha + 2\ell + 1)a_0 = 0 \Rightarrow a = 0 \quad \text{or} \quad a = -2\ell.$$

a_0 is arbitrary.

We select $\alpha = 0$, so when $j > 0$,

$$j(j+1+2\ell)a_j = (1+\ell-n)a_{j-1}, \text{ or:}$$

$$a_j = \frac{j+\ell-n}{j(j+1+2\ell)}a_{j-1} \tag{1.2}$$

Note that as $j \to \infty$, $a_j \sim \frac{a_{j-1}}{j}$, so $w(\rho) \sim e^{\rho}$ as $\rho \to \infty$. This would give $U_{E\ell}(\rho) \sim \rho^{\ell+1}e^{\rho/2}$ which is not normalisable! This means the series must terminate; this happens only if $n = 1, 2, 3, \ldots$ since $\ell = 0, 1, 2, \ldots$ and $j = 1, 2, 3, \ldots$

This means:

$$E_n = -\frac{1}{n^2}\frac{me^4}{2\hbar^2},$$

where $n = 1, 2, \ldots$

Energy levels are degenerate except for $n = 1$ (the ground state):

$$n = 1 \Rightarrow \ell = 0; \quad n = 2 \Rightarrow \ell = 0, 1; \quad n = 3 \Rightarrow \ell = 0, 1, 2; \quad \text{etc.}$$

For each n, $\ell = 0, 1, \ldots, n-1$. For each ℓ, $m = -\ell, \ldots, \ell$. So the degeneracy of E_n is:

$$\sum_{\ell=0}^{n-1}(2\ell+1) = n^2.$$

Degeneracy with respect to m is obvious because of invariance of H under rotation about the origin. Degeneracy of states with same n but different ℓ is peculiar to this particular potential however.

1.4.1 Hydrogenic wavefunctions

Recall that $\psi_{E\ell m}(r, \theta, \phi) = R_{E\ell}(r)Y_{\ell m}(\theta, \phi)$, $R_{E\ell}(r) = \frac{U_{E\ell}(r)}{r}$ and $U_{E\ell}(\rho) = \rho^{\ell+1}e^{-\rho/2}w(\rho)$. We will derive explicit expressions for ψ for $n = 1$ and $n = 2$.

The series expression of w from (1.2) gives:

$$w(\rho) = \begin{cases} a_0, & n = 1, \ell = 0 \\ a_0(1 - \frac{1}{2}\rho), & n = 2, \ell = 0 \\ a_0, & n = 2, \ell = 1. \end{cases}$$

Thus,

$$\begin{aligned} U_{10} &= a_0\rho e^{-\rho/2} \\ U_{20} &= \tfrac{a_0}{2}(2-\rho)\rho e^{-\rho/2} \\ U_{21} &= a_0\rho^2 e^{-\rho/2}. \end{aligned}$$

Recall:

$$r = \frac{n\hbar^2}{2me^2}\rho = \frac{n}{2}a\rho,$$

where a is the Bohr radius.

Thus,

$$R_{10} = c_{10}e^{-r/a}$$
$$R_{20} = c_{20}(2 - \tfrac{r}{a})e^{-r/2a}$$
$$R_{21} = c_{21}re^{-r/2a}$$

Normalising so that $\int_0^\infty r^2 R_{n\ell}^2\, dr = 1$,

$$R_{10} = \frac{2}{a^{3/2}}e^{-r/a}$$
$$R_{20} = \frac{1}{2\sqrt{2}a^{3/2}}\left(2 - \frac{r}{a}\right)e^{-r/2a}$$
$$R_{21} = \frac{r}{2\sqrt{6}a^{3/2}}e^{-r/2a}.$$

$\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r)Y_{\ell m}(\theta, \phi)$ is the complete wavefunction.

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$
$$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$
$$Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}.$$

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1.4.2 Example

Estimate E_0 for:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \beta r$$

where $\beta > 0$.

Solution:

$$E_0 \leqslant \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}.$$

$$\langle\psi|H|\psi\rangle = \frac{\hbar^2}{2mL^2} + \frac{3\beta L}{2} = f(L)$$

1.5 Peierls's theorem

Let $u_1, u_2, \ldots, u_N$ be a set of orthogonal functions, and let $H_{nm} = \langle u_n|H|u_m\rangle$. If $\{\lambda_i\}$ are the eigenvalues of the $N \times N$ matrix H_{nm} arranged in ascending order (i.e. $\lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_N$), then:

$$E_1 \leqslant \lambda_1, E_2 \leqslant \lambda_2, \ldots, E_N \leqslant \lambda_N.$$

That is, λ_i is an upper bound on the i^{th} eigenvalue of the Hamiltonian.

1.6 Identical particles and symmetry

The Hamiltonian for a system of n identical particles is completely symmetric under particle exchange. For example, the Hamiltonian of a helium atom is:

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}.$$

Let $\Psi(1, 2, \ldots, n)$ be any solution of the Schrödinger equation which depends on the coordinates – spatial and spin – of n identical particles. Let P_{ij} interchange particles i and j. Then:

$$P_{ij}H\Psi = HP_{ij}\Psi = EP_{ij}\Psi.$$

For a general Ψ which is a solution to the Schrödinger equation, $P_{ij}\Psi \neq \text{const.} \times \Psi$, i.e. exchange degeneracy. But nature favours nondegeneracy, and we have:

$$P_{ij}\Psi = \pm\Psi,$$

with $+$ for **bosons**: particles with integral spin (e.g. photons, mesons), and $-$ for **fermions**: particles with semi-integral spin (e.g. protons, electrons)

1.7 Examples

1.7.1 The helium atom

To estimate the ground-state energy of a helium atom (which has 0 total orbital angular momentum) we will select a trial wavefunction for each electron, built from hydrogenic wavefunctions:

$$\psi_{100}(r) = \left(\frac{Z}{a}\right)^{3/2} \frac{1}{\sqrt{\pi}} e^{-zr/a}$$

where Z is an adjustable parameter. This gives:

$$\langle\psi_{100}|\psi_{100}\rangle = 1$$

for $z > 0$.

Here, a is the Bohr radius and Z is the effective nuclear charge seen by an electron. Due to screening effects, we expect $1 < Z < 2$.

We introduce trial wavefunctions:

$$\psi_\uparrow = \psi_{100}(r)\begin{pmatrix}1\\0\end{pmatrix}, \quad \psi_\downarrow = \psi_{100}(r)\begin{pmatrix}0\\1\end{pmatrix}.$$

The trial wavefunction must be antisymmetric under exchange of electrons 1 and 2:

$$\Psi(1, 2) = -\Psi(2, 1).$$

If we put both electrons in ψ_{100}, their spin states must be different, so our trial wavefunction is:

$$\begin{aligned}\Psi(1, 2) &= \psi_{100}(1)\psi_{100}(2)\frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 - \begin{pmatrix}0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2\right] \\ &= -\Psi(2, 1).\end{aligned}$$

Also,

$$\int \Psi^\dagger(1,2)\Psi(1,2)\, d^3r_1\, d^3r_2 = 1.$$

The wavefunction can also be written:

$$\Psi(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_\uparrow(1) & \psi_\downarrow(1) \\ \psi_\uparrow(2) & \psi_\downarrow(2) \end{vmatrix}$$

Helium's Hamiltonian is spin-free, so:

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \int d^3r_1\, d^3r_2\, \psi^*_{100}(1)\psi^*_{100}(2) H \psi_{100}(1)\psi_{100}(2) \\ &= f(Z). \end{aligned}$$

We minimise f with respect to Z to obtain:

$$E_0 \leqslant f(Z)\Big|_{Z=Z_0}$$

This works out to be $E_0 \leqslant -77.5$ eV; compare this to the actual value $E_0 = -79.0$ eV.

1.7.2 The lithium atom

In order to estimate the ground-state energy, we construct a trial wavefunction $\Psi(1,2,3)$ from hydrogenic states.

$$H = \sum_{i=1}^{3} \left(-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{3e^2}{r_i} \right) + \frac{e^2}{r_{12}} + \frac{e^2}{r_{13}} + \frac{e^2}{r_{23}}$$

We will use:

$$\psi_{100} = ae^{-\alpha r}Y_{00}, \quad \psi_{200} = b\left[1 - \tfrac{1}{3}(\alpha+\beta)r\right] e^{-\beta r}$$

So $\langle \psi_{100} | \psi_{200} \rangle = 0$, and a and b are fixed by $\langle \psi_{100} | \psi_{100} \rangle = \langle \psi_{200} | \psi_{200} \rangle = 1$. α and β are adjustable parameters.

$\Psi(1,2,3)$ must be totally antisymmetric under electron exchange. Defining $\psi_{1\uparrow} \equiv \psi_{100}\binom{1}{0}$, etc., then:

$$\Psi(1,2,3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_{1\uparrow}(1) & \psi_{1\downarrow}(1) & \psi_{2\uparrow}(1) \\ \psi_{1\uparrow}(2) & \psi_{1\downarrow}(2) & \psi_{2\uparrow}(2) \\ \psi_{1\uparrow}(3) & \psi_{1\downarrow}(3) & \psi_{2\uparrow}(3) \end{vmatrix}$$

The determinant is antisymmetric under row exchange as required. Note that this also leads to the Pauli exclusion principle.

Calculate $E_0 \leqslant \langle \Psi | H | \Psi \rangle = f(\alpha, \beta)$ and minimise f with respect to α and β. This gives an answer of $E_0 < -200.8$ eV; compare this to the actual value of $E_0 = -202.5$ eV.

1.7.3 The H^- atom

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{r_{12}}.$$

The simplest wavefunction that achieves binding is:

$$\Psi(a,b) = c\left[e^{-ar_1 - br_2} + e^{-ar_2 - br_1}\right] \frac{1}{\sqrt{2}} \left[\binom{1}{0}_1 \binom{0}{1}_2 - \binom{0}{1}_1 \binom{1}{0}_2 \right]$$

H^-'s ground-state energy satisfies:

$$E_0 \leqslant \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

c is fixed in terms of a and b by $\langle \Psi | \Psi \rangle = 1$, so we minimise the right-hand side with respect to a and b.

This gives: $a = 1.03925$, $b = 0.28309$, so

$$E_0 \leqslant -1.026606 \underbrace{\left(\frac{me^4}{2\hbar^2} \right)}_{13.6\text{ eV}}$$

and this establishes binding, since ionising H^- takes energy $I = -13.6\,\text{eV} - E_0 = 0.36\,\text{eV}$. This means that the atom is bound, and indeed it does exist in the sun's photosphere.

Chapter 2

Scattering theory

2.1 Scattering theory in 1D

A particle moves from left to right with momentum p and energy $\frac{p^2}{2m}$. Its wavefunction is Ae^{ikx} where $k = p/\hbar$. It interacts with a potential $V(x)$ which is assumed to satisfy $V(\pm\infty) = 0$.

In regions where $V = 0$, the Schrödinger equation reads:

$$-\frac{\hbar^2}{2m}\psi'' = E\psi$$

and has solutions $e^{\pm ikx}$. Hence, the particle's wavefunction in the presence of V has asymptotic solutions:

$$\psi(x) \underset{x\to-\infty}{\sim} Ae^{ikx} + Be^{-ikx}, \quad \psi(x) \underset{x\to+\infty}{\sim} Ce^{ikx}$$

Note: If $V \to V_0$ as $x \to \infty$ (rather than $V \to 0$), then

$$\psi(x) \underset{x\to\infty}{\sim} Ce^{ik'x} \text{ where } k' = \sqrt{\frac{2m}{\hbar}(E - V_0)}$$

To interpret this formalism we need a QM continuity equation. We will work in 3D for generality.

The integral

$$\int_V |\psi|^2 \, d^3r$$

is the probability for finding the particle in a *finite* volume V. Then,

$$\begin{aligned}\frac{\partial}{\partial t}\int_V |\psi|^2 \, d^3r &= \int_V \left(\frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t}\right) d^3r \\ &= \frac{i}{\hbar}\int_V (\psi H^*\psi^* - \psi^* H\psi) d^3r\end{aligned}$$

where:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r).$$

Using the fact that:

$$\psi\nabla^2\psi^* - \psi^*\nabla^2\psi = \vec{\nabla}\cdot(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi)$$

and that $V^* = V$, we get:

$$\frac{\partial}{\partial t}\int_V |\psi|^2\, d^3r = -\int_V \vec{\nabla}\cdot\vec{S}\, d^3r,$$

where:

$$\vec{S} = \frac{i\hbar}{2m}(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi),$$

the **probability current density,** defined such that:

$$\frac{\partial}{\partial t}|\psi|^2 + \vec{\nabla}\cdot\vec{S} = 0.$$

Equivalently,

$$-\frac{\partial}{\partial t}\int_V |\psi|^2\, d^3r = \int_V \vec{\nabla}\cdot\vec{S}\, d^3r = \int_{\partial V}\vec{S}\cdot d\vec{A}$$

In words, the change in the probability of finding a particle in V = the net flow of probability in/out through the surface ∂V.

$\vec{S}\cdot d\vec{A}$ is the number of particles passing through $d\vec{A}$ per second, therefore $\vec{S}$ must have dimension $1/\mathrm{L}^2\mathrm{T}$, i.e. flux (in 3D).

For an energy eigenstate,

$$\psi = e^{-iEt/\hbar}\psi_E(\vec{r}),$$

we get

$$\frac{\partial|\psi|^2}{\partial t} = 0 \Rightarrow \vec{\nabla}\cdot\vec{S} = 0.$$

Now consider 1D again. For a particle with definite energy,

$$\vec{\nabla}\cdot\vec{S} = - \Rightarrow \frac{dS}{dx} = 0 \Rightarrow S = \text{const.}$$

So for $x \to -\infty$,

$$S = \frac{\hbar k}{m}|A|^2 - \frac{\hbar k}{m}|B|^2$$

and for $x \to \infty$

$$S = \frac{\hbar k}{m}|C|^2,$$

assuming $V(\infty) = 0$.

Hence,

$$\left|\frac{B}{A}\right|^2 + \left|\frac{C}{A}\right|^2 = 1,$$

or, in words,

$$\frac{\text{Reflected flux} + \text{transmitted flux}}{\text{Incident flux}} = 1.$$

2.2 Examples

2.2.1 Rectangular barrier

Determine the transmission coefficient for a rectangular potential barrier, where:

$$V(x) = \begin{cases} V_0 & \text{if } 0 < x < a \\ 0 & \text{otherwise} \end{cases}$$

We assume the particle is incident from the left with $E < V_0$. We already know that $|T|^2 + |R|^2 = 1$, where $T = B/A$ and $R = C/A$.

For $x < 0$:

$$-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x) \Rightarrow \psi(x) = e^{ikx} + Re^{-ikx}$$

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

For $0 < x < a$:

$$-\frac{\hbar^2}{2m}\psi''(x) + V_0\psi(x) = E\psi(x) \Rightarrow \psi(x) = Ae^{-\mu x} + Be^{\mu x}, \text{ where}$$

$$\mu = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

For $x > a$:

$$-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x) \Rightarrow \psi(x) = Te^{ikx}$$

The problem is to find T and R; ψ and ψ' must be continuous.

At $x = 0$,

$$1 + R = A + B$$
$$ik(1 - R) = \mu(-A + B)$$

and at $x = a$,

$$Ae^{-\mu a} + Be^{\mu a} = Te^{ika}$$
$$\mu(-Ae^{-\mu a} + Be^{\mu a}) = ikTe^{ika}$$

Or in matrix form,

$$\begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} 1 \\ R \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -\mu & \mu \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{2.1}$$

$$\begin{pmatrix} e^{-\mu a} & e^{\mu a} \\ -\mu e^{-\mu a} & \mu e^{\mu a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{ika} & 0 \\ ike^{ika} & 0 \end{pmatrix} \begin{pmatrix} T \\ 0 \end{pmatrix} \tag{2.2}$$

Solving for $\binom{A}{B}$ in (2.1):

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 - \frac{ik}{\mu} & 1 + \frac{ik}{\mu} \\ 1 + \frac{ik}{\mu} & 1 - \frac{ik}{\mu} \end{pmatrix} \begin{pmatrix} 1 \\ R \end{pmatrix}$$

Substituting this into (2.2):

$$Te^{ika}\begin{pmatrix}1\\ik\end{pmatrix}=\begin{pmatrix}\cosh\mu a+\frac{ik}{\mu}\sinh\mu a & \cosh\mu a-\frac{ik}{\mu}\sinh\mu a\\ \mu\sinh\mu a+ik\cosh\mu a & \mu\sinh\mu a-ik\cosh\mu a\end{pmatrix}\begin{pmatrix}1\\R\end{pmatrix}$$

Solving these two equations for R and T:

$$R=\frac{-i(\frac{k}{\mu}+\frac{\mu}{k})\sinh\mu a}{2\cosh\mu a+(\frac{\mu}{k}-\frac{k}{\mu})\sinh\mu a},\quad T=\frac{e^{-ika}}{\cosh\mu a+\frac{1}{2}(\frac{\mu}{k}-\frac{k}{\mu})\sinh\mu a}$$

This gives $|T|^2+|R|^2=1$.

For a high or broad barrier,

$$\mu a=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}a\gg 1.$$

So the transmission coefficient,

$$\begin{aligned}|T|^2&=\frac{1}{\cosh^2(\mu a)+\frac{1}{4}(\frac{\mu}{k}-\frac{k}{\mu})^2\sinh^2\mu a}\\&=\frac{k^2\mu^2}{k^2\mu^2+\frac{1}{4}(k^2+\mu^2)\sinh^2\mu a}\\&\approx 16e^{-2\mu a}\left(\frac{k\mu}{k^2+\mu^2}\right)^2\end{aligned}$$

since $\sinh(x\gg 1)\sim\frac{1}{2}e^x$.

2.2.2 Barrier of arbitrary shape

For a high broad barrier of length L, we found:

$$\begin{aligned}|T|^2&\approx e^{-2L\sqrt{\frac{2m}{\hbar^2}(V_0-E)}}\\&=e^{-2\times\text{barrier width}\times\text{barrier height}},\end{aligned}$$

where $16\left(\frac{k\mu}{k^2+\mu^2}\right)=O(1)$ provided $\frac{\mu}{k}=\sqrt{\frac{V_0-E}{E}}=O(5)$ (or more).

For an arbitrary barrier $V(x)$, find the average height and treat it as a rectangular barrier:

$$\text{Average barrier height}=\frac{\int_a^b dx\,\sqrt{\frac{2m}{\hbar^2}\,(V(x)-E)}}{\text{barrier width}}.$$

Thus,

$$|T|^2=e^{-2\int_a^b dx\sqrt{\frac{2m}{\hbar^2}(V(x)-E)}}$$

2.2.3 Controlled fusion

Controlled fusion in a Tokamak:

$$\mathrm{H}^2 + \mathrm{H}^3 \longrightarrow \underset{3.5\ \mathrm{MeV}}{\mathrm{He}^4} + \underset{14.1\ \mathrm{MeV}}{\mathrm{n}}$$

A blanket of lithium around the reactor core captures neutrons.

$$\mathrm{Li}^6 + \mathrm{n} \longrightarrow \mathrm{He}^4 + \underset{\text{recycled to reactor}}{\mathrm{H}^3} + \underset{\text{heat to turbine}}{4.8\ \mathrm{MeV}}$$

In order to react, the deuterium-tritium pair must be in range of the interparticle nuclear force:

$$R \sim \frac{e^2}{mc^2} \sim 3\ \mathrm{fm} \quad (1\ \mathrm{fm} = 10^{-13}\ \mathrm{cm})$$

A head-on collision will have $l = 0$, and so effective potential seen by deuterium/tritium is:

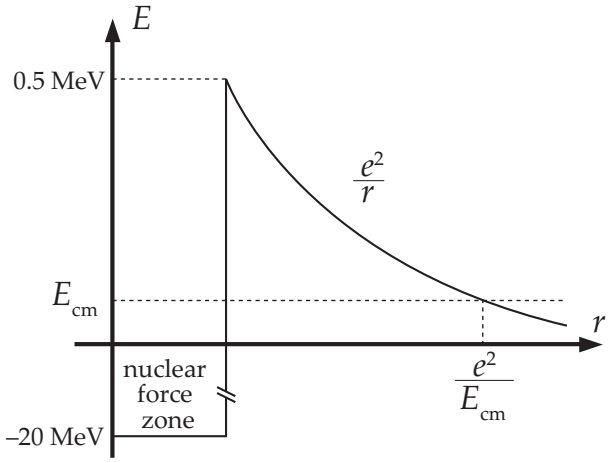

Figure 2.1: The potential seen by D-T pair

So the pair must overcome the Coulomb barrier of $mc^2 \sim 0.5$ MeV. Tokamak operates at $T \sim 10^8$ K $\Rightarrow E_{\mathrm{cm}} \sim 10$ keV. So the probability for barrier transmission is approximately:

$$\exp\left[-2\int_{e^2/mc^2}^{e^2/E_{\mathrm{cm}}} dr\,\sqrt{\frac{2m}{\hbar^2}\left(\frac{e^2}{r} - E_{\mathrm{cm}}\right)}\right]$$

2.3 Scattering theory in 3D

We define a differential scattering cross-section:

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = \frac{d^2N_{\mathrm{sc}}/d\Omega\,dt}{d^2N_{\mathrm{inc}}/dA\,dt}$$

where dN_{inc} is the number of particles crossing dA normal to incident beam, and dN_{sc} is the number of particles scattered into a solid angle $d\Omega$.

Thus, the number of particles scattered into $d\Omega$ per unit time is:

$$\begin{aligned}\frac{d^2N_{\text{sc}}}{d\Omega\, dt} &= \frac{d^2N_{\text{inc}}}{dA\, dt}\frac{d\sigma(\theta,\phi)}{d\Omega} \\ &= \text{incident flux} \times \left(\frac{\partial\sigma}{\partial\Omega}\right)\end{aligned} \tag{2.3}$$

σ has dimension of area, measured in barns. 1 barn $= 10^{-24}$ cm^2.

If the target is another particle, it recoils during collision. So we need to find a 2-body wavefunction in the centre of mass frame from Schrödinger equation:

$$\left[-\frac{\hbar^2}{2\mu} + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

where $\vec{r} = \vec{r}_1 - \vec{r}_2$. This can be writen as:

$$(\nabla^2 + k^2)\psi = U(\vec{r})\psi \tag{2.4}$$

where $U = \dfrac{2\mu V}{\hbar}$ and $E = \dfrac{\hbar^2k^2}{2\mu}$.

We must find a Green function such that:

$$(\nabla^2 + k^2)G(\vec{r} - \vec{r}') = -4\pi S(\vec{r} - \vec{r}')$$

so that the solution of (2.4) is:

$$\psi(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} = -\frac{1}{4\pi}\int d^3r'\, G(\vec{r} - \vec{r}')U(\vec{r}')\psi(\vec{r}') \tag{2.5}$$

We get:

$$G(\vec{r}) = -\frac{1}{\pi r}\frac{d}{dr}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} dp\, \frac{e^{ipr}}{p^2 + k^2 - i\epsilon}$$

This function has poles at $p = \pm\sqrt{k^2 + i\epsilon} = \pm(k + \frac{i\epsilon}{2k})$, so we choose this contour: By

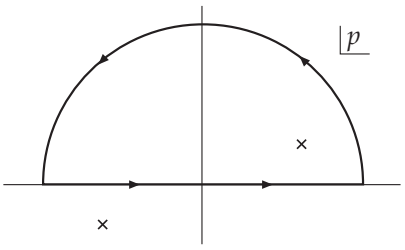

Figure 2.2: The contour used

Cauchy's theorem,

$$\begin{aligned}\oint dp\frac{e^{ipr}}{p^2 - k^2 - i\epsilon} &= \int_{-\infty}^{\infty} dp\frac{e^{ipr}}{p^2 - k^2 - i\epsilon} = 2\pi i + \sum \text{Res} \\ &= \frac{2\pi i + e^{i(k + i\epsilon/2k)}}{2k + i\epsilon/k} \\ &\to \frac{i\pi e^{ikr}}{k} \quad \text{as } \epsilon \to 0.\end{aligned}$$

So,

$$G(\vec{r}) = -\frac{i}{kr}\frac{d}{dr}e^{ikr} = \frac{e^{ikr}}{r}.$$

Hence, (2.5) is:

$$\psi_k^{(+)}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} = -\frac{1}{4\pi}\int d^3r\,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}U(\vec{r})\psi_k^{(+)}(\vec{r}). \tag{2.6}$$

The superscript (+) refers to our choice of G; see later.

We need $\psi_k^{(+)}$ for $r \to \infty$. Suppose $V(\vec{r})$ (and hence $U(\vec{r})$) has range a:

$$V(\vec{r}) \underset{\vec{r}\to\infty}{\sim} e^{-r/a} \quad \text{or} \quad V(\vec{r}) = 0 \text{ for } r > a.$$

Then,

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \underset{r\gg r'}{=} \frac{e^{ikr}e^{-ik\hat{r}\cdot\vec{r}'}}{r}$$

where $\hat{r} = \vec{r}/r$, and:

$$\psi_k^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} - \frac{e^{ikr}}{4\pi r}\int d^3r'\,e^{-ik\hat{r}\cdot\vec{r}'}U(\vec{r}')\psi_k^{(+)}(\vec{r})$$

since terms in the integral in (2.6) in region $r' \gtrsim r$ are suppressed due to rapid fall-off of $U(\vec{r})$ for $r' > a$.

Therefore, at $t = 0$, we have the incoming plane wave:

$$\psi_k(\vec{r}, 0) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} = \psi_{\text{inc}}$$

where $\vec{k} = k\hat{z}$, $E = \dfrac{\hbar^2k^2}{2\mu}$.

For $k > 0$, the particle interacts with the potential. For $t \to \infty$, the particle is scattered and is asymptotically free, with:

$$\begin{aligned}\psi_k^{(+)}(\vec{r}, t) &\underset{r\gg a}{\sim} \frac{1}{(2\pi)^{3/2}}\left(e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r}f(\vec{k}')\right)e^{-iEt/\hbar} \\ &= (\psi_{\text{inc}} + \psi_{\text{sc}})e^{-iEt/\hbar}\end{aligned}$$

where $\vec{k}' = k\hat{r}$; $\hat{r}$ isthe unit vector pointing from scattering centre to the observation point at $\vec{r}$.

So $\hbar k\hat{r} = \hbar\vec{k}'$ is the momentum of the particle scattered in direction $\hat{r}$.

2.3.1 Interpretation of f

The scattered wave is:

$$\psi_{\text{sc}} = \frac{fe^{ikr}}{(2\pi)^{3/2}r}$$

and the scattered flux density is:

$$\vec{S}_{\text{sc}} = \frac{i\hbar}{2\mu}(\psi_{\text{sc}}\vec{\nabla}\psi_{\text{sc}}^* - \psi_{\text{sc}}^*\vec{\nabla}\psi_{\text{sc}})$$

In spherical coordinates,

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\phi}}{r\sin\theta}\frac{\partial}{\partial \phi}$$

$$\Rightarrow \vec{\nabla}\psi_{\text{sc}} = \frac{f}{(2\pi)^{3/2} r}\vec{\nabla} e^{ikr} + O(\tfrac{1}{r^2})$$

$$= \frac{ikf}{(2\pi)^{3/2}} e^{ikr}\hat{r} + O(\tfrac{1}{r^2}).$$

Hence,

$$\vec{S}_{\text{sc}} = \frac{\hbar k |f|^2}{(2\pi)^3 \mu r^2}\hat{r} + (\tfrac{1}{r^3})$$

where $\frac{\hbar k}{\mu} = V =$ initial laboratory frame velocity of m_1.

So the number of particles crossing area $d\vec{A}$ per second of a large sphere centred at the scattering centre is:

$$\frac{d^2 N_{\text{sc}}}{dt} = \vec{S}_{\text{sc}} \cdot d\vec{A} = \frac{V|f|^2}{(2\pi)^3} d\Omega$$

(where $d\vec{A} = r^3 d\Omega\, \hat{r}$.)

ψ_{sc} is a radially outgoing scattered wave. This justifies our choice of boundary condition for G.

The incident particle flux is:

$$\psi_{\text{sc}} = \frac{V}{(2\pi)^{3/2}}\hat{z}$$

and the number of particles crossing $d\vec{A} = dA\,\hat{z}$ is normal to the incident beam is:

$$\frac{d^2 N_{\text{inc}}}{dt\, dA} = \frac{V}{(2\pi)^3} = \text{incident flux.}$$

By definition, differential cross-section is:

$$\frac{d\sigma}{d\Omega} = \frac{d^2 N_{\text{sc}}/d\Omega\, dt}{d^2 N_{\text{inc}}/dA\, dt} = |f|^2.$$

How to solve this problem with wave packets: start with a broad wave packet, centred at z-axis at $t = 0$. Expand in terms of eigenstates of H:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})\right]\psi_k^{(+)} = \frac{\hbar^2 k^2}{2\mu}\psi_k^{(+)}.$$

$$\psi_k^{(+)} \underset{r\to\infty}{\sim} \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} + \text{outgoing spherical wave } e^{ikr}/r.$$

$$\Rightarrow \psi(\vec{r}, 0) = \int d^3k\, \langle \psi_k^{(+)} | \psi(0)\rangle \psi_k^{(+)}(\vec{r}).$$

This requires justification, since $\{\psi_k^{(+)}\}$ may not be complete, V may form bound states. But $\psi_k^{(+)} \sim e^{i\vec{k}\cdot\vec{r}} + \ldots$ and $\{e^{i\vec{k}\cdot\vec{r}}\}$ *are* complete.

At later times,

$$\psi(\vec{r}, t) = \int d^3k\, \langle \psi_k^{(+)} | \psi(0)\rangle \psi_k^{(+)}(\vec{r}) e^{i\hbar k^2 t/2\mu}.$$

Examining this for large times ($Vt \gg a$) but small enough so that the packet has not spread appreciably, find that the initial packet, unchanged by V, still present in the scattered wave-function. There is however a lot of 'fine print', see Merzbacher 3 ed. pp. 286–290.

2.3.2 First Born approximation for f

Recall (2.6):

$$\psi_k^{(+)}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} = -\frac{1}{4\pi}\int d^3r\,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}U(\vec{r})\psi_k^{(+)}(\vec{r}).$$

If this is iterated once, i.e. replacing $\psi_k^{(+)}$ with $e^{i\vec{k}\cdot\vec{r}}/(2\pi)^{3/2}$, we get the **first Born approximation** to f from (2.6):

$$f = -\frac{\mu}{2\pi\hbar^2}\int d^3r\,e^{i\vec{r}'\cdot\vec{r}}V(\vec{r})e^{i\vec{k}\cdot\vec{r}},$$

renaming $r' \to r$, or:

$$f = -\frac{\mu}{2\pi\hbar^2}\underbrace{\int d^3r\,V(\vec{r})e^{-i\Delta\vec{k}\cdot\vec{r}}}_{\text{Fourier transform of } V}.$$

where $\Delta\vec{k} = \vec{k}' - \vec{k}$, the momentum transfer.

This is true for high energies or short-range potentials, and some other cases.

Example: Find the condition for this to be true for:

$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

Solution: One possibility is to demand small distortion even at $r = 0$:

$$\left|\frac{\psi_k^{(+)}(\vec{r}) - \psi_{\text{inc}}(\vec{r})}{\psi_{\text{inc}}(\vec{r})}\right|_{r=0} = \frac{\mu}{2\pi\hbar^2}\left|\int d^3r'\,\frac{e^{ikr'}}{r'}V(r')e^{i\vec{k}\cdot\vec{r}}\right|$$

Chapter 3

Angular momentum

3.1 Introduction

Assume an isolated system of particles. Then all spatial orientations of the system are equivalent. If external central fields are present, orientations about fields' centres are equivalent.

Isotropy of space requires the system's Hamiltonian to be invariant under rotation through an angle $\vec{\phi}$ (equivalent to rotating coordinate frame, however we will adopt the convention of rotating the system) using the right-hand rule for orienting $\vec{\phi}$.

Consider two experimenters O and O' using differently oriented coordinate systems with a common origin. Let R specify their relative orientation through $\vec{\phi}$. Let O prepare, for example, a neutron in state $|\alpha\rangle$ with momentum p moving parallel to x-axis. Let O' prepare a neutron state $|\alpha; R\rangle$ with momentum p moving parallel to the x'-axis.

If O carries out an experiment to determine the probability that state $|\alpha\rangle$ has a definite value of total angular momentum j with z-component m, then O will find this probability is $|\langle j\, m|\alpha\rangle|^2$.

But O can also carry out a similar experiment on the states $|\alpha; R\rangle$, $|j\, m; R\rangle$ prepared by O', and measure the probability $|\langle j\, m; R|\alpha; R\rangle|^2$.

As far as O is concerned, the neutron and measuring apparatus are rotated by R.

The assumption that the rotated state and measuring apparatus have precisely the same physical properties as the original state and measuring apparatus requires:

$$|\langle j\, m; R|\alpha; R\rangle|^2 = |\langle j\, m|\alpha\rangle|^2 .$$

By Wigner's theorem [see Gottfried 1 ed. pp. 226–228], states in O and O' are related by a unitary operator $R(\vec{\phi})$:

$$|\alpha; R\rangle = R(\vec{\phi})|\alpha\rangle, \quad |j\, m; R\rangle = R(\vec{\phi})|j\, m\rangle. \tag{3.1}$$

$R^\dagger = R^{-1}$.

For an infinitesimal rotation about the z-axis, we define:

$$R(\delta\phi_z) = \mathbb{1} - i\,\delta\phi_z \frac{J_z}{\hbar},$$

where J_z is a Hermitian operator with dimension of angular momentum. Note that $RR^\dagger = \mathbb{1} + O(\delta\phi^2)$.

J_z is defined as the *total* z-component of angular momentum and is the generator of rotations about the z-axis. Setting $\delta\phi_z = \frac{\phi_z}{N}$, a finite rotation can be obtained by compounding successive infinitesimal rotations about the z-axis:

$$\begin{aligned} R(\phi_z) &= \lim_{N\to\infty}\left(\mathbb{1} - \frac{iJ_z}{\hbar}\frac{\phi_z}{N}\right)^N \\ &= e^{iJ_z\phi_z/\hbar}. \end{aligned} \tag{3.2}$$

(Similarly for $R(\phi_x)$ and $R(\phi_y)$.

J_x, J_y and J_z operate on a Hilbert space of arbitrary dimension.

Example: An atom with spin up along z-axis is rotated by θ about the x-axis. New spin state is:

$$R|\uparrow\rangle = e^{-iJ_x\theta/\hbar}|\uparrow\rangle.$$

Example: Suppose a 3D vector $\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ is rotated b $\delta\phi_z$ about the z-axis. Physically $\vec{r}$ might represent the spin state of a spin-1 atom, for example. We now that:

$$\begin{aligned} R\vec{r} &= \begin{pmatrix} \cos(\delta\phi_z) & -\sin(\delta\phi_z) & 0 \\ \sin(\delta\phi_z) & \cos(\delta\phi_z) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ &= (1 + \delta\phi_z I_z)\vec{r} + O(\delta\phi_z)^2 \end{aligned} \tag{3.3}$$

where $I_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$.

$$R(\delta\phi_z) = 1 + \delta\phi_z I_z + \ldots \tag{3.4}$$

Similarly, for rotations about the x- and y-axes,

$$R(\delta\phi_x) = 1 + \delta\phi_x I_x + \ldots \tag{3.5}$$

$$R(\delta\phi_y) = 1 + \delta\phi_y I_y + \ldots \tag{3.6}$$

where $I_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$ and $I_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$, and $[I_x, I_y] = I_z$, etc.

Comparing (3.4), (3.5) and (3.6) with equivalents for infinitesimal ϕ, we get that in 3D:

$$J_l = i\hbar I_l, \qquad l = x, y, z$$

and

$$[J_x, J_y] = i\hbar J_z \quad (\text{+cyc.})$$

3.2 Commutation relations

Consider two sequences of infinitesimal rotations on a 3D vector $\vec{r}$:

1. $\delta\phi_x$ about x-axis followed by $\delta\phi_y$ about y-axis
2. $\delta\phi_y$ about y-axis followed by $\delta\phi_x$ about x-axis

Then get, from previous example,

$$\vec{r}' = (1 + \delta\phi_y I_y + \delta(\phi_y)^2)(1 + \delta\phi_x I_x + \delta(\phi_x)^2)\vec{r}$$
$$\vec{r}'' = (1 + \delta\phi_x I_x + \delta(\phi_x)^2)(1 + \delta\phi_y I_y + \delta(\phi_y)^2)\vec{r}$$

Hence,

$$\begin{aligned}\vec{r}'' - \vec{r}' &= \delta\phi_x\delta\phi_y[I_x, I_y]\vec{r} + O(\delta\phi^3) \\ &= \delta\phi_x\delta\phi_y I_z\vec{r} + O(\delta\phi^3)\end{aligned}$$

In terms of Js,

$$\begin{aligned}\vec{r}'' - \vec{r} &= \delta\phi_x\delta\phi_y\left[-\frac{iJ_x}{\hbar}, -\frac{iJ_y}{\hbar}\right]\vec{r} + O(\delta\phi^3) \\ &= \delta\phi_x\delta\phi_y\left(-\frac{iJ_z}{\hbar}\right) + O(\delta\phi^3)\end{aligned} \tag{3.7}$$

These rotations act on objects in 4D space. To each such rotation, there corresponds a unitary mapping in the Hilbert space of states.

Postulate that the analogue of (3.7) holds on the appropriate Hilbert space of more general states. So:

$$\begin{aligned}|\alpha''\rangle - |\alpha'\rangle &= \left[R(\delta\phi_x)R(\delta\phi_y) - R(\delta\phi_y)R(\delta\phi_x)\right]|\alpha\rangle \\ &= \delta\phi_x\delta\phi_y\left[-\frac{iJ_x}{\hbar}, -\frac{iJ_y}{\hbar}\right]|\alpha\rangle + O(\delta\phi^3) \\ &= \delta\phi_x\delta\phi_y\left[-\frac{iJ_z}{\hbar}\right]|\alpha\rangle + O(\delta\phi^3),\end{aligned}$$

by postulate.

Or,

$$[J_x, J_y] = i\hbar J_z \quad (\text{+cyc.})$$

i.e.

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k, \quad \{i, j, k\} = \{1, 2, 3\}$$

This is the basic condition on generators of rotations ($\equiv$ components of system's *total* angular momentum). No reference is made to the details of the structure of the system, only properties of rotations.

3.3 Quantisation of angular momentum

Set $\hbar = 1$ here, so $[J_x, J_y] = iJ_z$ etc.

Verify that J^2 verifies $[J^2, J_i] = 0$. Take J^2, J_z as a compatible set, and $|jm\rangle$ as eigenstates of J^2 *and* J_z. So,

$$J^2|jm\rangle = j(j+1)|jm\rangle$$
$$J_z|jm\rangle = m|jm\rangle$$

We have chosen the J^2 eigenvalue by convention. Since J^2 is positive semidefinite, $j(j+1) \geqslant 0$.

Let $J_\pm = J_x \pm iJ_y$. Then get:

$$[J_z, J_+] = J_+ \tag{3.8}$$
$$[J_z, J_-] = J_- \tag{3.9}$$
$$[J_+, J_-] = 2J_z \tag{3.10}$$
$$[J^2, J_\pm] = 0 \tag{3.11}$$
$$\tag{3.12}$$

Also,

$$\begin{aligned} J_+J_- &= (J_x + iJ_y)(J_x - iJ_y) \\ &= J_x^2 + J_y^2 + J_z \\ &= J^2 - J_z(J_z - 1) \end{aligned} \tag{3.13}$$

Likewise,

$$J_-J_+ = J^2 - J_z(J_z + 1) \tag{3.14}$$

Consider $J^2J_\pm|jm\rangle = J_\pm J^2|jm\rangle = j(j+1)J_\pm|jm\rangle$ [by (3.12)]. (3.9) and (3.10) give:

$$\begin{aligned} J_zJ_\pm|jm\rangle &= (J_\pm J_z \pm J_\pm)|jm\rangle \\ &= (m \pm 1)J_\pm|jm\rangle \end{aligned}$$

Thus,

$$J_\pm|jm\rangle = \text{eigenstates of } J^2,\ J_z \text{ with eigenvalues } j(j+1) \text{ and } m \pm 1 \text{ respectively.}$$

The norms of $J_+|jm\rangle$ $J_-|jm\rangle$ are, respectively,

$$\langle jm|J_-J_+|jm\rangle = \underbrace{[j(j+1) - m(m+1)}_{\text{ROOTS: } m=j, m=-j-1}\langle jm|jm\rangle \text{ [by (3.14)]}$$

$$\langle jm|J_+J_-|jm\rangle = \underbrace{[j(j+1) - m(m-1)}_{\text{ROOTS: } m=-j, m=j+1}\langle jm|jm\rangle \text{ [by (3.13)]}$$

Since these must both be non-negative,

$$-j \leqslant m \leqslant j. \tag{3.15}$$

Suppose $J_+|jm\rangle = 0$. A necessary and sufficient condition for this is the vanishing of the vector's norm, assuming $|jm\rangle \neq 0$.

$$\begin{aligned} & J_+|jm\rangle = 0 \\ \Leftrightarrow\ & j(j+1) - m(m+1) = 0 \\ \Rightarrow\ & m = j. \end{aligned} \tag{3.16}$$

Likewise,

$$\begin{aligned} & J_-|jm\rangle = 0 \\ \Leftrightarrow\ & j(j+1) - m(m-1) = 0 \\ \Rightarrow\ & m = -j. \end{aligned} \tag{3.17}$$

Consider $J_+^p|j,m\rangle \propto |j,m+p\rangle$ for $p = 0,1,2,\ldots$ Due to (3.15), $m+p \leqslant j$. Hence there is an integer $N \geqslant 0$ such that:

$$J_+^{N+1}|j,m\rangle \propto J_+|j,m+N\rangle = 0.$$
$$\Rightarrow m+N = j \text{ [from (3.16)]} \tag{3.18}$$

(Otherwise, $|j,m+N\rangle = 0$ which is extremely uninteresting)

Consider $J_-^q|j,m\rangle \propto |j,m-q\rangle$ for $q = 0,1,2,\ldots$ Due to (3.15), $m-q \leqslant -j$. Hence there is an integer $M \geqslant 0$ such that:

$$J_-^{M+1}|j,m\rangle \propto J_-|j,m-M\rangle = 0.$$
$$\Rightarrow m-M = j \text{ [from (3.17)]} \tag{3.19}$$

Combining (3.18) and (3.19) gives that $2j = M+N = 0,1,2,\ldots$

$$\Rightarrow j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots$$

Equations (3.15), (3.18) and (3.19) give:

$$m = -j, -j+1, \ldots, j.$$

Remember that j and m are in units of $\hbar$ here.

Note: In deriving these, we have used:

- $[J_x, J_y] = i\hbar J_z$
- J_i Hermitian
- $|jm\rangle$ is in a Hilbert space

…and that's all!

3.4 Conservation

The expectation of an observable A in a state $|\alpha'\rangle$ obtained by rotating the system about the z-axis is:

$$\langle\alpha'|A|\alpha'\rangle = \langle\alpha|e^{iJ_z\phi_z/\hbar}Ae^{-iJ_z\phi_z/\hbar}|\alpha\rangle$$

If $[J_z, A] = 0$, the result of measurement of A is independent of the system's orientation in x-y plane; and similarly for x- and y-axes. Hence, *an observable is rotation invariant if it commutes with J_x, J_y and J_z.* If a system's Hamiltonian is rotationally invariant,

$$[\vec{J}, H] = 0 \Longrightarrow \vec{J} = \text{constant}.$$

3.4.1 Degeneracy

If the system's Hamiltonian is rotationally invariant, $[\vec{J}, H] = 0$. Since $[J^2, J_z] = 0$, we can construct simultaneous eigenstates of H, J^2 and J_z, i.e.

$$H|Ejm\rangle = E|Ejm\rangle; \qquad J^2|Ejm\rangle = j(j+1)\hbar^2|Ejm\rangle; \qquad J_z|Ejm\rangle = m\hbar|Ejm\rangle.$$

Since $m = -j,\ldots,j$, each energy level with angular momentum j is $(2j+1)$-fold degenerate.

Proof that E is m-independent:
Suppose $H|Ejm\rangle = E(m)|Ejm\rangle$. Then:

$$\begin{aligned} J_+H|Ejm\rangle &= E(m)J_+|Ejm\rangle \\ &= H(J_+|Ejm\rangle) \\ &= E(m+1)J_+|Ejm\rangle \\ \Rightarrow E(m+1) &= E(m) \quad \text{QED.} \end{aligned}$$

3.5 Representations of $J_{x,y,z}$

We already found a representation of $J_{x,y,z}$ for the case $j = 1$. Recall:

$$J_x = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad J_y = \hbar \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad J_z = \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

So $[J_x, J_y] = J_z$ (+ cyc.) And $J^2 = 2\hbar^2 \Rightarrow j = 1$, since $J^2 = \hbar^2 j(j+1)$.

For general j, we know (from (3.14)):

$$J_\pm|j,m\rangle = c_\pm|j,m\pm 1\rangle$$

where $c_\pm$ are to be determined.

The norm of $J_+|jm\rangle$ is:

$$\begin{aligned} \langle jm|J_-J_+|jm\rangle &= \langle jm|J^2 - J_z(J_z+1)|jm\rangle \\ &= \hbar^2 j(j+1) - \hbar^2 m(m+1) \\ &= |c_+|^2. \end{aligned}$$

Set the phase of c_+ to zero. Then:

$$J_+|j,m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|j,m+1\rangle \tag{3.20}$$

Likewise, from (3.13),

$$J_-|j,m\rangle = \hbar\sqrt{j(j-1) - m(m-1)}|j,m-1\rangle \tag{3.21}$$

MEMORISE (3.20) AND (3.21)!

(3.20) and (3.21), together with $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{1}{2}(J_- - J_+)$, and $\langle jm|jm'\rangle = \delta_{m\,m'}$, can be used to find matrix representations of $J_{x,y,z}$.

3.5.1 Example

Find a matrix representation of $J_{\mathrm{x,y,z}}$ for $j = \frac{1}{2}$.
Suppose $j : |jm\rangle \to |m\rangle$. Then from (3.20) and (3.21):

$$\begin{aligned} \langle\tfrac{1}{2}|J_+|\tfrac{1}{2}\rangle &= 0 = \langle\tfrac{1}{2}|J_-|\tfrac{1}{2}\rangle \\ \langle-\tfrac{1}{2}|J_+|-\tfrac{1}{2}\rangle &= 0 = \langle-\tfrac{1}{2}|J_-|-\tfrac{1}{2}\rangle \\ \langle-\tfrac{1}{2}|J_+|\tfrac{1}{2}\rangle &= 0 = \langle\tfrac{1}{2}|J_-|-\tfrac{1}{2}\rangle \\ \langle\tfrac{1}{2}|J_+|-\tfrac{1}{2}\rangle &= \hbar = \langle-\tfrac{1}{2}|J_-|\tfrac{1}{2}\rangle \end{aligned}$$

Using $J_x = \frac{1}{2}(J_+ + J_-)$ and $J_y = \frac{1}{2}(J_- - J_+)$, get:

$$\langle \tfrac{1}{2}|J_x|\tfrac{1}{2}\rangle = 0 \qquad \langle \tfrac{1}{2}|J_x|-\tfrac{1}{2}\rangle = \tfrac{\hbar}{2}$$
$$\langle -\tfrac{1}{2}|J_x|\tfrac{1}{2}\rangle = \tfrac{\hbar}{2} \qquad \langle -\tfrac{1}{2}|J_x|-\tfrac{1}{2}\rangle = 0$$

and:

$$\langle \tfrac{1}{2}|J_y|\tfrac{1}{2}\rangle = 0 \qquad \langle \tfrac{1}{2}|J_y|-\tfrac{1}{2}\rangle = -\tfrac{i\hbar}{2}$$
$$\langle -\tfrac{1}{2}|J_y|\tfrac{1}{2}\rangle = \tfrac{i\hbar}{2} \qquad \langle -\tfrac{1}{2}|J_y|-\tfrac{1}{2}\rangle = 0$$

Finally,

$$\langle \tfrac{1}{2}|J_z|\tfrac{1}{2}\rangle = \tfrac{\hbar}{2} \qquad \langle \tfrac{1}{2}|J_z|-\tfrac{1}{2}\rangle = 0$$
$$\langle -\tfrac{1}{2}|J_z|\tfrac{1}{2}\rangle = 0 \qquad \langle -\tfrac{1}{2}|J_z|-\tfrac{1}{2}\rangle = -\tfrac{\hbar}{2}.$$

Hence,

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

3.6 Spherical harmonics

Consider the amplitude for finding a particle with angularm momentum ℓ, m in the direction $\hat{n}$ specified by spherical angles θ, ϕ.

$$\langle \hat{n}|\ell m\rangle = \langle \theta, \phi|\ell m\rangle = Y_{\ell m}(\theta, \phi).$$

We have, from (3.20) and (3.21),

$$L_\pm Y_{\ell m} = \hbar\sqrt{\ell(\ell \pm 1) - m(m \pm 1)}\, Y_{\ell m \pm 1}$$
$$L_\pm Y_{\ell m} = \hbar m Y_{\ell m},$$

where $\ell = 0, 1, 2, \ldots$ and $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$.

Even though $\vec{L}$ satisfies the basic commutator $[L_x, L_y] = i\hbar L_z$ etc. ℓ can only take values $0, 1, 2, \ldots$ Classical degrees of freedom have integer values of ℓ. See Gottfried 1 ed. p. 86.

3.7 Intrinsic angular momentum

There exist particles with nonvanishing angular momentum, **spin**, in their rest frames. Denote rest-frame angular momentum operator by $\vec{S}$. Then, $[S_x, S_y] = i\hbar S_z$, etc. Eigenvalues of $S^2 = S_x^2 + S_y^2 + S_z^2$ are $s(s+1)\hbar$, where $s = 0, \frac{1}{2}, 1, \ldots$ Integers for bosons, half-integers for fermions.

If a particle has orbital angular momentum $\vec{L}$, the total angular momentum operator is

$$\vec{J} = \vec{L} + \vec{S}.$$

$\vec{S}$ is not classical and cannot be represented by $\vec{r} \times \vec{p}$. Therefore, we expect:

$$[L_i, S_i] = 0.$$

3.7.1 Example

2-component spinors describe the spin states of non-relativistic spin-$\frac{1}{2}$ particles. Let:

$$|s = \tfrac{1}{2}, S_z = \tfrac{1}{2}\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right),$$
$$|s = \tfrac{1}{2}, S_z = -\tfrac{1}{2}\rangle = \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right).$$

Hence, with $S_z = \frac{\hbar}{2}\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$, then:

$$S_z|\tfrac{1}{2}, \tfrac{1}{2}\rangle = S_z\left(\begin{smallmatrix}1\\0\end{smallmatrix}\right) = \tfrac{\hbar}{2}|\tfrac{1}{2}, \tfrac{1}{2}\rangle$$
$$S_z|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = S_z\left(\begin{smallmatrix}0\\1\end{smallmatrix}\right) = -\tfrac{\hbar}{2}|\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

and:

$$S^2|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle = \tfrac{3}{4}\hbar^2|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle \Rightarrow s = \tfrac{1}{2}.$$

3.8 Addition of angular momenta

Assume two systems with independent momentum operators $\vec{J}_1$ and $\vec{J}_2$, with $[\vec{J}_1, \vec{J}_2] = 0$.

Problem: Construct the eigenkets and determine the allowed eigenvalues of the total angular momentum operator $\vec{J} = \vec{J}_1 + \vec{J}_2$. Note that since $[J_x, J_y] = iJ_z$, etc., the allowed values of j are $0, \frac{1}{2}, 1, \ldots$

Solution: Two complete sets of angular momentum operators for the complete system are:

(a) $J_1^2, J_{1z}, J_2^2, J_{2z}$

(b) J^2, J_z, J_1^2, J_2^2

Kets associated with set (a) are known:

$$|j_1 m_1\, j_2 m_2\rangle = |j_1 m_1\rangle|j_2 m_2\rangle$$

which we will denote $|m_1 m_2\rangle$ for simplicity.

These satisfy:

$$J_i^2|m_1 m_2\rangle = j_i(j_i + 1)|m_1 m_2\rangle$$
$$J_{iz}|m_1 m_2\rangle = m_i|m_1 m_2\rangle$$

where $i = 1, 2$.

The kets $|j_1 j_2 jm\rangle$ (which we will write as $|jm\rangle$) associated with set (b) are unknown. By definition, they satisfy:

$$J^2|jm\rangle = j(j+1)|jm\rangle$$
$$J_z|jm\rangle = m|jm\rangle$$
$$J_i^2|jm\rangle = j_i(j_i+1)|jm\rangle$$

(We assume $\langle jm|jm\rangle = 1$.)

Since

$$J_1^2|j_1 j_2 jm\rangle = j_1(j_1+1)|j_1 j_2 jm\rangle,$$

and

$$J_1^2|j_1' m_1 j_2 m_2\rangle = j_1'(j_1'+1)|j_1' m_1 j_2 m_2\rangle,$$

then:

$$\langle j_1 j_2 jm|j_1' m_1 j_2 m_2\rangle = \langle jm|m_1 m_2\rangle = 0$$

unless $j_1 = j_1'$.

The set $\{|m_1 m_2\rangle\}$ spans a $(2j+1)(2j+1)$-dimensional subspace of the infinite-dimensional Hilbert space of states, i.e.:

$$\sum |m_1 m_2\rangle\langle m_1 m_2| = \mathbb{1}$$

where the sum is over $-j_1 \leqslant m_1 \leqslant j_1$ and $-j_2 \leqslant m_2 \leqslant j_2$. Therefore, the unknown kets $|jm\rangle$ in this subspace can be represented in terms of the known kets $|m_1 m_2\rangle$:

$$|jm\rangle = \sum_{m_1 m_2} |m_1 m_2\rangle\langle m_1 m_2|jm\rangle \tag{3.22}$$

where $\langle m_1 m_2|jm\rangle = \langle j_1 m_1 j_2 m_2|j_1 j_2 jm\rangle$ are called **Clebsch–Jordan coefficients**.

Since $J_z = J_{1z} + J_{2z}$,

$$(J_{1z} + J_{2z})|jm\rangle = m|jm\rangle$$
$$(J_{1z} + J_{2z})|m_1 m_2\rangle = (m_1 + m_2)|m_1 m_2\rangle.$$

Hence,

$$\langle jm|m_1 m_2\rangle = 0$$

unless $m = m_1 + m_2$. So m must equal $m_1 + m_2$.

Since $\langle jm|m_1 m_2\rangle = 0$, the largest value of $m = j_1 + j_2$, $\Rightarrow$ the largest value of j is $j_1 + j_2$. Otherwise, $|J_\pm|jm\rangle| = 0$ (see earlier). There is only one state with $j = j_1 + j_2$ and $m = j$:

$$\begin{aligned} |j\,j\rangle &= |j_1 j_2\rangle \\ &\equiv |j_1\,j_1\rangle|j_2\,j_2\rangle \end{aligned}$$

We have adopted the phase convention for the CG coefficient: $\langle j_1 j_2|jj\rangle = \mathbb{1}$.

There are two linearly independent kets $|m_1 m_2\rangle$ with $m = j_1 + j_2 - 1$:

$$|m_1 m_2\rangle = |j_1, j_2 - 1\rangle, \qquad |m_1 m_2\rangle = |j_1 - 1, j_2\rangle$$

One linear combination must be associated with $j = j_1 + j_2$, and the other is associated with $j = j_1 + j_2 - 1$. Hence, we can generate a table:

Value of m	**Allowed values of j**	**No. of kets**
$j_1 + j_2$	$j_1 + j_2$	1
$j_1 + j_2 - 1$	$j_1 + j_2$, $j_1 + j_2 - 1$	2
$j_1 + j_2 - 2$	$j_1 + j_2$, $j_1 + j_2 - 1$, $j_1 + j_2 - 3$	3
$\vdots$	$\vdots$	$\vdots$

For each allowed value of j_1 there are $2j+1$ kets $|jm\rangle$. These kets, for the allowed values of j, also span the $(2j_1+1)(2j_2+1)$-dimensional subspace.

That is,

$$|m_1 m_2\rangle = \sum_{j\,m} |jm\rangle\langle jm|m_1 m_2\rangle$$

Note: This implies that the CG coefficients are matrix elements of a unitary operator connecting two alternative bases in the $(2j_1+1)(2j_2+1)$-dimensional Hilbert space.

There is only one linearly independent ket $|jm\rangle$ for each value jm. Why?

Because there is no independent Hermitian operator constructed from $\vec{J}_1$, $\vec{J}_2$ that commutes with J^2, J_z, J_1^2, J_2^2. If there were such an operator, say K, then we could have simultaneous eigenstates $|j_1 j_2 jmk\rangle$ giving degeneracy due to the allowed values of $k = k_1, k_2, \ldots$ with $\langle jmk_i|jmk_j\rangle = \delta_{ij}$. But there is no such operator.

So we must have:

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

where $j_{\min} + N = j_1 + j_2$, $N = 1, 2, \ldots$

Use formula:

$$\sum_{n=M-N}^{M} (2n+1) = (2M-N+1)(N+1) \tag{3.23}$$

Hence,

$$\sum_{j=j_1+j_2-N}^{j_1+j_2} (2j+1) = (2j_1+2j_2-N+1)(N+1) = (2j_1+1)(2j_2+1)$$

or,

$$(N-2j_1)(N-2J-2) = 0 \Rightarrow N = 2j_1, \text{ or } 2j_2.$$

Must have $j_{\min} = j_1 + j_2 - N \geqslant 0$ since $j = 0, \frac{1}{2}, \ldots$ So:

$$N = \begin{cases} 2j_2 \text{ if } j_1 > j_2 & \Rightarrow j_{\min} = j_1 - j_2 \\ 2j_1 \text{ if } j_2 > j_1 & \Rightarrow j_{\min} = j_2 - j_1 \end{cases}$$

So we conclude: The spectrum of J^2, where $\vec{J} = \vec{J}_1 + \vec{J}_2$ is:

$$j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|.$$

Eigenstates are given by:

$$|jm\rangle = \sum_{\substack{-j_1 \leqslant m_1 \leqslant j_1 \\ -j_2 \leqslant m_2 \leqslant j_2}} \langle m_1 m_2|jm\rangle |m_1 m_2\rangle$$

where $m = m_1 + m_2$.