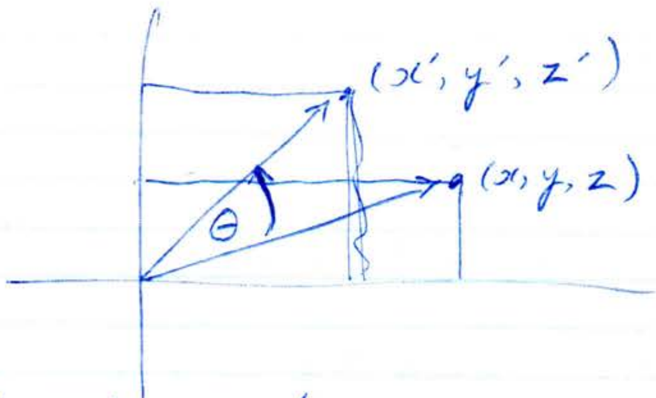

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\left.\begin{array}{l} x' = \cos\theta\, x - \sin\theta\, y \rightarrow x - \theta y \\ y' = \sin\theta\, x + \cos\theta\, y \rightarrow y + \theta x \end{array}\right\} \theta \ll 1.$$
$$z' = z$$

Problem - work out 2×2 representation of D_θ in spinor space.

Commutation Rules for $\underline{J}$

$D_\alpha = 1 - i\alpha J_z$ rotates a system through infinitesimal angle α about z-axis. Suppose $\underline{A}$ is a vector operator with expectation value

$$\langle \underline{A} \rangle = \langle A_x\rangle \hat{i} + \langle A_y\rangle \hat{j} + \langle A_z\rangle \hat{k}.$$

$\langle A_x\rangle' = \langle A_x\rangle - \alpha\langle A_y\rangle$

$\langle A_y\rangle' = \langle A_y\rangle + \alpha\langle A_x\rangle$

$\langle A_z\rangle' = \langle A_z\rangle$

The rule for transforming operators is

$$A_x' = D_\alpha^\dagger A_x D_\alpha$$

$$A_x' = (1 + i\alpha J_z) A_x (1 - i\alpha J_z)$$

$$= A_x + i\alpha (J_z A_x - A_x J_z)$$

ie $\langle A_x' \rangle = \langle A_x \rangle + i\alpha \langle [J_z, A_x] \rangle$

$$\therefore \; i\alpha [J_z, A_x] = -\alpha A_y$$

or $[J_z, A_x] = i A_y$

- We have only used the requirement that J_z generate rotations.

Problem - verify the above if $\underset{\sim}{A} = \underset{\sim}{P}$.

If $\underset{\sim}{A} = \underset{\sim}{J}$, then

$$\left.\begin{aligned} [J_z, J_x] &= i J_y \\ [J_x, J_y] &= i J_z \\ [J_y, J_z] &= i J_x \\ [J_i, J_j] &= i \varepsilon_{ijk} J_k \end{aligned}\right\} \quad \underset{\sim}{J} \times \underset{\sim}{J} = i \underset{\sim}{J} .$$

- Note that we have assumed nothing about $\underset{\sim}{J}$, other that it generate rotations.

Other Symmetry Operations

1/ Parity - reflection through the origin.

$$\left.\begin{aligned} x &\to -x \\ y &\to -y \\ z &\to -z \end{aligned}\right\} \quad \underset{\sim}{r} \to -\underset{\sim}{r}$$

$$\therefore \; \underset{\sim}{P} = \frac{\hbar}{i} \nabla \to -\underset{\sim}{P}$$

$\underset{\sim}{l} = \underset{\sim}{r} \times \underset{\sim}{p}$ is unchanged.

U_p = parity operator.

$U_p^\dagger \underset{\sim}{r} U_p = -\underset{\sim}{r}$

but $U_p^\dagger \underset{\sim}{l} U_p = \underset{\sim}{l}$

$\therefore [U_p, \underset{\sim}{l}] = 0.$

Since U_p commutes with $H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$, L^2, L_z, the simultaneous eigenfunctions are characterized by definite parity.

ie $U_p |\gamma l m\rangle = c|\gamma l m\rangle$

Since $U_p^2 = 1$, $c = \pm 1$.

eg. $U_p Y_l^m = (-1)^l Y_l^m$

since Y_l^m contains only odd powers of $\sin\theta$ or $\cos\theta$ for l odd and

$\sin(\theta+\pi) = -\sin\theta$, $\cos(\theta+\pi) = -\cos\theta$.

Magnetic fields - invariant under parity.

Electric fields - change sign under parity.

As a result, parity violating transitions are induced by the Stark effect.

β-decay.

Time Reversal.

~~...~~ Time reversal ~~operation~~ symmetry arises from the observation that if $\Psi(\underline{r}, t)$ satisfies

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\underline{r})\Psi$$

then $\Psi^*(\underline{r}, -t)$ satisfies the same equation, provided $V(\underline{r})$ is real.

Θ = time reversal operator.

$$\Theta \underline{r} \Theta^{-1} = \underline{r}$$

$$\Theta \underline{p} \Theta^{-1} = -\underline{p}$$

$$\Theta \underline{J} \Theta^{-1} = -\underline{J}.$$

If initial conditions are the same, then

$$\Psi^*(\underline{r}, -t) = \Psi(\underline{r}, t)$$

$$\Psi(\underline{r}, -t) = \Psi^*(\underline{r}, t) = \Theta\Psi(\underline{r}, t)$$

For stationary states,

$$\Psi(\underline{r}, t) = \psi(\underline{r}) e^{-iEt/\hbar}$$

Thus the stationary states can always be chosen such that $\psi(\underline{r})$ is real. (in co-ord. rep.)

Θ has the properties

$$\Theta \Psi(\underline{r}, t) = \Psi^*(\underline{r}, t)$$

If the time development is given by

$$\Psi(t) = e^{-iHt/\hbar}\,\Psi(0)$$

then the time-reversed solution evolves into

$$\Theta\Psi(-t) = e^{-iHt/\hbar}\,\Theta\Psi(0)$$

or $\Theta\Psi(t) = e^{iHt/\hbar}\,\Theta\Psi(0)$

Thus $\Theta e^{-iHt/\hbar} = e^{iHt/\hbar}\,\Theta$.

If Θ is unitary, then

$$-\Theta H = H\Theta$$

$\Rightarrow$ for every stationary state with energy E, there is another stationary state with energy $-E$. This contradicts observation.

$\therefore$ Θ is anti-unitary.

$$\left.\begin{aligned}\Theta(\Psi_1 + \Psi_2) &= \Theta\Psi_1 + \Theta\Psi_2 \\ \Theta a\Psi_1 &= a^*\Theta\Psi_1\end{aligned}\right\}$$ antilinear.

If $|\alpha\rangle$ is an arbitrary vector which is invariant under time reversal, then

$$\Theta|\alpha\rangle = |\alpha\rangle$$

Suppose $|m\rangle$ is a complete set of stationary eigenfunctions of H.

$\Theta|m\rangle = |m\rangle$ if H is real.

$$|\alpha\rangle = \sum_m |m\rangle\langle m|\alpha\rangle$$

$$\Theta|\alpha\rangle = \sum_m |m\rangle\langle m|\alpha\rangle^* = |\alpha\rangle$$

$\therefore$ the expansion coefs. $\langle m|\alpha\rangle$ are real.

eg. suppose $|\alpha\rangle = A|n\rangle$

$$\Theta|\alpha\rangle = \Theta A\Theta^{-1}\Theta|n\rangle$$

ie let $|\alpha\rangle = A|n\rangle$
Then $\Theta|\alpha\rangle = |\alpha\rangle$
if $\Theta A\Theta^{-1} = A$

If $\Theta A\Theta^{-1} = A$, then

$$\langle m|A|n\rangle^* = \langle m|A|n\rangle$$

ie. any operator which is invariant under time reversal can be represented by a real matrix.

(go to p. 11)

Group Representations

- An abstract set of group elements can always be represented by $n \times n$ matrices for one or more values of n, resulting in an n-dimensional representation.

- What do we mean by representation?

~~To~~ For every element a, there is an $n \times n$ matrix $R(a)$ such that if $c = ab$

$$R(c) = R(a)\,R(b)$$

- All groups are represented by the identity ~~mat~~ representation.

Books on group theory

1. Meijer and Bauer "Group Theory, the application to Q.M." (North Holland, 1962).

2. Hammermesh "Group Theory and its applications to physical problems" (Addison Wesley, 1962).

3. Tinkham "Group Theory and Q.M." (McGraw-Hill, 1964).

4. H. Weyl "The Theory of Groups and Q.M." (Dover, 1931).

- What is the relevance of group theory to Q.M.?

Suppose that H has an n-fold degenerate eigenvalue E. Then the corresponding eigenvectors $|E i\rangle$ $i = 1, \ldots, n$ span a subspace $\mathcal{M}_E$ of Hilbert space.

Let ϕ_E be any vector in $\mathcal{M}_E$ and S ~~an~~ a symmetry transform - ie $HS = SH$.

Then $HS\phi_E = SH\phi_E = ES\phi_E$

ie if ϕ_E is an eigenvector of H lying in $\mathcal{M}_E$, then so is $S\phi_E$, since the eigenvalue is still E. ie. all possible symmetry operations map $\mathcal{M}_E$ into itself.

The transformation of vectors in $\mathcal{M}_E$ into itself is represented by the matrix elements $\langle i|S|j\rangle$ of the vectors $|i\rangle$ which span $\mathcal{M}_E$.

ie. suppose $|a\rangle$ is any state in $\mathcal{M}_E$.

$$|a\rangle = \sum_i a_i |i\rangle \quad , \quad a_i = \langle a|i\rangle$$

Then $S|a\rangle = \sum_i a_i S|i\rangle$

but $S|i\rangle = \sum_j |j\rangle\langle j|S|i\rangle$

$$\therefore \quad S|a\rangle = \sum_{ij} a_i |j\rangle\langle j|S|i\rangle = \sum_j b_j |j\rangle$$

ie. $b_j = \sum_i \langle j|S|i\rangle a_i = \sum_i S_{ji} a_i$

The matrices S_{ji} form a representation of the symmetry group.

Theorem

To every n-fold degenerate eigenvalue of the Hamiltonian, there corresponds an n-dimensional representation of the symmetry group. The converse is also true. The study of group theory is useful in classifying and labelling the eigenvalues.

Different linear combinations of basis vectors lead to different matrix representations for the symmetry operations, but these are considered equivalent. They differ by only a unitary transform or similarity transform.

Reduction of Representation.

- If the vector space $\mathcal{M}$ is composed of two parts ~~such that~~ $\mathcal{M}_1$ and $\mathcal{M}_2$ such that $\mathcal{M}_1$ transforms into itself and $\mathcal{M}_2$ transforms into itself, with no intermixing, then a set of basis vectors can be found such that the matrix representations assume a block-diagonal form.

$|1\rangle \cdots |r\rangle$ span $\mathcal{M}_1$
$|r+1\rangle \cdots |n\rangle$ span $\mathcal{M}_2$

$$S_{ij} = \begin{pmatrix} S_{11} & \cdots & S_{1r} & & & \\ \vdots & & \vdots & & & \\ S_{r1} & \cdots & S_{rr} & & & \\ & & & S_{r+1,r+1} & \cdots & S_{r+1,n} \\ & & & \vdots & & \vdots \\ & & & S_{n,r+1} & \cdots & S_{nn} \end{pmatrix}$$

$$= \begin{pmatrix} S_1 & 0 \\ 0 & S_2 \end{pmatrix}$$

$$T = \begin{pmatrix} T_1 & 0 \\ 0 & T_2 \end{pmatrix} \qquad ST = \begin{pmatrix} S_1T_1 & 0 \\ 0 & S_2T_2 \end{pmatrix}$$

ie. the submatrices S_1, T_1 and S_2, T_2 themselves form representations of the group.

We need only choose the basis vectors such that each one lies entirely in $\mathfrak{M}_1$ or in $\mathfrak{M}_2$.

Irreducible Representations of Rotation Group.

J_x, J_y, and J_z are the generators of infinitesimal rotations. Since an arbitrary rotation can be composed out of these, we want to find a set of eigenfunctions which is irreducible w r t J_x, J_y and J_z.

- Introduce operators $J_\pm = J_x \pm i J_y$

From commutation rules:

$$J_\pm J_z - J_z J_\pm = \mp\hbar J_\pm .$$

and $J^2 = J_x^2 + J_y^2 + J_z^2 = J_- J_+ + J_z^2 + J_z = J_+ J_- + J_z^2 - J_z$

~~Suppose $|j\rangle$ is an eigenvector~~

Since J_z and J^2 commute, we can find simultaneous eigenvectors $|\lambda m\rangle$ such that

$$J_z |\lambda m\rangle = m\hbar |\lambda m\rangle$$

$$J^2 |\lambda m\rangle = \lambda\hbar^2 |\lambda m\rangle .$$

I. - First prove that for a given λ, there is a largest m; in fact $\lambda \geq m^2$.

$$J^2 - J_z^2 = \frac{1}{2}(J_+ J_- + J_- J_+) = \frac{1}{2}(J_+ J_+^\dagger + J_+^\dagger J_+)$$

The expectation value of any operator of the form $AA^\dagger$ is ≥ 0

$$(\langle\lambda m| J^\dagger)(J|\lambda m\rangle) = \langle\Phi|\Phi\rangle \geq 0 .$$

$\therefore \langle \lambda m | J^2 - J_z^2 | \lambda m \rangle$

$= \hbar^2(\lambda - m^2) \langle \lambda m | \lambda m \rangle \geq 0.$

II - Let j be the largest eigenvalue of J_z

Then $J_z J_- |\lambda j\rangle = J_- J_z |\lambda j\rangle - J_- |\lambda j\rangle$

$= \hbar(j-1) J_- |\lambda j\rangle$

$\therefore J_- |\lambda j\rangle$ is an eigenfunction of J_z with eigenvalue $(j-1)\hbar$. Similarly

$(J_-)^r |\lambda j\rangle$ is an eigenfunction of J_z with eigenvalue $(j-r)\hbar$.

In the same way, $J_z J_+ |\lambda j\rangle = (j+1) J_+ |\lambda j\rangle$.

But since ~~Mj~~ j is largest eigenvalue, $J_+ |\lambda j\rangle = 0$.

Since $J^2 = J_x^2 + J_y^2 + J_z^2$

$= J_- J_+ + J_z^2 + J_z \; (= J_+ J_- + J_z^2 - J_z)$

it follows that

$J^2 |\lambda j\rangle = (J_- J_+ + J_z^2 + J_z) |\lambda j\rangle = j(j+1) |\lambda j\rangle$

III. Since $[J^2, J_-] = 0$, $J^2 |\lambda, j-r\rangle = j(j+1) |\lambda, j-r\rangle$

Put $\lambda = j(j+1)$

The sequence of ~~eigenvalues~~ eigenfns $|\lambda, j\rangle, |\lambda, j-1\rangle, \ldots, |\lambda, j-r\rangle$ must eventually terminate since $\lambda \geq (j-r)^2$

ie. suppose $J_- |\lambda, j-n\rangle = 0$.

Then $J^2|\lambda, j-n\rangle = (J_+J_- + J_z^2 - J_z)|\lambda, j-n\rangle$

$$= (J_z^2 - J_z)|\lambda, j-n\rangle$$

$$= \{(j-n)^2 - (j-n)\}|\lambda, j-n\rangle$$

$$= j(j+1)|\lambda, j-n\rangle$$

$\therefore (j-n)(j-(n+1)) = j(j+1)$

$\Rightarrow j = \frac{n}{2}$

ie j is integral or half-integral.

- The operators J_+, J_- and J_z, which are the infinitesimal generators of all possible rotations, transform the $|\lambda\, j\rangle$, $|\lambda\, j-1\rangle$, ... $|\lambda, -j\rangle$

amongst themselves and thus form the basis for an irreducible representation of the rotation operators.

- Replace λ by j, so that the states are labelled ~~according to~~ $|jm\rangle$.

$\langle jm|J_z|jm\rangle = m\hbar$

$\langle jm\pm1|J_\pm|jm\rangle = [(j\pm m+1)(j\mp m)]^{1/2}$

$(2j+1)$ dimensional matrix representation of infinitesimal rotation operators D_α.

If $J_+|jm\rangle = c\,|j\,m+1\rangle$, then

$c^2 = \langle jm|J_-J_+|jm\rangle = \langle jm|J^2 - J_z^2 - J_z|jm\rangle$

$= j(j+1) - m^2 - m = (j-m)(j+m+1)$

<u>Representation of $|jm\rangle$ for integral $j = l$</u>

$$\underset{\sim}{L} = \underset{\sim}{r} \times \underset{\sim}{P}$$

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

$$L_\pm = \pm e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

(see, e.g. Merzbacher)

$$\langle\theta,\phi|lm\rangle = Y_l^m(\theta,\phi)$$

$$Y_l^m(\theta,\phi) = (-1)^m\left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\phi}$$

- Orthonormal basis set so that

$$\iint Y_{l'}^{m'*}\, Y_l^m \sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'}$$

- Notice that $Y_l^{m*} = (-1)^m Y_l^{-m}$.

Also define $C_{lm}(\theta,\phi) = \sqrt{\frac{4\pi}{2l+1}}\; Y_l^m(\theta,\phi)$

$$C_{l0}(\theta,\phi) = P_l(\cos\theta)$$

$$C_{lm}(0,\phi) = \delta_{m0}.$$