Advanced Quantum Mechanics

Rajdeep Sensarma

sensarma@theory.tifr.res.in

Lecture #5

Symmetries and Quantum Mechanics

Recap of Last Class

- Vibrational Modes of NH3 : Matrix Elements
- Continuous Symmetry: Parametrization
- Infinitesimal transformations and Generators (Translation and Rotation as e.g.)
- Finite Transformations
- Properties of Generators : Lie Brackets (Ang. Momentum Commutation Relations)

Generators and Lie Brackets

- The generators of an Abelian group commute, so structure constants are all 0 E.g.: $[\hat{p}_x, \hat{p}_y] = 0$

Will focus on 3D Rotation from now on

Lie Brackets and Structure Constants for 3D Rotation

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R_{\hat{n}}(\theta) \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \quad R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

For infinitesimal rotations, $\cos\theta \sim 1 - \theta^2/2, \quad \sin\theta \sim \theta$

$$R_z(\theta) = \begin{pmatrix} 1-\theta^2/2 & -\theta & 0 \\ \theta & 1-\theta^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\theta^2/2 & -\theta \\ 0 & \theta & 1-\theta^2/2 \end{pmatrix} \quad R_y(\theta) = \begin{pmatrix} 1-\theta^2/2 & 0 & \theta \\ 0 & 1 & 0 \\ -\theta & 0 & 1-\theta^2/2 \end{pmatrix}$$

Note: We can choose any representation to calculate this

Lie Brackets for 3D Rotation

$$R_z(\theta) = \begin{pmatrix} 1-\theta^2/2 & -\theta & 0 \\ \theta & 1-\theta^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\theta^2/2 & -\theta \\ 0 & \theta & 1-\theta^2/2 \end{pmatrix} \quad R_y(\theta) = \begin{pmatrix} 1-\theta^2/2 & 0 & \theta \\ 0 & 1 & 0 \\ -\theta & 0 & 1-\theta^2/2 \end{pmatrix}$$

$$R_x(\theta)R_y(\theta) = \begin{pmatrix} 1-\theta^2/2 & 0 & \theta \\ \theta^2 & 1-\theta^2/2 & -\theta \\ -\theta & \theta & 1-\theta^2 \end{pmatrix} \qquad R_y(\theta)R_x(\theta) = \begin{pmatrix} 1-\theta^2/2 & \theta^2 & \theta \\ 0 & 1-\theta^2/2 & -\theta \\ -\theta & \theta & 1-\theta^2 \end{pmatrix}$$

$$R_x(\theta)R_y(\theta) - R_y(\theta)R_x(\theta) = \begin{pmatrix} 0 & -\theta^2 & 0 \\ \theta^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = R_z(\theta^2) - 1$$

Rotation Operator for finite rotations $\mathcal{D}(\hat{n},\theta) = e^{-i\vec{L}\cdot\hat{n}\theta}$

$$[1 - iL_x\theta - L_x^2\theta^2/2][1 - iL_y\theta - -L_y^2\theta^2/2] - [1 - iL_y\theta - L_y^2\theta^2/2][1 - iL_x\theta - L_x^2\theta^2/2]$$

$$= 1 - iL_z\theta^2 - 1 \qquad \Rightarrow [L_x, L_y] = iL_z$$

Evaluating other commutators in similar fashion

Angular Momentum commutation relations

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

Choice of EigenStates

L_x,L_y,L_z are all conserved, and their eigenstates would be H eigenstates (provide quantum no.s)

But they do not commute with each other, so cannot write simultaneous eigenstates of all 3.

Need to make a choice which eigenstate to use.

Casimir Operator $$L^2 = L_x L_x + L_y L_y + L_z L_z$$

Use

$$[L^2, L_i] = 0 \qquad\qquad [L_i, L_j] = i\epsilon_{ijk} L_k$$

Common eigenstates of L^2 and L_z

$$L_z |l, m\rangle = m|l, m\rangle \qquad\qquad L^2|l, m\rangle = l|l, m\rangle$$

Undetermined (for now) l (>0) and m

Raising/Lowering Operators

Raising-Lowering Operators $L^{\pm} = L_x \pm iL_y$

Use

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

$$[L_z, L^{\pm}] = iL_y \pm L_x = \pm(L_x \pm iL_y) = \pm L^{\pm}$$

Eigenstate of L_z $\quad L_z|m\rangle = m|m\rangle$

$$L_z L^{\pm}|m\rangle = (L^{\pm}L_z \pm L^{\pm})|m\rangle = L^{\pm}(m \pm 1)|m\rangle$$

So, raising/lowering operators increase/decrease the eigenvalue of L_z by 1

Eigenstate of L^2 $\quad L^2|l\rangle = l|l\rangle$

Since $[L^2, L_i]=0$, $[L^2, L^+]=0$ and $[L^2, L^-]=0$ $\quad L^2 L^{\pm}|l\rangle = L^{\pm}L^2|l\rangle = lL^{\pm}|l\rangle$

So, raising/lowering operators conserve the eigenvalue of L^2

Now $\quad L_z L^{\pm}|l,m\rangle = (m \pm 1)L^{\pm}|l,m\rangle$ $\quad$ and $\quad L^2 L^{\pm}|l,m\rangle = lL^{\pm}|l,m\rangle$

So $\quad L^{\pm}|l,m\rangle = c_{\pm}|l, m \pm 1\rangle$

Applying L^+ increases eigenvalue of L_z by 1, while keeping eigenvalue of L^2 fixed. Can we keep increasing eigenvalue of L_z like this forever?

Common eigenstates of L^2 and L_z

$$\langle l,m|L^2 - L_z^2|l,m\rangle = \langle l,m|L_x^2 + L_y^2|l,m\rangle = \frac{1}{2}\langle l,m|L^+L^- + L^-L^+|l,m\rangle \geq 0$$

So $$l - m^2 \geq 0$$

We cannot keep applying raising operator to the eigenstates ad infinitum since it raises m values without changing l values

$$L^+|l,m_{max}\rangle = 0 \quad L^-|l,m_{min}\rangle = 0$$

$$L^-L^+|l,m_{max}\rangle = 0 \Rightarrow (L_x - iL_y)(L_x + iL_y)|l,m_{max}\rangle = 0 \Rightarrow L_x^2 + L_y^2 + i[L_x,L_y]|l,m_{max}\rangle = 0$$

$$\Rightarrow L^2 - L_z^2 - L_z|l,m_{max}\rangle = 0 \Rightarrow l - m_{max}^2 - m_{max}|l,m_{max}\rangle = 0$$

$$l = m_{max}(m_{max}+1)$$

$$L^+L^-|l,m_{min}\rangle = 0 \Rightarrow (L_x + iL_y)(L_x - iL_y)|l,m_{min}\rangle = 0 \Rightarrow L_x^2 + L_y^2 - i[L_x,L_y]|l,m_{min}\rangle = 0$$

$$\Rightarrow L^2 - L_z^2 + L_z|l,m_{min}\rangle = 0 \Rightarrow l - m_{min}^2 + m_{min}|l,m_{min}\rangle = 0$$

$$l = m_{min}(m_{min}-1)$$

Common eigenstates of L^2 and L_z

$$L_z|l,m\rangle = m|l,m\rangle \qquad L^2|l,m\rangle = l|l,m\rangle$$

For a given l $\quad L^+|l,m_{max}\rangle = 0 \quad L^-|l,m_{min}\rangle = 0$

$$l = m_{max}(m_{max}+1) \qquad l = m_{min}(m_{min}-1)$$

Since | l, m_{max}> can be reached from |l, m_{min}> by applying L^+ successively , $m_{max}-m_{min}$ =n (non-negative integer)

$$m_{max}^2 + m_{max} = m_{min}^2 - m_{min}$$

$$m_{max} + m_{min} = 0$$

$$(m_{max}+m_{min})(m_{max}-m_{min}+1) = 0$$

$$m_{max} = -m_{min} = n/2$$

Half Integer

$$(m_{max}+m_{min})(n+1) = 0$$

Common eigenstates of L^2 and L$_z$

Defining $j = m_{max}$ $\quad L_z|j,m\rangle = m|j,m\rangle \quad L^2|j,m\rangle = j(j+1)|j,m\rangle \quad \langle j',m'|j,m\rangle = \delta_{jj'}\delta_{mm'}$

Matrix Elements: $\langle j',m'|L^2|j,m\rangle = j(j+1)\delta_{jj'}\delta_{mm'}$ $\quad \langle j',m'|L_z|j,m\rangle = m\delta_{jj'}\delta_{mm'}$

$$L^{\pm}|j,m\rangle = c^{\pm}_{jm}|j,m\pm 1\rangle \qquad \langle j',m'|L^{-}L^{+}|j,m\rangle = |c^{+}_{jm}|^2\delta_{jj'}\delta_{mm'}$$

$$\langle j',m'|L^{-}L^{+}|j,m\rangle = \langle j',m'|L^2 - L_z^2 - L_z|j,m\rangle = j(j+1) - m(m+1)\delta_{jj'}\delta_{mm'}$$

$$c^{+}_{jm} = \sqrt{(j-m)(j+m+1)} \qquad c^{-}_{jm} = \sqrt{(j+m)(j-m+1)}$$

$$\langle j',m'|e^{-i\vec{L}.\hat{n}\theta}|j,m\rangle \sim \delta_{jj'}$$

The irreps of rotation group are labeled by half-integers, j= 0, 1/2, 1, 3/2, 2,.....

2j+1 dimensional invariant subspace of the rotation group

j labels the irreps/invariant subspaces and |m> states provide a basis in this subspace

Rotation Operator: $\mathcal{D}(\alpha,\beta,\gamma) = \mathcal{D}_z(\alpha)\mathcal{D}_y(\beta)\mathcal{D}_z(\gamma) = e^{-iL_z\alpha}e^{-iL_y\beta}e^{-iL_z\gamma}$

$$\mathcal{D}^{(j)}_{mm'}(\alpha,\beta,\gamma) = \langle j,m'|e^{-iL_z\alpha}e^{-iL_y\beta}e^{-iL_z\gamma}|j,m\rangle = e^{-i(m'\alpha+m\gamma)}\underline{\langle j,m'|e^{-iL_y\beta}|j,m\rangle}$$

$d^{(j)}_{mm'}(\beta)$

Orbital Angular momentum

$\vec{L} = \vec{r} \times \vec{p}$ Spherical Polar Co-ordinates: $(r, \theta, \phi) = (r, \hat{n})$

Infinitesimal rotation about x axis: $1 - iL_x\chi|r, \hat{n}\rangle = |r, \hat{n} + \hat{x} \times \hat{n}\chi\rangle \ = |r, \theta + \delta\theta, \phi + \delta\phi\rangle$

Now $\hat{n} = \sin\theta\cos\phi\hat{x} + \sin\theta\sin\phi\hat{y} + \cos\theta\hat{z}$

So $\delta\hat{n} = \chi(\hat{x} \times \hat{n}) = -\chi\cos\theta\hat{y} + \chi\sin\theta\sin\phi\hat{z}$

On the other hand

$$\hat{n} + \delta\hat{n} = \sin(\theta + \delta\theta)\cos(\phi + \delta\phi)\hat{x} + \sin(\theta + \delta\theta)\sin(\phi + \delta\phi)\hat{y} + \cos(\theta + \delta\theta)\hat{z}$$

Expanding to linear order in small changes

$$\delta\hat{n} = (\cos\theta\cos\phi\delta\theta - \sin\theta\sin\phi\delta\phi)\hat{x} + (\cos\theta\sin\phi\delta\theta + \sin\theta\cos\phi\delta\phi)\hat{y} - \sin\theta\delta\theta\hat{z}$$

Comparing, $\delta\theta = -\chi\sin(\phi)$ $\delta\phi = -\chi\cot(\theta)\cos(\phi)$

Orbital Angular momentum

$$\delta\theta = -\chi \sin(\phi) \qquad \delta\phi = -\chi \cot(\theta)\cos(\phi)$$

$$\langle r, \theta, \phi | 1 + i L_x \chi | \alpha \rangle = \langle r, \theta + \delta\theta, \phi + \delta\phi | \alpha \rangle = \langle r, \theta, \phi | \alpha \rangle + \delta\theta \partial_\theta \langle r, \theta, \phi | \alpha \rangle + \delta\phi \partial_\phi \langle r, \theta, \phi | \alpha \rangle$$

$$L_x = \frac{-1}{i}[\sin(\phi)\partial_\theta + \cot(\theta)\cos(\phi)\partial_\phi]$$

Similarly

$$L_y = \frac{1}{i}[\cos(\phi)\partial_\theta - \cot(\theta)\sin(\phi)\partial_\phi] \qquad L_z = \frac{1}{i}\partial_\phi$$

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

$$\langle \hat{n} | L^2 | l, m \rangle = l(l+1)\langle \hat{n} | l, m \rangle \Rightarrow \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + l(l+1)\right]\langle \hat{n} | l, m \rangle$$

Spherical Harmonics $Y_l^m(\theta, \phi)$ are the wfn.s of basis states of irreps of Rotation group

Particle in a spherically symmetric potential

$$\left[-\frac{\nabla^2}{2m} + V(r) - E\right]\psi(r,\theta,\phi) = 0 \qquad = \left[\frac{1}{2m}\partial_r^2 + E - V(r) - \frac{L^2}{2mr^2}\right]\psi = 0$$

Criterion for Symmetry: Hamiltonian commutes with all the generators of the Lie group

Irreducible basis functions for (θ,φ) are the spherical Harmonics $\psi_{nm}^{(l)}(\vec{r}) = R_n^{(l)}(r) Y_l^m(\theta,\phi)$

Degeneracy corresponding to rotational symmetry: ϵ_{nl} is independent of m.

(2l+1) fold degeneracy corresponding to the dimension of the irrep.

Atomic Physics Nomenclature: l=0 --> s-wave, l=1 --> p-wave, l=2 --> d-wave etc.

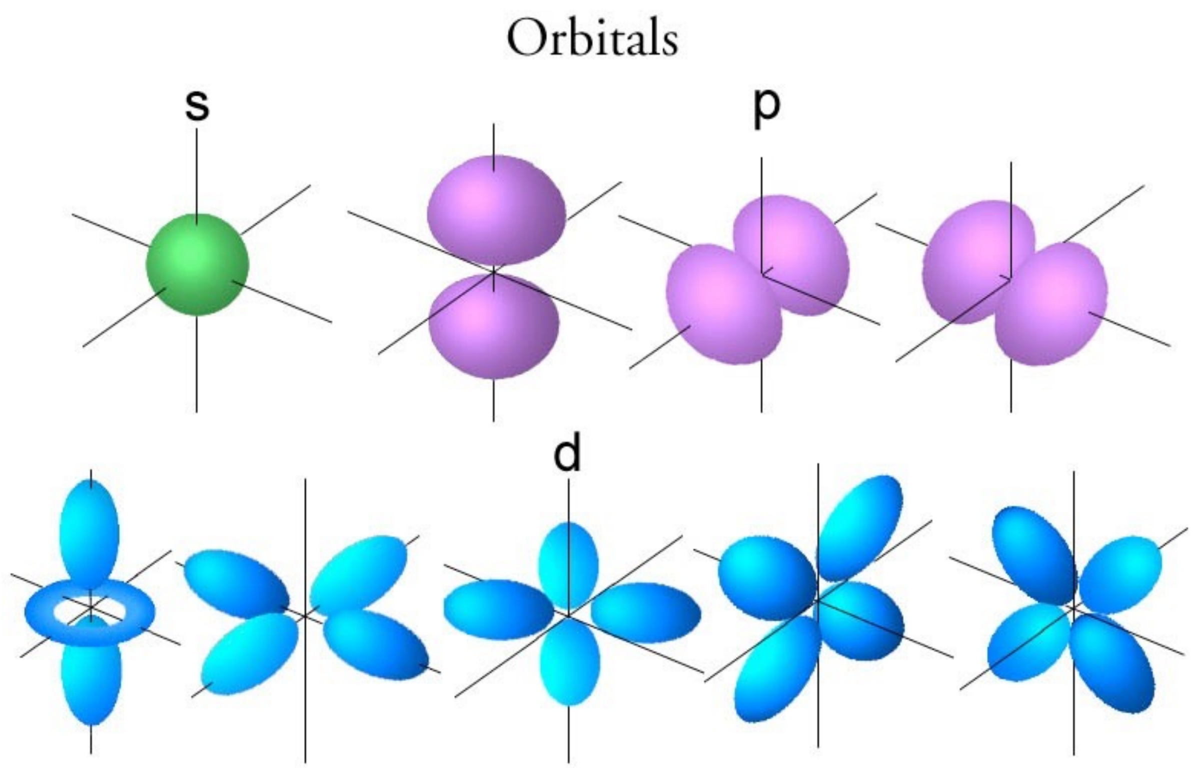
s-wave orbitals are non-degenerate, p-wave is 3-fold degenerate (p_x,p_y,p_z), d-wave is 5-fold degenerate (d_{z^2} $d_{x^2-y^2}$, d_{xy}, d_{yz}, d_{xz}) etc.

p-wave basis fn.s: $p_x \sim Y^1_1+Y^{-1}_1 \sim x$, $p_y \sim -i(Y^1_1-Y^{-1}_1) \sim y$, $p_z \sim Y^0_1 \sim z$,

d-wave basis fn.s: $d_{z^2} \sim Y^0_2 \sim z^2$, $d_{x^2-y^2} \sim Y^2_2 + Y^{-2}_2 \sim x^2-y^2$

$d_{xz} \sim Y^1_2 + Y^{-1}_2 \sim xz$, $d_{yz} \sim -i(Y^1_2 - Y^{-1}_2) \sim yz$, , $d_{xy} \sim -i(Y^2_2 - Y^{-2}_2) \sim xy$

Particle in a spherically symmetric potential



In H atom, the energy does not depend even on l, $E_n \sim 1/n^2$. Is this accidental or are we missing something?

- What about half-integer values of l ? Orbital Angular momentum only allows integer irreps.
- The states/co-ordinates corresponding to half-integer irreps are not related to rotn. of spatial co-ord.
- This will be generically called spin-degrees of freedom (spin degrees allow integer valued irreps)

j = 1/2 and Spin

2 dimensional irrep of rotation group. Basis states are $|1/2, 1/2\rangle = |+\rangle$ *and* $|1/2, -1/2\rangle = |-\rangle$

The Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0^* \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

correspond to the angular momentum (spin) operators through $S_i = \frac{1}{2}\sigma_i$

S_i satisfies angular momentum commutation relations $[S_i, S_j] = i\varepsilon_{ijk}S_k$

Rotation operator: $\mathcal{D}(\alpha, \beta, \gamma) = e^{-\frac{i}{2}\sigma_z\alpha}e^{-\frac{i}{2}\sigma_y\beta}e^{-\frac{i}{2}\sigma_z\gamma}$

Rotation operator: $\mathcal{D}(\hat{n}, \theta) = e^{-i\hat{n}\cdot\vec{\sigma}\frac{\theta}{2}} = \begin{pmatrix} \cos(\theta/2) - in_z\sin(\theta/2) & -(n_y + in_x)\sin(\theta/2) \\ (n_y - in_x)\sin(\theta/2) & \cos(\theta/2) + in_z\sin(\theta/2) \end{pmatrix}$

Rotation by 2π leads to a negative sign $\mathcal{D}(\hat{n}, 2\pi) = \cos(\pi) = -1$

Need a 4π rotation to come back to original state.

j = 1/2 and Spin

Spin Precession and 4π rotations

Spins in magnetic field: $H = g\mu_B \vec{B} \cdot \vec{S} = \omega S_z$ $\qquad \omega = g\mu_B B$ $\qquad$ Larmor Frequency

Time Evolution: $U(t) = e^{-i\omega S_z t} = \mathcal{D}(\hat{z}, \omega t)$

Evolution of state vector: $|\alpha(t)\rangle = e^{-i\omega t/2}|+\rangle\langle+|\alpha\rangle + e^{i\omega t/2}|-\rangle\langle-|\alpha\rangle$ $\qquad$ Precesses with 4π/ω

Evolution of expectation values:

$$\langle S_x(t)\rangle = \langle S_x(0)\rangle \cos(\omega t) - \langle S_y(0)\rangle \sin(\omega t)$$

$$\langle S_y(t)\rangle = \langle S_y(0)\rangle \cos(\omega t) + \langle S_x(0)\rangle \sin(\omega t)$$

Precesses with 2π/ω

Measured in Neutron interferometry experiments

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Observation of the Phase Shift of a Neutron Due to Precession in a Magnetic Field*

S. A. Werner
Physics Department, University of Missouri, Columbia, Missouri 65201

and

R. Colella and A. W. Overhauser
Physics Department, Purdue University, Lafayette, Indiana 47907

and

C. F. Eagen
Scientific Research Staff, Ford Motor Company, Dearborn, Michigan 48121

(Received 27 August 1975)

We have directly observed the sign reversal of the wave function of a fermion produced by its precession of 2π radians in a magnetic field using a neutron interferometer.

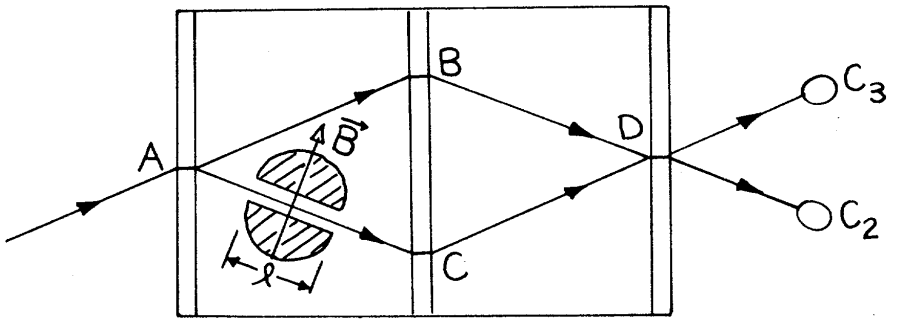

FIG. 1. A schematic diagram of the neutron interferometer. On the path AC the neutrons are in a magnetic field B (0 to 500 G) for a distance l (2 cm).

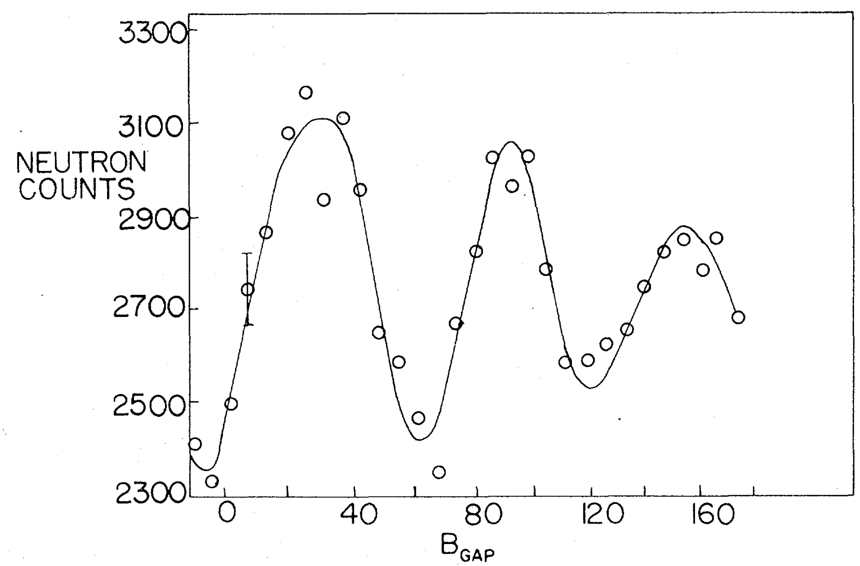

FIG. 3. The difference count, $I_2 - I_3$, as a function of the magnetic field in the magnet air gap in gauss. Approximate counting time was 40 min per point.

Magnetic Field phase shifts the state of A-C-D beam.
Interference between phase shifted and non-phase shifted beam
The B field is changed to obtain successive maxima.This corresponds to $\delta\omega=4\pi$. $\delta\omega=2\pi$ gives minima corresponding to π phase shift.