

# Quantum Mechanics

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February 27, 2023

## 1 Course Contents

1. Free Particle: (9 lectures)
  - (a) Schroedinger Equation, Hamiltonian, Commutation Relations, Wave functions, Probability Interpretation, Currents, Measurement, Plane waves, Normalization, Boundary conditions, Discrete Space and Regularization, delta function, Wave packets, group velocity. (1 1/2 lectures)
  - (b) Postulates of QMech, Bra-ket notation, Fourier Transform, Vector Space. (1 1/2 )
  - (c) Matrices, Hermitian, Unitary, Tensor Product, Projection Operator.(1)
  - (d) Schroedinger and Heisenberg Representation, Evolution Operator.(1)
  - (e) Feynman Path Integral.(2)
  - (f) Density Operator, Quantum Statistical Mechanics. (2)
2. Spin-1/2 system:(3 lectures)
  - (a) Stern Gerlach, Illustrating q mech., Atom in a magnetic field, Dynamics of two level systems. (2)
  - (b) Quantum Computer.(1)
3. Rotation Group: (4 lectures)
  - (a) Symmetries and Conservation Laws, Lie Groups, Rotation, Lorentz, Poincare, Global and local invariances (gauge invariance).(2)

- (b) Spin and Orbital Angular Momentum, Spherical harmonics.(2)
  - (c) Discrete Symmetries:C,P,T. (1)
4. Harmonic Oscillator: (4 lectures)
    - (a) Path Integral treatment. (2)
    - (b) Anharmonic Oscillator.(1/2)
    - (c) Coherent states.(1/2)
    - (d) Introduction to field theory.(1)
  5. Perturbation Theory: (5 lectures)
    - (a) Time Independent (Degenerate and Non-degenerate Pert. Theory).(1)
    - (b) Time Dependent Perturbation Theory, Sinusoidal perturbations, Fermi Golden Rule.(1)
    - (c) Scattering Theory.(3)
  6. Interaction of Charged Particles:(11 lectures)
    - (a) Hamiltonian and Lagrangian, Gauge Invariance. (1/2)
    - (b) Bohm-Aharanov Effect.
    - (c) Path Integral.(1 1/2)
    - (d) Hydrogen Atom, Diatomic Molecule. (2)
    - (e) Atom in an Electric and Magnetic Field, NMR. (2)
    - (f) Fine and Hyperfine Structure, Lamb Shift.(1)
    - (g) Electron in a Magnetic Field. , Landau levels, QHE (Q Hall Effect).(1)
    - (h) QED, Scattering, Dipole Radiation.(3)
  7. Dirac Equation and Klein Gordon Equation.(4 lectures)

## **Text Books:**

1. Cohen-Tannoudji....
2. Landau and Lifshitz....
3. Feynman and Hibbs ....

These notes follow these books quite closely.

## **Grading Policy:**

Homework	: 30 %
Mid-term examination:	: 20 %
Final Examination:	: 50 %
Total	: 100 %

## **Other points:**

1. Homework assignments will be given out once a week and will be due back in exactly one week. Homeworks handed in late will not be graded. You may consult with each other on the homework problems (indeed this is a very good thing), but the final solution should be yours. You may also be asked occasionally to work out problems on the board.
2. Basic knowledge of quantum mechanics is assumed. The aim of the course is to extend your formalistic and mathematical skills and also develop physical intuition.
3. Although text books have been specified we will not follow the order of presentation of any particular book. In terms of material Cohen-Tannoudji will be followed quite closely. For path integrals Feynman and Hibbs. The quasi-classical approximation is taken from Landau-Lifshitz. There are many other good books, such as those by Dirac, Schiff, Sakurai...

## 2 Free Particle

### 2.1 Basics

In classical mechanics a free particle is described by specifying its mass  $m$ , position  $x$  and momentum  $p$ . The Hamiltonian is given by

$$H = \frac{p^2}{2m} \quad (1)$$

In **Heisenberg's formulation** this equation continues to be true but  $x, p$  are non-commuting *operators* that satisfy

$$[x, p] = i\hbar \quad (2)$$

**Dimensions:**  $xp$  has dimensions  $L^2T^{-1}M$  - dimensions of angular momentum. This is also  $ML^2T^{-2}T$  which is *energy*  $\times$  *time*. This has dimensions of "action". In q.mech. we often use units where  $\hbar = 1$ . Then  $E \approx T^{-1}$ . Also  $P \approx L^{-1}$ . Then action can be said to be dimensionless. In relativistic systems it is common to set  $c = 1$  ( $c$ =vel. of light). (So  $\hbar = c = 1$ ).  $L \approx T \approx E^{-1} \approx P^{-1} \approx M^{-1}$ . Thus in these units,  $p, E, m$  all have dimensions of  $1/\text{length}$ . However for non-relativistic quantum mech we usually keep the constants.

(H.W: Show that  $\frac{e^2}{4\pi\epsilon_0\hbar c}$  is dimensionless. What is its value? Can you define something analogous using the other important constants in nature:  $G$  gravitational constant? Should the fundamental constants in nature be dimensionful or dimensionless? What if we had a universe where  $\hbar$  has twice its present value, and all other (dimensionless nos.) are the same. What would be different? Think about these things.)

$$e = 1,6 \times 10^{-19} \text{ Coul}$$

$$\hbar = 1.05 \times 10^{-34} \text{ J} \cdot \text{s}$$

$$c = 3 \times 10^8 \text{ m/s}$$

$$\frac{1}{4\pi\epsilon_0} = 8.98 \times 10^9 \frac{\text{Nm}^2}{\text{coul}^2}$$

$$G = 6.6 \times 10^{-11} \frac{\text{Nm}^2}{\text{kg}^2}$$

In this formulation the possible values that can result when momentum is **measured**(what does this mean??) are the eigenvalues of the operator

$p$ . Same for  $x$ . Operators can be represented by matrices. Eigenvalues of  $H$  are thus the measured values of energy. In particular at the end of a measurement the particle has that measured value i.e. it is in an *eigenstate* of that operator. As  $x$  and  $p$  do not commute, it follows that the particle cannot be simultaneously an eigenstate of both. Therefore if it has a precise value of momentum, it *cannot* have a precise value of position, and vice versa. This observation is embodied in the “**Heisenberg Uncertainty Relation**”

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (3)$$

In the Heisenberg formalism one has to diagonalise matrices.

(Do they know Fourier Transforms?) This is trivially a consequence of the mathematical properties of FT.

In the **Schroedinger formulation** one has to solve a *linear* differential equation:

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (4)$$

where  $H$  is a linear differential operator. It is equal to  $-\frac{1}{2m} \frac{\partial^2}{\partial x^2}$  From studying differential equations we know that this also reduces to an eigenvalue problem. Thus the space of solutions of Schroedinger’s equation forms a vector space on which  $H, p, x$  can be represented as (**infinite dimensional**, why?) matrices. These matrices satisfy Heisenberg’s commutation relations.

In a nutshell these are the two (equivalent) descriptions of quantum mechanics discovered in the 1920’s. **R.P. Feynman** discovered (1940?) another formulation called the path integral formulation. We will discuss this soon. This idea is used a lot in Quantum Field Theory.

Schroedinger’s formulation is more convenient for Non-relativistic QM.

Things you should know:

1. The wave function represents what? Born’s probability interpretation:  
 $dP \propto |\psi|^2 dx$

1.1. Given a wave function, physical quantities that can be calculated are expectation values of operators such as  $x, p, ..$  and functions thereof:

$$\int_{-\infty}^{+\infty} \psi^* O \psi dx = \langle O \rangle$$

2. Normalization :  $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$ . This is a physical requirement and constrains the solutions of SE.

3. In this representation  $p$  is represented by  $-i\hbar \frac{\partial}{\partial x}$ .

3.1. Proof of uncertainty reln.: Consider for  $\alpha$  real:

$$\int_{-\infty}^{+\infty} \left| \alpha x \psi + \frac{\partial}{\partial x} \psi \right|^2 dx \geq 0$$

The three terms are:

$$\alpha^2 \int x^2 |\psi|^2 dx = \alpha^2 (\Delta x)^2$$

$$\int \left| \frac{\partial}{\partial x} \psi \right|^2 dx = \frac{(\Delta p)^2}{\hbar^2}$$

$$\int \alpha x (\psi \frac{\partial}{\partial x} \psi^* + \psi^* \frac{\partial}{\partial x} \psi) dx = -\alpha$$

They add up to

$$\alpha^2 (\Delta x)^2 - \alpha + \frac{(\Delta p)^2}{\hbar^2} \geq 0$$

This means the discriminant has to be  $\leq 0$ . So

$$1 - 4(\Delta x)^2 \frac{(\Delta p)^2}{\hbar^2} \leq 0$$

This gives

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$$

4. The eigenfns of  $p$  are  $Ae^{ikx}$  and have ev  $\hbar k$ . “plane waves”

5. These plane waves are not normalizable.  $\int_{-\infty}^{+\infty} |\psi|^2 dx = \infty$ . Dirac introduced a “delta function” to deal with these. The Dirac Delta Function  $\delta(x)$  is zero everywhere except at  $x = 0$  where it is infinite. It also satisfies  $\int dx \delta(x) = 1$ . And  $\int dx f(x) \delta(x) = f(0)$ . Using this notation one can show that (HW)  $\int_{-\infty}^{+\infty} |\psi|^2 dx = |A|^2 2\pi \delta(0)$ . (for plane wave states). These are called “plane wave normalizable”. Although these states are not allowed strictly speaking we will use them as an approximation and for practical convenience.

Another way to deal with plane waves is to put it in a box:

Size  $L$ . So if  $\Psi(x) = A^{ikx}$  is plane wave, then  $|A|^2 = \frac{1}{\sqrt{L}}$ . This is **infrared regularization**. What is the smallest value: Depends on bc. If we have standing waves, then we have states with  $\sin kx$  and  $k = \frac{n\pi}{L}$ . (Periodic?)

**Ultraviolet gularizatipon** assume  $k$  has a max. As in a crystal with spacing  $a$ .  $k \leq \frac{2\pi}{a}$ . And  $Na = L$ . So  $k$  takes  $N$  values.

$dx \rightarrow \sum_{n=1}^N a$ .  $dk \rightarrow \sum_{m=1}^N \frac{2\pi}{L}$ . Try evaluationg  $\int dx e^{ikx}$  and  $\int dk \int dx e^{ikx}$  and figure out properties of delta-function.

6. Probability density of finding a particle in such a state (=constant)

7. Probability current:

$$J_x = \frac{\hbar}{2im} [\psi^* \partial_x \psi - c.c.] = \underbrace{\frac{\hbar k}{m}}_{\text{velocity}} \underbrace{|A|^2}_{\text{number density}} \quad (5)$$

8. Current Conservation  $\partial_x J_x - \partial_t J_t = 0$  where  $J_t = \psi^* \psi =$  number density.

9. States havind a definite time dependence  $e^{-iEt}$  satisfy the time independent SE  $H\psi = E\psi$ . For plane wave states clearly  $E = \frac{(\hbar k)^2}{2m}$ .

10. We usually require  $E$  to be real. what if it is not? Calculate  $\partial_t(\psi^* \psi)$ .

11. Continuous versus discrete  $E$ . Confining potentials and bound states. Particle in a box. HW.

12. Prove current conservation using SE. Starting with  $-\frac{\hbar^2 \partial^2 \psi}{2m \partial x^2} = i \frac{\hbar \partial \psi}{\partial t}$  we get (multiply by  $\psi^*$ , integrate by parts and subtract c.c)  $-\partial_x J_x$  on the LHS and  $i \partial_t(\psi^* \psi)$  on the RHS. QED.

12. HW problem with particle leaking out of a box.

13. Given a wave function, physical quantities that can be calculated are expectation values of operators such as  $x, p, ..$  and functions thereof:

$$\int_{-\infty}^{+\infty} \psi^* O \psi dx = \langle O \rangle$$

14. For a plane wave what is  $\langle x \rangle, \langle x^2 \rangle$ ? What does it mean?

15. Given the above, how does one construct a classical looking particle? ANS "wave packet". Superpose different harmonics: Draw. eg  $\psi(x) = A e^{-\frac{(x-vt)^2}{2b^2}}$ . Do you know how to fix A? This represents a particle moving along the trajectory  $x = vt$ . At least initially. After some time? calculate!

16. Group velocity is  $\frac{d\omega}{dk}$  is  $\frac{k}{m}$ . But what is  $k$ ?  $\psi$  is peaked around some  $k$ . Consider the wave fn.

$$\psi = A \int dk e^{ikx} e^{-\frac{b^2(\hbar k - mv)^2}{2}} e^{-i \frac{\hbar^2 k^2 t}{2m}} \quad (6)$$

This represents a superposition of plane waves of momentum  $\hbar k$  and the appropriate time dependence.  $k$  peaked around  $mv$ . Do the integral. Set

$\hbar = 1$ . The exponent is:

$$\begin{aligned} & -k^2\left(\frac{b^2}{2} + i\frac{t}{2m}\right) + k(b^2mv + ix) - \frac{m^2v^2b^2}{2} \\ & = -\left(\frac{b^2}{2} + i\frac{t}{2m}\right)\left(k - \frac{(b^2mv + ix)}{(b^2 + i\frac{t}{m})}\right)^2 + \frac{(b^2mv + ix)^2}{2(b^2 + i\frac{t}{m})} - \frac{m^2v^2b^2}{2} \end{aligned}$$

After doing the  $k$  integral we are left with a term in the exponent:

$$\frac{(b^2mv + ix)^2}{2(b^2 + i\frac{t}{m})} - \frac{m^2v^2b^2}{2}$$

We expand this for large  $m$  but small  $mb$  to get

$$\psi \approx e^{-\frac{(x-vt)^2}{2b^2} - it\frac{mv^2}{2} + imvx} \quad (7)$$

We can also calculate  $|\psi|$  by adding to the exponent its c.c. to get

$$|\psi| \approx e^{-\frac{b^2(x-vt)^2}{(b^4 + \frac{t^2}{m^2})}} \quad (8)$$

This clearly represents a ‘semi-classical’ wave function of a particle moving along a trajectory with vel  $v$ . The  $t$  and  $x$  dependences give the classical energy and momentum respectively.

The Feynman Path Integral (FPI) approach is best suited to demonstrate this. Later.

## 2.2 Postulates of Q.M.

1. The space of allowed “wave-fns” is a vector space over complex nos. (Hilbert space). The wave fns have to be square integrable and smooth.

i) Superposition:  $\psi = a_1\psi_1 + a_2\psi_2$ ,  $a_1, a_2 \in \mathcal{C}$  is also a physical state.

ii) Scalar product  $\int d^3r \phi^*(r)\psi(r) = \langle \phi | \psi \rangle$  has the following props:

a)  $\langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle$

b) Linear  $\langle \phi | a_1\psi_1 + a_2\psi_2 \rangle = a_1 \langle \phi | \psi_1 \rangle + a_2 \langle \phi | \psi_2 \rangle$

c) anti linear  $\langle a_1\psi_1 + a_2\psi_2 | \phi \rangle = a_1^* \langle \psi_1 | \phi \rangle + a_2^* \langle \psi_2 | \phi \rangle$

d) Norm  $\langle \phi | \phi \rangle = \int d^3r \phi^* \phi > 0$  and is  $=0$  iff  $\phi = 0$ . 2. Dirac’s

Notation:

$|\psi\rangle$  represents a state. Inner product of  $|\psi\rangle$  and  $|\phi\rangle$  is denoted by  $\langle \phi | \psi \rangle$



Thus

$$\psi(r) \leftrightarrow |\psi\rangle$$

“ket”

$$\int d^3r \phi^*(r) \psi(r) \leftrightarrow \langle \phi | \psi \rangle$$

Dual space: The space of linear functionals:

defn of lin fnl:  $\chi$  is a linear fnl  $\Rightarrow$  it assigns a complex no. to every ket  $|\psi\rangle$ .

$$\chi(|\psi\rangle) = c$$

The space of  $\chi$ 's is the dual vector space.

Linear i.e.  $a\chi_1(|\psi\rangle) + b\chi_2(|\psi\rangle) = a\chi_1 + b\chi_2(|\psi\rangle)$

Hilbert space and its dual are isomorphic. (Except for plane wave states!)

A particular linear functional  $\psi^{dual}$  can be associated with a ket  $|\psi\rangle$  by:

$$\psi^{dual}(|\phi\rangle) \equiv \langle \psi | \phi \rangle$$

This defines the bra  $\langle \phi | \equiv \phi^{dual}$ .

3. Basis vectors:  $|e_i\rangle$   $i = 1, N$  for an  $N$  dim space. Completeness.

Discrete and continuous.

Orthonormal:  $\langle e_n | e_m \rangle = \delta_{nm}$  or  $\langle e(\lambda) | e(\lambda') \rangle = \delta(\lambda - \lambda')$

Thus usual wave fn  $\psi(r) = \langle r | \psi \rangle$

$$|\psi\rangle = \int d^3r \psi(r) |r\rangle$$

$\langle r | r \rangle = \delta(0) = \infty$  not normalizable.

Momentum basis:

$$\psi(r) = \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(p) e^{ip \cdot r}$$

“Fourier transform”

$$\tilde{\psi}(p) = \int d^3r e^{-ip \cdot r} \psi(r)$$

Check .

Define  $|p\rangle$  by  $\tilde{\psi}(p) = \langle p | \psi \rangle$ . and

$$|\psi\rangle = \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(p) |p\rangle$$

This requires  $\langle p | \partial' \rangle = (2\pi)^3 \delta^3(p - p')$

$$\begin{aligned} |\psi\rangle &= \int d^3r \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(p) |r\rangle \\ &= \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(p) \underbrace{\int d^3r e^{ip \cdot r}}_{|p\rangle} |r\rangle \end{aligned}$$

Thus  $\langle r | p \rangle = e^{ip \cdot r}$ .

Thus inserting  $\int \frac{d^3p}{(2\pi)^3} |p\rangle \langle p|$  or  $\int d^3r |r\rangle \langle r|$  is equivalent to FT.

4. Operators: Linear operator:  $A | \psi \rangle = | \phi \rangle$  and correspondingly  $\mathcal{A}\psi(r) = \phi(r)$  where  $\mathcal{A}$  is a differential operator.

$$\mathcal{A}\psi(r) = \langle r | A | \psi \rangle = \int d^3r' \langle r | A | r' \rangle \psi(r')$$

$\langle r | A | r' \rangle$  are matrix elements. Operators are represented by matrices. Discrete or continuous depends on basis.

eg  $\mathcal{A}$  is  $-id/dx$  what is  $A$ ?

$$\begin{aligned} -id/dx \psi(x) &= \int dx' id/dx' \delta(x - x') \psi(x') \\ &= \int dx' id/dx' \langle x | x' \rangle \psi(x') \\ &= \int dx' [\langle x | id/dx' | x' \rangle] \psi(x') \end{aligned}$$

$$\langle x | A | x' \rangle = \langle x | id/dx' | x' \rangle = id/dx' \delta(x - x')$$

. (Note the sign change)

$$\langle p | A | p' \rangle = \int dx p' e^{i(p' - p)x} = 2\pi \delta(p' - p) p'$$

5. Hermiticity:  $A = A^\dagger$

$$\langle \chi | A\psi \rangle^* = \langle \psi | A^\dagger | \chi \rangle$$

$$\int dx (\chi^* A\psi)^* = \int dx \psi^* A^\dagger \chi = \int dx (A\psi)^* \chi$$

eg  $A = d/dx$ :

$$\int (\chi^*(x) d\psi/dx)^* = \int d\psi^*/dx \chi(x) = - \int dx \psi^* d\chi/dx$$

Note - sign. We have "integrated by parts". (What boundary conditions are required?) Thus  $A^\dagger$  here is  $-d/dx$ . Thus it is anti-Hermitian. Thus  $i\frac{d}{dx}$  is Hermitian.

6. Eigenvalues and eigenvectors.

If  $A|\psi_n\rangle = a_n|\psi_n\rangle$  then  $a_n$  is an eigenvalue and  $|\psi_n\rangle$  is an eigen vector.

### 2.3 Matrices

If  $e_i \approx |i\rangle$  are a orthonormal basis then the matrix  $A_{ij} = \langle i|A|j\rangle$  is the matrix representation of the operator  $A$ . Thus

$$A|j\rangle = \sum_k A_{kj}|k\rangle$$

$$\langle i|A|j\rangle = \sum_k A_{kj} \langle i|k\rangle = A_{ij}$$

Thus if  $|\psi\rangle = \sum a_n|n\rangle$  the column vector  $(a_n)$  represents the state  $|\psi\rangle$ . Then

$$A|\psi\rangle = \sum_i A|i\rangle \langle i|\psi\rangle = \sum_i a_i A|i\rangle$$

$$= \sum_i a_i \sum_j |j\rangle \langle j|A|i\rangle$$

$$= \sum_j (\sum_i A_{ji} a_i) |j\rangle$$

So the numbers  $\sum_i A_{ji} a_i$  represents  $A|\psi\rangle$ .

Diagonal rep of matrix : Choose a (orthonormal) basis consisting of eigenvectors of  $A$ . In this basis  $A$  is a diagonal matrix:  $A = \text{diag}(a_1, a_2, a_3 \dots a_N)$ . Then  $A = A^\dagger$  implies that the eigenvalues are real. Physical (i.e. experimentally measurable) quantities must be represented by Hermitian matrices. eg. energy, momentum, ... Hermitian means real symmetric, or imaginary antisymmetric. eg Pauli matrices.

Unitary matrices:  $UU^\dagger = U^\dagger U = I$ .

They are important - they preserve norm:

$$\langle U\psi|U\psi\rangle = \langle \psi|U^\dagger U|\psi\rangle = \langle \psi|\psi\rangle$$

$$\text{Det}(UU^\dagger) = \text{Det}U \text{Det}U^\dagger = |\text{Det}U|^2 = 1$$

So  $\text{Det}U = \pm 1$ . If we diagonalise  $U$  then since  $U^{-1} = U^\dagger = U^*$  the diagonal elements must be of the form  $e^{i\theta_n}$  where  $\theta_n$  is real.

Thus  $U = e^{iA}$  where  $A$  is hermitian. ( $iA$  is anti Hermitian).

If  $A$  is small, the  $U = 1 + iA$ , and  $U^\dagger = 1 - iA$ . A Unitary transformation is

$$\begin{aligned} UFU^\dagger &= (1 + iA)F(1 - iA) \\ &= F + i[A, F] \end{aligned}$$

Thus

$$\delta F = i[A, F]$$

is the form of the infinitesimal transformation. eg  $e^{i\epsilon \frac{P}{\hbar}}$  is a translation by  $\epsilon$ .

$$\begin{aligned} \delta F &= i\epsilon \left[ \frac{P}{\hbar}, F \right] = i\epsilon \left( -i \frac{dF}{dx} \right) \\ &= \epsilon \frac{dF}{dx} \end{aligned}$$

## 2.4 Tensor Products

$V_1, V_2$  are two vector spaces. The tensor product is a vector space  $V_1 \otimes V_2$ . If  $|e_i^1\rangle, i = 1 - N_1, |e_j^2\rangle, j = 1 - N_2$  are the bases of  $V_1, V_2$ , then the  $N_1 N_2$  states  $|e_i^1\rangle \otimes |e_j^2\rangle$  are the basis states of  $V_1 \otimes V_2$ .

eg  $|p_x, p_y, p_z\rangle$  actually is a state in the tensor product space  $|p_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle$ . Similarly, multiparticle states.

1.

$$\lambda[|\phi_1\rangle \otimes |\chi_2\rangle] = \lambda[|\phi_1\rangle] \otimes |\chi_2\rangle = |\phi_1\rangle \otimes \lambda[|\chi_2\rangle]$$

2.

$$|\phi_1\rangle \otimes [|\chi_1\rangle + |\chi_2\rangle] = |\phi_1\rangle \otimes |\chi_1\rangle + |\phi_1\rangle \otimes |\chi_2\rangle$$

3. If  $|\phi_1\rangle = \sum_{n=1}^{N_1} a_n |e_n^1\rangle$  and  $|\chi_1\rangle = \sum_{m=1}^{N_2} b_m |e_m^2\rangle$ , then  $|\phi_1\rangle \otimes |\chi_1\rangle = \sum_{n=1}^{N_1} \sum_{m=1}^{N_2} \underbrace{a_n b_m}_{N_1 N_2} |e_n^1\rangle \otimes |e_m^2\rangle$

4. But the general state is  $|\Psi\rangle = \sum_{n=1}^{N_1} \sum_{m=1}^{N_2} \underbrace{c_{n,m}}_{N_1 N_2} |e_n^1\rangle \otimes |e_m^2\rangle$

5. Scalar product  $|\phi_1\rangle \otimes |\chi_1\rangle$  and  $|\phi_2\rangle \otimes |\chi_2\rangle$

is  $\langle \phi_2 | \phi_1 \rangle \langle \chi_1 | \chi_2 \rangle$ .

6. Similarly operators: If  $A$  acts on  $V_1$  and  $B$  in  $V_2$ . and

$A|\phi_1\rangle = |\phi_2\rangle$  and  $B|\chi_1\rangle = |\chi_2\rangle$  then  $A \otimes B|\phi_1\rangle \otimes |\chi_1\rangle = A|\phi_1\rangle \otimes B|\chi_1\rangle = |\phi_2\rangle \otimes |\chi_2\rangle$

Similarly on a general state (i.e. not a direct product) act on the individual basis states which are direct products.

Thus we should actually write  $\tilde{A} = A \otimes I$  and  $\tilde{B} = I \otimes B$  and  $\tilde{A}\tilde{B} = AI \otimes IB = A \otimes B$ .

**Example:** Two spins 1/2 . The basis states are

$$|+\rangle \otimes |+\rangle$$

$$|+\rangle \otimes |-\rangle$$

$$|-\rangle \otimes |+\rangle$$

$$|-\rangle \otimes |-\rangle$$

Another notation:

$$|+, +\rangle, |+, -\rangle, |-, +\rangle, |-, -\rangle,$$

Operators  $\vec{S}_1, \vec{S}_2$  - Pauli matrices.

Let  $S_{1x} = \sigma_x$  etc. As matrices  $\sigma_{ij}, i, j = 1, 2$

Let  $S_{2x} = \tau_x$  etc. As matrices  $\tau_{ab}, a, b = 1, 2$

Then

$$\begin{aligned} \vec{S}_1 \cdot \vec{S}_2 &= S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z} \\ &= S_{1x} \otimes S_{2x} + S_{1y} \otimes S_{2y} + S_{1z} \otimes S_{2z} \\ &= \sigma_{xij}\tau_{xab} + \sigma_{yij}\tau_{yab} + \sigma_{zij}\tau_{zab} \end{aligned}$$

Action on states:

$$S_{1x}S_{2x} = S_{1x} \otimes S_{2x}[|+\rangle \otimes |+\rangle] = \sigma_x \otimes \tau_x[|+\rangle \otimes |+\rangle] = [ |-\rangle \otimes |-\rangle ]$$

On the other hand

$$\sigma_x \sigma_x = I$$

This is not a tensor product.

$\sigma \otimes \tau$  can be written as a 4X4 matrix.

## 2.5 CSCO

Complete Set of Commuting Observables: How do you specify a state completely?

Let the eigenvectors of  $A$  be  $|a_n\rangle$ , i.e.  $A|a_n\rangle = a_n|a_n\rangle$ . There may be many of these. So label by another index:  $|a_n, i\rangle, i : 1 - N_n$ . How does one label them? Use another observable  $B$  such that  $[A, B] = 0$ .  $B$  will not change  $A$  eigenvalue. So

$$B|a_n, i\rangle = \sum_j b_{ij}|a_n, j\rangle$$

Thus  $B$  is block diagonal. Draw. Let us diagonalise  $B$  in each block. So instead of  $i$  use  $b_m$ , Thus the states are labelled by  $|a_n, b_m\rangle, m : 1 - N_b$ . If  $N_b = N_n$  then we have a distinct eigenvalue for each state. If  $N_b < N_n$  then then we have many states with same values  $a_n, b_m$ . Thus we call them  $|a_n, b_m, k\rangle$  where  $k : 1 - N_{n,m}$ . Find another operator  $C$  such that  $[A, C] = [B, C] = 0$ . This is block diagonal in the block labelled by  $a_n, b_m$ . Diagonalise it. Let the ev be  $c_p$ . If all ev are distinct we are done. Otherwise keep going. In this way we get a CSCO:  $A, B, C, D, \dots$  and a set of labels that uniquely specify the state  $|a_n, b_m, c_p, d_q, \dots\rangle$ . The set is not unique.

eg Plane waves in three dimensions.

## 2.6 Projection Operators

$P$  is a projection operator if  $P^2 = P$ . Eigenvalues are 1,0.

Projector into a state  $|\psi\rangle$  is  $\frac{|\psi\rangle\langle\psi|}{\sqrt{\langle\psi|\psi\rangle}}$

## 2.7 Schroedinger, Heisenberg and Interaction Representation

1.

$$\psi(x, t) = e^{-\frac{i}{\hbar}Ht}\psi(x, 0) \quad (9)$$

if  $H$  is time independent.

2.

$$\psi(x, t) = \underbrace{Pe^{-\frac{i}{\hbar}\int_0^t H(t')dt'}}_{\text{EvolutionOperator}} \psi(x, 0) \quad (10)$$

if  $H$  is time dependent.  $P$  stands for “**Path Ordering**”.

3. The evolution operator  $U(t, 0)$  is unitary if  $H$  is Hermitian.  $U(t, 0) = U(t, t_1)U(t_1, 0)$ .

4. Defn of Path ordering:  $U(t, t - \Delta t) = e^{-iH\Delta t}$  when  $\Delta t \rightarrow 0$ . Also  $U(t, 0) \equiv U(t, t - \Delta t)U(t - \Delta t, t - 2\Delta t)\dots U(\Delta t, 0)$ . (Note that  $e^A e^B \neq e^{A+B}$ ).
5. Check Schroedinger eqn.
6. Why Path ordering is imp for time dependent  $H$  only:  $H = H_0 + f(t)H_1$  with  $[H_0, H_1] \neq 0$ .

$$[H_0 + f(t_1)H_1, H_0 + f(t_2)H_1] = (f(t_1) - f(t_2))[H_1, H_0]$$

7. Use bra-ket notation:  $|\psi(t)\rangle_S = U(t, t_0)|\psi(t_0)\rangle_S$  "S"=Schrodinger.  
 $\langle\psi(t_0)|_S U^\dagger(t, t_0) = \langle\psi(t)|_S$

$$\langle\psi(t)|_S \mathcal{O}_S(t) |\psi(t)\rangle_S = \langle\mathcal{O}_S(t)\rangle_t$$

is exp value at time "t". The t-dep in O is because of some *explicit* time dependence.

$$\langle\psi(0)|_S U^\dagger(t, 0) \mathcal{O}_S U(t, 0) |\psi(0)\rangle_S = \langle\mathcal{O}\rangle_t$$

8. H = Heisenberg. Define  $U^\dagger \mathcal{O}_S(t) U(t, 0) = \mathcal{O}_H(t)$

$$|\psi(0)\rangle_S = |\psi\rangle_H$$

Heisenberg states have no time dep.

$$\langle\mathcal{O}_H(t)\rangle_t = \langle\psi|\mathcal{O}_H(t)|\psi\rangle_H = \langle\psi(t)|\mathcal{O}_S(t)|\psi(t)\rangle_S = \langle\mathcal{O}_S(t)\rangle_t$$

At  $t = 0$  both reps are identical. H-operators have all the time dep. S-op only have explicit time dep. H-states have no time dep.

9. Calculate  $\mathcal{O}_H(t + \Delta t) - \mathcal{O}_H(t)$  using U's to get

$$\begin{aligned} \frac{d\mathcal{O}_H}{dt} &= U^\dagger \frac{d\mathcal{O}_S}{dt} U + \frac{i}{\hbar} U^\dagger [H_S, \mathcal{O}_S] U \\ &= \left(\frac{d\mathcal{O}_S}{dt}\right)_H + \frac{i}{\hbar} [H_H, \mathcal{O}_H(t)] \end{aligned}$$

10.  $-i\hbar \frac{dX_H}{dt} = -i\hbar \frac{P_H}{m}$   
 $i\hbar \frac{dP_H(t)}{dt} = -i\hbar V'(X_H)$

## 2.8 Path Integral

1. Instead of starting with a wave function one defines directly a probability amplitude for a particle to go from a point  $x_i$  at time  $t_i$  to a point  $x_f$  at time  $t_f$ . Call it  $K(x_f, t_f; x_i, t_i)$ . Feynman defined the following formula for it: Motivation: double slit experiment.

$$K(x_f, t_f; x_i, t_i) = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp\left(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t))\right) \quad (11)$$

Note that this is not the probability amplitude of a measurement, it is the probability amplitude of an *event*.

2. Draw pictures and show classical limit. Principle of stationary phase. Derive Lagrange's eqn.

3. How do you actually calculate: What does  $\mathcal{D}x(t)$  mean? Divide  $t_f - t_i$  into  $N$  intervals  $\epsilon = t_{j+1} - t_j$  with  $t_0 = t_i$  and  $t_f = t_N$ . Let  $x_j = x(t_j)$ . Then  $\mathcal{D}x(t) \approx dx_1 dx_2 \dots dx_j \dots dx_{N-1}$ . There will in general a constant of proportionality (possibly infinite). Thus

$$K(f, i) = K(x_f, t_f; x_i, t_i) = \mathcal{N} \int_{x_0=x_i}^{x_N=x_f} [dx_1 dx_2 \dots dx_{N-1}] e^{\frac{i}{\hbar} S(f, i)}$$

Where  $S$  is the action and  $\mathcal{N}$  is a normalization constant.

2. The composition law  $K(a, b) = \int dx_c K(b, c) K(c, a)$ : Draw figure.  $K$  is called Kernel. This can be iterated.

3. Get

$$K(x_f, t_f; x_i, t_i) = \int dx_1 \int dx_2 \dots \int dx_{N-1} K(f, N-1) K(N-1, N-2) \dots K(j+1, j) \dots K(1, i) \quad (12)$$

4. Do the integral  $\int dx_i K(j+1, j) K(j, j-1)$

$$\begin{aligned} & e^{\frac{i}{\hbar} \frac{m}{2} \left[ \frac{x_{j+1} - x_j}{\epsilon} \right]^2 + \frac{m\epsilon}{2} \left[ \frac{x_j - x_{j-1}}{\epsilon} \right]^2} \\ = & e^{\frac{im}{\hbar\epsilon} \left[ \left( x_j - \frac{x_{j+1} + x_{j-1}}{2} \right)^2 + \left( \frac{x_{j+1} - x_{j-1}}{2} \right)^2 \right]} \\ = & \sqrt{\frac{i\hbar\epsilon 2\pi}{2m}} e^{\frac{i2\epsilon m}{\hbar 2} \left( \frac{x_{j+1} - x_{j-1}}{2\epsilon} \right)^2} \end{aligned}$$



This is clearly proportional to  $K(j+1, j-1)$ . The factor in square root is the normalization factor. If we use the Gaussian normalization factor for each of the unit K's, i.e.  $\sqrt{\frac{m}{2\pi\epsilon\hbar i}}$ , we get the final result

$$\sqrt{\frac{m}{2\pi 2\epsilon\hbar i}} e^{\frac{i2\epsilon m}{\hbar^2} \left(\frac{x_{j+1}-x_{j-1}}{2\epsilon}\right)^2}$$

which has the correct normalization.

Clearly this process can be iterated to replace  $2\epsilon$  by  $N\epsilon = t_f - t_i$ . Thus

$$K(x_f, t_f; x_i, t_i) = \sqrt{\frac{m}{2\pi(t_f - t_i)\hbar i}} e^{\frac{i(t_f - t_i)m}{\hbar^2} \left(\frac{x_f - x_i}{(t_f - t_i)}\right)^2} \quad (13)$$

### 5. Relation to wave functions - evolution operator.

$$\psi(x_f, t_f) = e^{-i \int_{t_i}^{t_f} H dt} \psi(x_i, t_i) = \int K(x_f, t_f; x_i, t_i) \psi(x_i, t_i) dx_i \quad (14)$$

### 5.5) Expansion of $K(x_f, t_f; x_i, t_i)$ in terms of wave functions

$$K(x_f, t_f; x_i, t_i) = \sum_n \psi_n(x_f) \psi_n^*(x_i) e^{-i \frac{E_n(t_f - t_i)}{\hbar}}$$

### 6. Derivation of Schroedinger's eqn.

Consider infinitesimal evolution from  $t$  to  $t + \epsilon$ . The evolution operator is

$$K(x_f, t_f; x_i, t_i) = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp\left(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t))\right)$$

We set  $t_f = t_i + \epsilon$  to get

$$\psi(x_f, t_i + \epsilon) = \int_{x(t_i)=x_i}^{x(t_i+\epsilon)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_i+\epsilon} dt L(x(t), \dot{x}(t))\right) \psi(x_i, t_i) dx_i$$

For infinitesimal evolution

$$\psi(x_f, t_i + \epsilon) = \mathcal{N} \int e^{\frac{i}{\hbar} \frac{m}{2} \epsilon \left[\frac{x_f - x_i}{\epsilon}\right]^2} \psi(x_i, t_i) dx_i$$

$\mathcal{N}$  is chosen so that the gaussian integral gives 1. bLHS is  $\psi(x_f, t_i) + \epsilon \frac{\partial \psi}{\partial t_i}$ .  
 Letting  $x_f - x_i = y$  and  $\psi(x_f, t_i) = \psi(x_i, t_i) + y \frac{\partial \psi}{\partial y} + \frac{y^2}{2} \frac{\partial^2 \psi}{\partial y^2}$  (we get (linear term vanishes by symmetry)

$$i\hbar \frac{\partial \psi}{\partial t_i} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial y^2}$$

(After multiplying by  $\hbar$  on both sides.) This is SE. QED.

Note that  $K(x_f, t_f; x_i, t_i)$  satisfies SE. Also the bc  $\lim_{t_f \rightarrow t_i} K(x_f, t_f; x_i, t_i) = \delta(x_f - x_i)$ .

7. getting semi classical energy, momentum. Using  $\sqrt{\frac{m}{2\pi(t_f - t_i)\hbar i}} e^{\frac{i(t_f - t_i)m}{\hbar^2} (\frac{x_f - x_i}{(t_f - t_i)})^2}$  we can understand semi classical limit : Change in phase wrt change in  $x_f$  gives momentum and change wrt  $t_f$  gives energy. Use  $K(x_f, t_f; x_i, t_i)$  and study variation wrt  $x_f$ . Prove that  $\frac{\partial}{\partial x} S_{cl} = p$ .

a)

$$\begin{aligned} S + \delta S &= \int_{t_a}^{t_b} L(x + \delta x, \dot{x} + \delta \dot{x}) dt \\ \delta S &= \int_{t_a}^{t_b} \frac{d}{dt} \left[ \delta x \frac{\partial L}{\partial \dot{x}} \right] dt + \int dt [\text{eqn of motion}] \\ \delta S &= \delta x \frac{\partial L}{\partial \dot{x}} \Big|_{t_b}^{t_b} \\ \frac{\partial S}{\partial x_b} &= \frac{\partial L}{\partial \dot{x}} \Big|_{t_b} = P_b \end{aligned}$$

b) Same thing for energy:

$$S + \delta S = \int_{t_a}^{t_b + \delta t_b} dt L(t, x'_{cl}, \dot{x}'_{cl})$$

$x'$  is the modified classical solution.  $x'_{cl}(t_b + \delta t_b) = x_{cl}(t_b) = x_b$ .

$$\begin{aligned} S + \delta S &= \int_{t_a}^{t_b + \delta t_b} L(x'_{cl}, \dot{x}'_{cl}) dt \\ &= \int_{t_a}^{t_b} L(x'_{cl}, \dot{x}'_{cl}) + \delta t_b L(x'_{cl}, \dot{x}'_{cl}) \\ \delta S &= \delta t_b L(x'_{cl}, \dot{x}'_{cl}) + \int_{t_a}^{t_b} [L(x'_{cl}, \dot{x}'_{cl}) - L(x_{cl}, \dot{x}_{cl})] dt \end{aligned}$$

The term in square brackets is after integrating by parts and using equations of motion  $\delta x_{cl} \frac{\delta L}{\delta \dot{x}}$ .

Using bc we get  $x'_{cl}(t_b) + \dot{x}'_{cl} \delta t_b = x_{cl}$ . So  $x'_{cl} - x_{cl} = -\dot{x}'_{cl} \delta t_b$ . All this gives:

$$\begin{aligned} \delta S &= L \delta t_b + \int^{t_b} dt [L(t, x'_{cl}, \dot{x}'_{cl}) - L(t, x_{cl}, \dot{x}_{cl})] \\ &= L \delta t_b + \frac{\partial L}{\partial \dot{x}} (x'_{cl} - x_{cl}) = L \delta t_b - p \dot{x}_{cl} \delta t_b = -E \delta t_b. \end{aligned}$$

c) Understand normalization:  $\frac{m}{2\pi\hbar T} dx = P(b) dx$ .

$$\frac{mb}{T} < p < \frac{m(b+dx)}{T}$$

Range of momentum  $dp = \frac{m dx}{T}$ . Thus the probability is of the form  $P(p) dp = \text{const } dp$  where const is  $\frac{1}{2\pi\hbar}$ .

7.5) Do the Gaussian slit - Feynman - and repeat results of wave packet spreading etc. - Perhaps as HW.

8. Include potential term  $V(x)$ . **Harmonic oscillator** approx. Add  $-V(x(t))$  to  $L$ . Then calculate PI all over again. Stationary phase gives the usual classical equations of motion. In general cannot

be done exactly. Expand  $V(x)$  in power series near minimum. Quadratic term gives harmonic oscillator. Can be done exactly.

The kernel for the harmonic oscillator can be found exactly:

$$\int_{X(0)=X_i}^{X(T)=X_f} \mathcal{D}X(t) e^{\frac{im}{2\hbar} \int_0^T (\dot{x}^2 - \omega^2 x^2) dt}$$

Expand  $X(t) = X_{classical}(t) + y(t)$ , where  $x_{cl}(t)$  is the classical solution that satisfies the boundary conditions. Expand. Purely classical piece give the classical action. This is

$$\exp\left\{\frac{im\omega}{2\hbar \sin\omega T} [(x_f^2 + x_i^2) \cos\omega T - 2x_f x_i]\right\}$$

What remains is a Gaussian integral over  $y(t)$

$$\int_{Y(0)=0}^{Y(T)=0} \mathcal{D}Y(t) e^{\frac{im}{2\hbar} \int_0^T (\dot{Y}^2 - \omega^2 Y^2) dt}$$

Expand  $y(t) = \sum_n a_n \sin(\frac{n\pi t}{T})$

$$KE = T \sum_n a_n^2 \frac{1}{2} \left(\frac{n\pi}{T}\right)^2$$

$$PE = T \sum_n \frac{1}{2} a_n^2 \omega^2$$

Do integral over  $a_n$  (Jacobian is a constant) : the integral is of the form  $e^{-const a_n^2 ((\frac{n\pi}{T})^2 - \omega^2)}$ . The constant is independent of  $\omega$  and has the same value when  $\omega = 0$ . This integral is  $const' \times (1 - \frac{\omega^2 T^2}{n^2 \pi^2})^{-\frac{1}{2}}$ . Product over all  $n$  gives  $(\frac{\sin \omega T}{\omega T})^{-1/2}$ . Comparing with free particle gives  $const' = (\frac{m}{2\pi i \hbar T})^{1/2}$ .

The final result:

$$\left(\frac{m\omega}{2\pi i \hbar \sin \omega T}\right)^{1/2} \exp\left\{\frac{i m \omega}{2 \hbar \sin \omega T} [(x_f^2 + x_i^2) \cos \omega T - 2 x_f x_i]\right\}$$

9. Do with forcing function. Only classical action will be different.

10. **Several degrees of freedom.**  $K(x_f, X_f, t_f; x_i, X_i, t_i)$ . The convenience of the formalism. Separable systems.  $S(x, X) = S_1(x) + S_2(X)$ . The concept The final result:

$$\left(\frac{m\omega}{2\pi i \hbar \sin \omega T}\right)^{1/2} \exp\left\{\frac{i m \omega}{2 \hbar \sin \omega T} [(x_f^2 + x_i^2) \cos \omega T - 2 x_f x_i]\right\}$$

9. Do with forcing function. Only classical action will be different.

10. **Several degrees of freedom.**  $K(x_f, X_f, t_f; x_i, X_i, t_i)$ . The convenience of the formalism. Separable systems.  $S(x, X) = S_1(x) + S_2(X)$ . The concept of "integrating out" degrees of freedom. When would you want to do that: unobservables : eg ren group - effective actions, thermodynamic heat bath or the rest of the universe,

## 2.9 Statistical Mechanics and the Density Matrix

1. Elementary Quantum Stat Mech: Expectation value of an operator in equilibrium so that states are weighted with Boltzmann factor  $\langle A \rangle = \sum_i p_i A_i$  where  $p_i = \frac{1}{Z} e^{-\beta E_i}$

$Z$  The partition fn. Free energy.  $F(T, V, N)$  or  $E(S, V, N)$ .

2. Other infmn  $P(x)$ ? Need the unintegrated form of the partition fn i.e. density matrix.

$$3. P(x) = \frac{1}{Z} \sum_i \phi_i^*(x) \phi_i(x) e^{-\beta E_i}$$

Similarly

$$\begin{aligned} \langle A \rangle &= \frac{1}{Z} \sum_i A_i e^{-\beta E_i} \\ &= \frac{1}{Z} \sum_i \phi_i^*(x) A \phi_i(x) e^{-\beta E_i} = \frac{1}{Z} \sum_i \langle \phi_i | A | \phi_i \rangle e^{-\beta E_i} \end{aligned}$$

Define

$$\begin{aligned} \rho(x', x) &= \sum_i \phi_i(x') \phi_i^*(x) e^{-\beta E_i} \\ \rho &= \sum_i | \phi_i \rangle \langle \phi_i | e^{-\beta E_i} \\ &= \underbrace{\sum_i | \phi_i \rangle \langle \phi_i |}_1 e^{-\beta H} \\ &= 1 \cdot e^{-\beta H} \end{aligned}$$

“Density Matrix”.

$$\langle A \rangle = \frac{1}{Z} \text{Tr}[A\rho] = \int dx A \rho(x', x) \delta(x - x')$$

where  $Z = \text{Tr}[\rho] = \int dx \rho(x, x)$

4. Consider

$$K(x_f, t_f; x_i, t_i) = \sum_n \psi_n(x_f) \psi_n^*(x_i) e^{-\frac{i}{\hbar} E_n (t_f - t_i)}$$

If we let  $i(t_f - t_i) = \beta \hbar$  we have the density matrix!

Thus can use path integral with  $i\hbar$  replaced by  $u$  to evaluate  $\rho$ :

$$\rho(x', x) = K(x', \beta \hbar; x, 0) = \int_{x(0)=x, x(\beta \hbar)=x'} \left( \exp\left\{ -\frac{1}{\hbar} \int_0^\beta \hbar \left[ \frac{m}{2} \dot{x}^2(u) + V(x) \right] du \right\} \right) \mathcal{D}x(u)$$

To calculate  $Z = \text{Tr}[\rho]$  set  $x' = x$  and integrate over  $x$ , i.e. sum over all *periodic* paths.

5. Density operator in general:

a) Pure case :  $\rho_k = | \psi_k \rangle \langle \psi_k |$ . Assume normalized.  $\rho^2 = \rho$ .  $\text{Tr} \rho = 1$ .

In terms of some energy eigenstates (say):  $| \psi_k \rangle = \sum_n c_n | \phi_n \rangle$  with  $\sum_n c_n^* c_n = 1$ . So

$$\rho_k = \sum_{n,m} c_n^* c_m | \phi_m \rangle \langle \phi_n |$$

$Tr\rho = 1$  clearly. Off diagonal elements are “coherences”.

Time evolution:  $\rho_k(t) = |\psi_k(t)\rangle\langle\psi_k(t)|$  So  $\frac{d\rho}{dt} = \frac{1}{i\hbar}[H, \rho]$ .

Note that only coherences have non zero time dependence.

b) Mixed case

$$\rho = \sum_k p_k \rho_k$$

$p_k$  is a probability :  $\sum_k p_k = 1$ . Motivation for this can be from thermo or from integrating out.

$Tr\rho = 1$  obviously. But  $\rho^2 \leq \rho$ . Equals sign only in pure case.

Time evolution: same as pure case. In the case of  $e^{-\beta H}$  obviously time dependence is not there.

6. Several variables and partial traces - that discussion can be carried over to density matrices. Tensor product. In general the density matrix is not a direct product of two density matrices. If the systems are physically independent it will be a direct product.

i) Direct product:  $\rho = \rho_\phi \otimes \rho_\xi$

$$\rho_\phi = p_1 |\phi_1\rangle\langle\phi_1| + p_2 |\phi_2\rangle\langle\phi_2|$$

$$\rho_\xi = q_1 |\xi_1\rangle\langle\xi_1| + q_2 |\xi_2\rangle\langle\xi_2|$$

Partial trace over  $\phi$  gives  $\rho_\xi$  and vice versa.

ii) Consider

$$\rho = p_1 |\phi_1\rangle\langle\xi_1| + p_2 |\phi_2\rangle\langle\xi_2|$$

$Tr_\phi \rho = \rho_\xi$  defined above, and vice versa but this  $\rho$  is not a direct product.

iii) Start with pure state dm:  $\frac{1}{\sqrt{2}}(|\phi_1\rangle\langle\xi_1| + |\phi_2\rangle\langle\xi_2|)$

$$Tr_\phi \rho = \frac{1}{2}(|\xi_1\rangle\langle\xi_1| + |\xi_2\rangle\langle\xi_2|)$$

which is not a pure state.

### 3 Spin half system

#### 3.1 Stern Gerlach

1. Force on silver atoms in a non-uniform magnetic field  $\vec{F} = \nabla(\vec{\mu} \cdot \vec{B})$ .  $\mu \propto S(\text{spin})$ . Classically spin is in a random direction. The no. of spins  $dN(\theta)$  aligned at an angle  $\theta$  w.r.t.  $z$ -axis is  $\propto 2\pi \sin\theta d\theta$  (solid angle). Force is  $\propto S_z$  and thus the displacement  $\Delta z$  is also  $\propto S_z = S_{max} \cos\theta$ . So  $d\Delta z \propto \sin\theta d\theta$ . Thus we get that  $dN(\theta) \propto \sin\theta d\theta \propto d(\Delta z)$ . So  $dN(\Delta z) = \text{const } d(\Delta z)$ . In other word a constant no. density fn. What is observed are two peaks corresponding to  $S_z = \pm 1/2 \hbar$ .  $\Rightarrow$  **quantization of spin.**

2. So we have a two state Hilbert space spanned by  $| + \rangle, | - \rangle$ . Can obviously apply all postulates of QM. Except need an evolution operator.
3. CSCO is either  $S_z, S_x$ , or  $S_y$ , or some linear combination.
4. Thus  $S.u$  where  $\vec{u}$  is a unit vector measures spin along  $\vec{u}$ .

$$S.u = \cos\theta\sigma_z + \sin\theta\cos\phi\sigma_x + \sin\theta\sin\phi\sigma_y$$

This is obtained by rotating  $\sigma_z$ . Thus consider rotating by  $\theta$  around the  $y$ -axis. This is done by

$$e^{-\frac{i\theta\sigma_y}{2}}\sigma_z e^{\frac{i\theta\sigma_y}{2}} = (\cos\theta\sigma_z + \sin\theta\sigma_x)$$

Rotate further by  $\phi$  around  $z$ -axis and get  $S.u$ . Thus  $R\sigma_z R^\dagger$  with  $R = e^{-\frac{i\phi\sigma_z}{2}} e^{-\frac{i\theta\sigma_y}{2}}$  gives the answer.

5. The corresponding eigenvectors are thus  $|\pm\rangle_u = R|\pm\rangle$  Thus

$$\begin{aligned} |+\rangle_u &= \\ e^{-\frac{i\phi\sigma_z}{2}} (\cos\frac{\theta}{2} - i\sin\frac{\theta}{2}\sigma_y) |+\rangle &= e^{-\frac{i\phi}{2}} \cos\frac{\theta}{2} |+\rangle + e^{\frac{i\phi}{2}} \sin\frac{\theta}{2} |-\rangle \\ |-\rangle_u &= \\ e^{-\frac{i\phi\sigma_z}{2}} (\cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\sigma_y) |-\rangle &= e^{\frac{i\phi}{2}} \cos\frac{\theta}{2} |-\rangle - e^{-\frac{i\phi}{2}} \sin\frac{\theta}{2} |+\rangle \end{aligned}$$

6. Polarizer analyser sequence. Start with  $|+\rangle$ . Analyser in some other direction  $\vec{u}$ . Find various probabilities.

Basic expressions :

$$\begin{aligned} \langle + | + \rangle_u &= e^{-\frac{i\phi}{2}} \cos\frac{\theta}{2} \\ \langle - | + \rangle_u &= e^{\frac{i\phi}{2}} \sin\frac{\theta}{2} \\ \langle + | - \rangle_u &= -e^{-\frac{i\phi}{2}} \sin\frac{\theta}{2} \\ \langle - | - \rangle_u &= e^{\frac{i\phi}{2}} \cos\frac{\theta}{2} \end{aligned}$$

What is  $\langle + | S_z | + \rangle_u$ ? ANS  $\cos^2\theta/2 - \sin^2\theta/2 = \cos\theta$  which is the classical answer. Similarly  $\langle S_x \rangle, \langle S_y \rangle$ .

7. Back to Stern Gerlach. Prepare  $|\pm\rangle_u$  state. Then analyze into  $|\pm\rangle$  states.

$$\langle + | - \rangle_u = -e^{-\frac{i\phi}{2}} \sin \frac{\theta}{2}$$

When does measurement take place? Even after the magnetic field there is a wave packet which has split into two - representing the two possible outcomes. Even after they hit the screen? After we observe it?

If it doesn't hit the screen it is possible to recombine them into a single beam and get back  $|\pm\rangle_u$  state. This is a physical explanation of "complete set of states".

8. **Precession in a magnetic field.** "Larmor precession." Quantum mechanical evolution in a constant magnetic field Rotating frame.

i)  $H = -\gamma \mathbf{S} \cdot \mathbf{B}$  and assume  $\mathbf{B}$  is const.

Classically  $\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \mathbf{B}$  If  $-\gamma \vec{B} = \vec{\omega}$ , then  $\frac{d\vec{m}}{dt} = \vec{\omega} \times \vec{m}$ .

Larmor Precession.

ii) Effect of going to a rotating frame  $(\frac{d\vec{m}}{dt})_X = (\frac{d\vec{m}}{dt})_x - \vec{\omega} \times \vec{m}$

iii) Quantum mechanically  $U = e^{i/2\gamma \vec{B} \cdot \vec{\sigma} t}$   $\vec{\omega} = -\gamma \vec{B}$ . So if  $B_x$  is there then  $U = e^{-i/2\omega_x \sigma_x t}$  which is a rotation about the x-axis by an angle  $\omega t$  - time dependent rotation - Larmor precession.

eg  $H = H_z \sigma_z$ . If  $\psi_+(t) = \langle + | \psi(t) \rangle$  and  $\psi_-(t) = \langle - | \psi(t) \rangle$  then

$$|\psi(t)\rangle = e^{-\frac{iH_z t}{\hbar}} |+\rangle \psi_+(0) + e^{+\frac{iH_z t}{\hbar}} |-\rangle \psi_-(0)$$

Compare with

$$|+\rangle_u = e^{-\frac{i\phi}{2}} \cos \frac{\theta}{2} |+\rangle + e^{+\frac{i\phi}{2}} \sin \frac{\theta}{2} |-\rangle$$

If we set  $\cos \theta/2 = \psi_+(0)$  and  $\sin \theta/2 = \psi_-(0)$  and  $\phi = \frac{H_z t}{\hbar}$  then they are the same. Thus the solution is just a rotated state.

iv) Generalize to the case where there is both  $B_z$  and some  $B_x$ .

Step1 : Determine  $\theta, \phi$ .

Step2 Find  $|\pm\rangle_u$  and the eigenvalues are  $\pm |\gamma B|$ . where  $|B|^2 = B_x^2 + B_z^2$ .  $\omega_1 = -\gamma B_x$  and  $\Delta\omega = \gamma B_z$

Step3. Start with  $|\psi(0)\rangle = |+\rangle = |+\rangle_u \cdot u \langle + | + \rangle + |-\rangle_u \cdot u \langle - | + \rangle$

Step 4.  $|\psi(t)\rangle = e^{-i\omega_+ t} |+\rangle_u \cdot u \langle + | + \rangle + e^{-i\omega_- t} |-\rangle_u \cdot u \langle - | + \rangle$

$$= e^{i\phi/2 - i\omega_+ t} \cos\theta/2 |+\rangle_u - e^{-i\phi/2 - i\omega_- t} \sin\theta/2 |-\rangle_u$$

Step5: Calculate  $\langle - | \psi(t) \rangle$  to get  $e^{i\phi} \sin\theta/2 \cos\theta/2 (e^{i\Delta\Omega t} - e^{-i\Delta\Omega t}) e^{-i\omega_{avg} t}$



Prob (t) =  $\sin^2\theta\sin^2\Delta\Omega t$  where  $(\Delta\Omega)^2 = (\Delta\omega)^2 + \omega_1^2$  and  $\tan\theta = \frac{\omega_1}{\Delta\omega}$

9. Rotating magnetic field. Classical picture of resonance. Quantum picture. **NMR.**  $\frac{d\vec{m}}{dt} = \gamma\vec{m} \times (B_z\hat{e}_z + B_1\cos\omega t\hat{e}_x + B_1\sin\omega t\hat{e}_y)$

Go to rotating frame where  $B_1(t)$  is time independent.

$$\left(\frac{d\vec{m}}{dt}\right)_X = \left(\frac{d\vec{m}}{dt}\right)_x - \vec{\omega} \times \vec{m}$$

If  $\gamma B_z = -\omega_0$  then we get

$$\left(\frac{d\vec{m}}{dt}\right)_X = \vec{m} \times (\omega - \omega_0)\hat{e}_z - \vec{m} \times \omega_1\hat{e}_x$$

.

**qm:** Time dependent Hamiltonian!

.

$$H = \hbar/2 \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{+i\omega t} & \omega_0 \end{pmatrix} \quad (15)$$

Going to rotating frame qm is done by  $|\psi\rangle = e^{-i\omega t/2\sigma_z}|\chi\rangle$  is a definition of  $|\chi\rangle$  where Hamiltonian becomes time independent.

Equation becomes (Use  $e^{-i\omega t\sigma_z/2}\sigma_x e^{+i\omega t/2} = \cos\omega t\sigma_x + i\sin\omega t\sigma_y$ )

$$i\hbar\frac{\partial}{\partial t}e^{-i\omega t/2\sigma_z}|\chi\rangle = e^{-i\omega t/2\sigma_z}\hbar/2(\omega_0\sigma_z + \omega_1\sigma_x)|\chi\rangle$$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}|\chi\rangle = \hbar/2[(\omega_0 - \omega)\sigma_z + \omega_1\sigma_x]|\chi\rangle$$

$$\mathcal{P}_{+-}(t) = \frac{\omega_1^2}{\omega_1^2 + (\Delta\omega)^2} \sin^2(\sqrt{\omega_1^2 + \Delta\omega^2}t/2)$$

When  $\Delta\omega = 0$ , the probability becomes 1 at some time. This is when resonance occurs. So  $\omega_0 = \omega$ .  $\omega$  is the energy of the photon corresponding to oscillating field.  $\omega_0$  is the energy difference. So  $\hbar\omega = \Delta E$ .

10. Other 2-level systems... ( $K^0 - \bar{K}^0$  system). **“Regeneration”**. General two level system and Spin 1/2 analogy.

## 4 Rotation Group

### 4.1 Symmetries and Conservation Laws

1. Physical idea of symmetry - translation, rotation, Lorentz transformation. Connection to coordinate transformation - the idea of manifest invariance of equations/Hamiltonian/Lagrangian. Distinction between active and passive transformation - one involves a physical movement whereas the other is a change of coordinates. But ultimately they amount to the same thing because “if the coordinate change leaves  $H$  invariant “you can’t tell from within the system that you have moved”.

If  $H$  is invariant under translations, then  $[P, H] = 0$ . But this also means  $P$  is constant in time. Conservation of momentum.

2. Transformation of other quantities: eg. background fields. If  $B \neq 0$  then rotation is not a symmetry, unless you rotate  $B$  also.

3. Practical application:i) when you choose a convenient coordinate system.

ii)Intuitive idea that the final result cannot contain such and such term: e.g by rotation/reflection symmetry the energy of a magnetic field cannot contain  $B_x$ . It must be  $B^2$ .

These ideas are made precise by group theory.

4. Groups: mathematical objects that describe symmetry operations. Multiplication, inverse, identity, closure. Discrete vs continuous. (Note:  $gh \neq hg$  in general - non commutative, but associative)

5. Discrete vs continuous groups. Lie groups. Lie algebras (addition is also included). Illustrate with translations.  $D_x(a) = e^{iaP_x}$  The idea of exponentiation.

Generator =  $P_x$

Similarly  $D_y(b)$ .  $P_x, P_y$  form an algebra.  $D_x, D_y$  form a group. Commutation relation for algebra. Commutative (Abelian) vs Non abelian groups.

$$D_x(a)D_x(b) = D_x(a + b) = D_x(b)D_x(a)$$

....

$$D_x(a)D_y(b) = D_y(b)D_x(a)$$

Equivalent to

$$[P_x, P_y] = 0$$

Explain the action on coordinates, wave functions, etc.

$D_x(a) : x \rightarrow x + a$  and  $D_x(a)x D_x^{-1} = x + a$  (prove to second order)

$$[P_x, x] = -i$$

Here  $x$  is being treated as an operator.

$[iP_x, x] = \partial_x x = 1$  is a particular representation of the operators in  $x$ -space. Then  $D_x(a) = e^{a\partial_x}$

Acting on functions  $D_x(a)\psi(x) = \psi(x + a)$ .

Rotations:

$$x' = x\cos\theta + y\sin\theta$$

$$y' = -x\sin\theta + y\cos\theta$$

Can write as a matrix.  $R(\theta) = \dots$  Also abelian - any one generator group is abelian by defn.

6. Implications for qm:  $[G, H] = 0$   $G$  is the generator of a transformation. Degeneracy.  $R(orG) | 1 \rangle = | 2 \rangle$ ,  $| 2 \rangle$  have same energy.  $R | 2 \rangle = | 3 \rangle \dots$  It will probably end somewhere if the group is **compact**. This defines an **irrep**. Dimension of the irrep is known from group theory. eg for rotation group. eg of spin  $1/2$ .  $2j + 1$ .

How does one define transf of wave fns.

$$\psi'(r') = \psi(r)$$

Why? Defines a **scalar**. If  $r' = \mathcal{R}r$  Then

$$\psi'(r') = \psi(\mathcal{R}^{-1}r')$$

$$\Rightarrow \psi'(r) = R\psi(r) = \psi(\mathcal{R}^{-1}r)$$

eg Translations:

$$\psi'(x) = R\psi(x) = \psi(x - a) = e^{-a\partial_x}\psi(x)$$

where  $R$  is the effect of a translation by  $+a$  on the state. This gives

$$R = D_x(-a) = e^{-a\partial_x} = e^{-iaP_x}$$

**Note the signs.**

Action on kets:

$$| \psi' \rangle = R | \psi \rangle$$

$$\Rightarrow \langle r | \psi' \rangle = \langle r | R | \psi \rangle = \langle \mathcal{R}^{-1}r | \psi \rangle$$

Thus

$$R^\dagger | r \rangle = | \mathcal{R}^{-1}r \rangle$$

Clearly  $R^\dagger R = RR^\dagger = I$  So  $R$  is **unitary**. It is obviously linear. So on states it is represented by a unitary matrix and the generators by a Hermitian matrix.

Action on operators  $A' = RAR^\dagger$ .

7. Let us use this to find  $R$  for rotations: eg

$$\psi'(r) = R\psi(r) = \psi(\mathcal{R}^{-1}r) = \psi(x+yd\phi, y-xd\phi) = [1-d\phi(x\partial_y - y\partial_x)]\psi(x, y)$$

Let

$$x\partial_y - y\partial_x = \frac{i}{\hbar}L_z$$

Thus

$$R = 1 - d\phi \frac{i}{\hbar}L_z$$

This can be defined as the action of (infinitesimal) rotation about z on states. For finite rotations  $R_z(\phi) = e^{\frac{-i\phi L_z}{\hbar}}$ . Physically: Rotates your coordinate system by  $+\phi$ . Or physical system by  $-\phi$ .

So if Hamiltonian is rotationally invariant about Z- axis  $[L_z, H] = 0$ . What is  $L_z$ ? It is angular momentum. Check : Classically  $\mathbf{L} = \mathbf{r} \times \mathbf{P}$ . So  $L_z = xP_y - yP_x = -i\hbar(x\partial_y - y\partial_x)$

Similarly

$$\begin{aligned} \frac{i}{\hbar}L_x &= y\partial_z - z\partial_y \\ \frac{i}{\hbar}L_y &= z\partial_x - x\partial_z \end{aligned}$$

Commutation relations

$$[L_i, L_j] = i\hbar\epsilon^{ijk}L_k$$

8. Implications for matrix elements. eg for integration : even and odd fns. The analog of this for more complicated groups. eg  $\int e^{in\theta}d\theta$  Using **invariance of measure**  $d\theta$  under  $\theta \rightarrow \theta + a$  show that integral must be zero. So only singlets can be integrated to get non zero answer.

$$\int_0^{2\pi} d\theta f(\theta) = \int_0^{2\pi} d\theta' f(\theta')$$

Choose  $\theta' = \theta + a$ . Consider  $I_n = \int_0^{2\pi} d\theta e^{in\theta}$ . By change of variables  $I_n = \int_0^{2\pi} d\theta' e^{in\theta'} = \int_0^{2\pi} d\theta e^{in(\theta+a)} = e^{ina}I_n$ . We have used  $d\theta = d\theta'$ .  $\Rightarrow I_n[1 - e^{ina}] = 0$ . So either  $n = 0$  or  $I_n = 0$ .

Get result that the integral is zero unless  $f$  is a singlet.  
 Similarly for rotation gr.

$$\int d^3x f_a(x, y, z) = \int d^3x' f_a(x'..) = \int d^3x f_a(\mathcal{R}(\theta, \phi)x..) = \int d^3x R_{ab}^{-1} f_b(x..) \\ \Rightarrow (\delta_{ab} - R_{ab}^{-1}(\theta, \phi)) \int d^3x f_b(x, y, z) = 0$$

eg of functions that transform are  $e^{in\phi} \cos m\theta$ .

Cannot be zero for all  $\theta, \phi$  unless i)  $R$  is the identity or ii) the integral is zero. QED.

9. Using above result one can make statements about matrix elements

$$\int d^3x \psi_n^*(x) O(x, \partial_x) \psi_m(x)$$

. Multiplying two irreps. the general answer is complicated - but known. Q  
 nos add. again eg of  $Y_{lm}$  and  $e^{im\phi}$ .

10. Before we turn to rotation group what are the other symmetries?

Lorentz group

$$x' = \gamma(x - \beta t)$$

$$t' = \gamma(t - \beta x)$$

$$y' = y$$

$$z' = z$$

( $\gamma = \frac{1}{\sqrt{1-\beta^2}}$ ). In units where  $c=1$ .  $SO(3)$ - rotations.  $SO(3,1)$  Lorentz group.  
 Poincare group includes translations.

11. Internal symmetries: Best known example : electric charge! Phase of the wave function can be changed. Overall phase is not important. Actually this corresponds to particle number.

12. Local vs. global symmetries. "gauge" symmetries.

## 4.2 Rotation Group and Angular Momentum

1. Commutation relns:

$$[J_i, J_j] = i\epsilon_{ijk} J_k$$

$$[J^2, J_i] = 0$$

$$J_+ = J_x + iJ_y$$

$$J_- = J_x - iJ_y$$

$$[J_z, J_\pm] = \pm J_\pm$$

$$[[J_+, J_-] = 2J_z$$

2. CSCO

3. How nonlinearity fixes normalization. Thus  $\sigma_i$  do **not** satisfy the commutation relns:  $\frac{\sigma_i}{2}$  do. Unlike Abelian case.

4.  $J_\pm$  are raising lowering operators.

$$J_+ |m\rangle = \text{const} |m+1\rangle.$$

5. Show that  $|j, m\rangle$  and  $|j, m \pm 1\rangle$  are orthogonal using  $J_z, J_\pm$  commutation. Thus the states generated by rotations span a vector space of some dimensionality that can be worked out. This is the **representation**. Explain the concept of a representation.

$$\text{Fix const by using } |J_- |j, m\rangle|^2 = \langle j, m | J_+ J_- |j, m\rangle$$

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

Eigenvalue of  $J^2$  being  $j(j+1)$  is a convention.  $j$  is a real number.

$$|J_+ |j, m\rangle|^2 = \langle j, m | J_- J_+ |j, m\rangle$$

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

So

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

.

6. Show

$$\text{:i) } -j \leq m \leq j$$

$$\text{ii) } J_- |j, -j\rangle = 0 \text{ but } J_- |j, -j + \epsilon\rangle \neq 0.$$

$$J_+ |j, j\rangle = 0 \text{ but } J_+ |j, m - \epsilon\rangle \neq 0.$$

iii) The value of  $m$  closest to  $-j$ , if it is a little larger than  $-j$  (can always be made to lie between  $-j, -j+1$ ) we get a contradiction. Because on the one hand  $J_-$  acting on that has to give zero, because

$m - 1 < -j$ . On the other hand the norm of  $J_-|j, m\rangle$  is not zero if  $m > -j$ . Only possibility is that the  $m$  must be precisely  $= -j$ .

Thus the difference between  $-j$  and  $m$  must be an integer. Similarly between  $j$  and  $m$ . Thus we have  $m - p = -j$  and  $m + q = j$ .

Therefore  $j = (q + p)/2 \Rightarrow j$  is integer or half integer

7. Matrix elements :

$$\langle j, m | J_z | j', m' \rangle = \delta_{j,j'} \delta_{m,m'}$$

$$\langle j, m | J_{\pm} | j', m' \rangle = \delta_{j,j'} \delta_{m,m' \pm 1} \sqrt{j(j+1) - m(m \pm 1)}$$

As an example of the group theoretic selection rule.

8. Examples of representations:  $j=0, 1/2, 1$ . What they act on.

### 4.3 Orbital Angular Momentum and $Y_{lm}$

1.

$$L_x = \frac{\hbar}{i}(y\partial_z - z\partial_y)$$

etc. Physical idea of orbital vs spin.

Write this in terms of  $\theta, \partial_\theta, \phi, \partial_\phi$

2. Change of variables:  $x, y, z \rightarrow r, \theta, \phi$ . Volume element  $d^3x = r^2 dr d\Omega = r^2 dr d\phi d(\cos\theta)$

$$Y_{lm} = \langle \theta, \phi | l, m \rangle$$

This is the definition. Like

$$\langle x | k \rangle = e^{ikx}$$

3. Just as  $e^{ikx}$  is a soln of  $\partial_x \psi(x) = k\psi(x)$  we need eqns for  $Y_{lm}$ .

$$L_+ Y_{lm} = 0$$

$$L_z Y_{lm} = m Y_{lm}$$

4. Need  $L_j$  expressions in spherical coordinates.

$$L_x = i(\sin\phi\partial_\theta + \frac{\cos\phi}{\tan\theta}\partial_\phi)$$

$$L_y = i(-\cos\phi\partial_\theta + \frac{\sin\phi}{\tan\theta}\partial_\phi)$$

$$L_z = -i\partial_\phi$$

$$L_+ = e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi)$$

$$L_- = e^{-i\phi}(-\partial_\theta + i\cot\theta\partial_\phi)$$

$$L^2 = -(\partial_\theta^2 + \frac{1}{\tan\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2)$$

$$z = r\cos\theta, \quad \rho = r\sin\theta, \quad x = \rho\cos\phi, \quad y = \rho\sin\phi$$

Consider functions that don't depend on  $r$ .

$$f(x, y, z) = f(r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta) \equiv g(\theta, \phi)$$

$$\frac{\partial f}{\partial x} = \frac{\partial g}{\partial x} = \frac{\partial g}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial g}{\partial \phi} \frac{\partial \phi}{\partial x}$$

$$\tan \theta = \frac{\sqrt{x^2 + y^2}}{z}$$

$$\sec^2 \theta d\theta = -\frac{\rho}{z^2} dz + \frac{2xdx + 2ydy}{2\rho z}$$

$$\frac{\partial \theta}{\partial z} = -\frac{\rho}{z^2} \cos^2 \theta = -\frac{1}{r} \sin \theta$$

$$\frac{\partial \theta}{\partial x} = \cos^2 \theta \frac{x}{\rho z} = \frac{1}{r} \cos \theta \cos \phi$$

$$\frac{\partial \theta}{\partial y} = \cos^2 \theta \frac{y}{\rho z} = \frac{1}{r} \cos \theta \sin \phi$$

$$\frac{x}{y} = \cot \phi \Rightarrow \frac{dx}{y} - \frac{xdy}{y^2} = -\operatorname{cosec}^2 \phi d\phi$$



$$\begin{aligned}
\frac{\partial \phi}{\partial x} &= -\frac{\sin^2 \phi}{y} = -\frac{\sin \phi}{r \sin \theta} \\
\frac{\partial \phi}{\partial y} &= \frac{x \sin^2 \phi}{y^2} = \frac{\cos \phi}{r \sin \theta} \\
\frac{\partial g}{\partial x} &= \frac{1}{r} \cos \theta \cos \phi \frac{\partial g}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial g}{\partial \phi} \\
y \frac{\partial g}{\partial x} &= \sin \theta \cos \theta \sin \phi \cos \phi \frac{\partial g}{\partial \theta} - \sin^2 \phi \frac{\partial g}{\partial \phi} \\
\frac{\partial g}{\partial y} &= \frac{\partial g}{\partial \theta} \frac{\partial \theta}{\partial y} + \frac{\partial g}{\partial \phi} \frac{\partial \phi}{\partial y} \\
\frac{\partial g}{\partial y} &= \frac{\partial g}{\partial \theta} \frac{1}{r} \cos \theta \sin \phi + \frac{\partial g}{\partial \phi} \frac{\cos \phi}{r \sin \theta} \\
x \frac{\partial g}{\partial y} &= \sin \theta \cos \theta \sin \phi \cos \phi \frac{\partial g}{\partial \theta} + \cos^2 \phi \frac{\partial g}{\partial \phi} \\
L_z g &= x \frac{\partial g}{\partial y} - y \frac{\partial g}{\partial x} = \frac{\partial g}{\partial \phi}
\end{aligned}$$

Similarly

$$\begin{aligned}
\frac{\partial g}{\partial y} &= \frac{1}{r} \cos \theta \sin \phi \frac{\partial g}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial g}{\partial \phi} \\
\frac{\partial g}{\partial z} &= -\frac{\sin \theta}{r} \frac{\partial g}{\partial \theta} \\
-L_x g &= z \frac{\partial g}{\partial y} - y \frac{\partial g}{\partial z} = \sin \phi \frac{\partial g}{\partial \theta} + \cos \phi \cot \theta \frac{\partial g}{\partial \phi} \\
L_y g &= z \frac{\partial g}{\partial x} - x \frac{\partial g}{\partial z} = \cos \phi \frac{\partial g}{\partial \theta} - \cot \theta \sin \phi \frac{\partial g}{\partial \phi}
\end{aligned}$$

Thus we get a realization in terms of Hermitian differential operators (multiplying by  $-i$ ):

$$L_z = -i \frac{\partial}{\partial \phi}, \quad L_x = i \sin \phi \frac{\partial}{\partial \theta} + i \cos \phi \cot \theta \frac{\partial}{\partial \phi}, \quad L_y = -i \cos \phi \frac{\partial}{\partial \theta} + i \sin \phi \cot \theta \frac{\partial}{\partial \phi}$$

5. Using  $L_z$  get  $Y_{lm}(\theta, \phi) = F_{lm}(\theta)e^{im\phi}$

and

$$L_+ Y_{ll} = 0 \Rightarrow [-\partial_\theta + \cot\theta l] F_{ll} = 0$$

$$dF = \frac{ld(\sin\theta)}{\sin\theta} F$$

$$F = c(\sin\theta)^l$$

$$Y_{ll} = ce^{il\phi} \sin^l \theta$$

Get the rest by using lowering operators.

**Example:**

$$Y_{11}(\theta, \phi) = c e^{i\phi} \sin \theta$$

where  $c$  is a normalization constant.

$$L_- Y_{11} = e^{-i\phi} (\partial_\theta + i \cot \theta \partial_\phi) (c e^{i\phi} \sin \theta)$$

$$\Rightarrow \sqrt{2} Y_{10} = -2c \cos \theta$$

$$Y_{10} = c\sqrt{2} \cos \theta$$

$$L_- Y_{10} = \sqrt{2} Y_{1-1} = \sqrt{2} c e^{-i\phi} \sin \theta$$

$$\Rightarrow Y_{1-1} = c e^{-i\phi} \sin \theta$$

6. Orthogonality:

$$\int d\Omega Y_{lm}^*(\theta, \phi) Y_{lm}(\theta', \phi') = \delta_{ll'} \delta_{mm'}$$

Closure:

$$\sum_{l=0}^{\infty} Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi') = \delta(\cos\theta - \cos\theta') \delta(\phi - \phi')$$

The delta fns satisfy  $\int d\Omega \delta^2 = 1$

7. Explicit expressions:

$$Y_{1,\pm 1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

Cartesian representation x,y,z !!!

Similarly  $Y_{2,m}(\theta, \phi)$  are essentially  $x_i x_j$  these five.

Check that they satisfy  $R\psi(r) = \psi(\mathcal{R}^{-1}r)$

8. Observables transform as  $A' = RAR^\dagger$

$[V, J_i] = 0 \Rightarrow V$  is a scalar

$[V_i, J_j] = i\epsilon_{ijk} V_k \Rightarrow \mathbf{V}$  is a vector.

$\mathbf{J}$  itself is therefore a vector.

9. **Spin** vs Orbital ang momentum. eg. If  $\psi$  itself happens to be a vector,  $\psi'(\mathcal{R}r) = \mathcal{R}\psi(r)$ . Thus  $\psi'(r) = \mathcal{R}\psi(\mathcal{R}^{-1}r)$ . The  $\mathcal{R}$  outside is implemented by  $\vec{d}\phi \times \vec{\psi}$ . Which is  $-i\vec{d}\phi \cdot \vec{S}$  where  $S$  is  $i$  times the matrix that implements the cross product. eg

$$S_z = i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (16)$$

implements rotation about z-axis.  $(-i \cdot i = 1)$ . The  $\mathcal{R}^{-1}$  inside is implemented as already seen by  $-i\vec{d}\phi \cdot \vec{L}$ . So total generator is  $S + L$ .  $S$  is spin.

10. Addition of Angular Momentum - Clebsch Gordan coeff.

The product of two representations must be a representation - in the sense that the generators will not take you out of that set. But it may be **reducible**. Thus:

$$\sum_j c(j) |j, m(= m_1 + m_2)\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

The max value on RHS is  $m_1 = j_1$  and  $m_2 = j_2$ . So max on LHS is  $m_{max} = j_1 + j_2$ . This must be the max value of  $m$  of some  $j_{max}$  Thus

$j_{max} = j_1 + j_2$ . No other (smaller) value of  $j$  can give this  $m$ . Thus we have

$$|j_1 + j_2, j_1 + j_2\rangle = |j_1, j_1\rangle \otimes |j_2, j_2\rangle$$

Use  $J_{\pm} |j, m\rangle = \sqrt{j(j+1) - m(m\pm 1)} |j, m\pm 1\rangle$  Get

$$|j_1 + j_2, j_1 + j_2 - 1\rangle = \sqrt{\frac{j_1}{j_1 + j_2}} |j_1 - 1\rangle \otimes |j_2\rangle + \sqrt{\frac{j_2}{j_1 + j_2}} |j_1\rangle \otimes |j_2 - 1\rangle$$

The orthogonal state is

$$|j_1 + j_2 - 1, j_1 + j_2 - 1\rangle = \sqrt{\frac{j_2}{j_1 + j_2}} |j_1 - 1\rangle \otimes |j_2\rangle - \sqrt{\frac{j_1}{j_1 + j_2}} |j_1\rangle \otimes |j_2 - 1\rangle$$

**Example: spin 1/2**

$$|1, 1\rangle = |++\rangle$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}} [|+-\rangle + |-+\rangle]$$

$$|1, -1\rangle = |--\rangle$$

The orthogonal combination:

$$|0, 0\rangle = \frac{1}{\sqrt{2}} [|+-\rangle - |-+\rangle]$$

The above was an example of calculation of Clebsch-Gordan coefficients.

## 11. Clebsch-Gordan:

$$|J, M\rangle = \sum_{m_1, m_2} |j_1, m_1; j_2, m_2\rangle \underbrace{\langle j_1, m_1; j_2, m_2 | J, M \rangle}_{\text{Clebsch-Gordan}}$$

$$|j_1 - j_2| \leq J \leq j_1 + j_2$$

**Recursion reln for C-G:**

Act with  $J_-$  on LHS and  $J_{1-} + J_{2-}$  on RHS and apply  $\langle m'_1, m'_2 |$  to get

$$\sqrt{J(J+1) - M(M-1)} \langle m'_1, m'_2 | J, M-1 \rangle$$

$$= \sqrt{j_1(j_1 + 1) - m'_1(m'_1 + 1)} \langle m'_1 + 1, m'_2 | J, M \rangle \\ + \sqrt{j_2(j_2 + 1) - m'_2(m'_2 + 1)} \langle m'_1, m'_2 + 1 | J, M \rangle$$

Another reln where +1 and -1 are interchanged. General procedure:

As in the example above we started with  $|j_1 + j_2, j_1 + j_2 \rangle$  and got  $|j_1 + j_2, j_1 + j_2 - 1 \rangle$ . Then by orthogonality we got  $|j_1 + j_2 - 1, j_1 + j_2 - 1 \rangle$ .

Continue: Use these relations to get  $|j_1 + j_2, j_1 + j_2 - 2 \rangle$ ,  $|j_1 + j_2 - 1, j_1 + j_2 - 2 \rangle$ . Then by orthogonality get  $|j_1 + j_2 - 2, j_1 + j_2 - 2 \rangle$ . Keep going and work out all the C-G's.

12. Wigner-Eckart:

i). Scalar operator A: Using  $[J^2, A] = 0 = [J_i, A]$  we can show that

$$\langle j', m' | A | j, m \rangle = \delta_{jj'} \delta_{mm'} a(j)$$

From

$$\langle j', m' | [J^2, A] | j, m \rangle = 0 = \langle j', m' | [J_z, A] | j, m \rangle$$

we see that  $j = j'$  and  $m = m'$ .

To see that the matrix element doesn't depend on  $m$ :

$$\langle j, m | J_- A J_+ | j, m \rangle = [j(j+1) - m(m+1)] \langle j, m+1 | A | j, m+1 \rangle$$

Also:

$$\langle j, m | J_- A J_+ | j, m \rangle = \langle j, m | A J_- J_+ | j, m \rangle = [j(j+1) - m(m+1)] \langle j, m | A | j, m \rangle$$

Thus the matrix elements do not depend on  $m$ . So any two scalars matrix elements are proportional in the entire  $(j, m)$  subspace.

ii) For vectors  $\vec{V}$ : Can show that:

$$\langle j, m' | \vec{V} | j, m \rangle = a(j) \langle j, m' | \vec{J} | j, m \rangle$$

i.e. the prop const is ind of  $m$ :

Use  $[V_+, J_+] = 0$  and the fact that  $V_+$  has  $m = 1$ . Thus

$$\langle j, m+2 | V_+ J_+ | j, m \rangle = \langle j, m+2 | J_+ V_+ | j, m \rangle$$

Insert complete set of states: Only  $|j, m + 1\rangle$  contribute. so

$$\langle j, m + 2 | V_+ | j, m + 1 \rangle \langle j, m + 1 | J_+ | j, m \rangle = \langle j, m + 2 | J_+ | j, m + 1 \rangle \langle j, m + 1 | V_+ | j, m \rangle$$

Thus

$$\frac{\langle j, m + 2 | V_+ | j, m + 1 \rangle}{\langle j, m + 2 | J_+ | j, m + 1 \rangle} = \frac{\langle j, m + 1 | V_+ | j, m \rangle}{\langle j, m + 1 | J_+ | j, m \rangle} = C_+(j)$$

Similarly with  $V_-$  we get  $C_-$ .

Finally, using  $[V_+, J_-] = 2V_z$  we find on inserting a complete set of states,  $\langle j, m | V_z | j, m \rangle = C_+ m$ . If we use  $[V_-, J_+] = -2V_z$  we get  $\langle j, m | V_z | j, m \rangle = C_- m$ . Thus  $C_+ = C_-$ .

Thus if  $P$  is proj operator into  $j$ -subspace:

$$PJVP = a(j)PJJP = a(j)j(j+1)P$$

$$\Rightarrow a(j) = \frac{J \cdot V}{j(j+1)}$$

in the given subspace.

Useful: iii) spinning electron in a magnetic field:  $H_1 = w_l(L_z + 2S_z)$ .

$$J = L + S$$

CSCO:  $J_z, J^2, L^2, S^2$

Thus if we neglect mixing between different values of  $j$  for small B-field.

$$\begin{aligned} \langle J, M, S, L | H_1 | J, M, S, L \rangle &= w_l \frac{\langle J \cdot L \rangle + 2 \langle S \cdot L \rangle}{J(J+1)} J_z \\ &= (3/2 + \frac{S(S+1) - L(L+1)}{2J(J+1)}) M w_l \end{aligned}$$

“Lande’s g-factor” - splits the degeneracy.

iv) General Wigner-Eckart: matrix elements of  $T_{Q,K}$  are proportional to Clebsch-Gordan:

$$\langle j, m | T_{Q,K} | j', m' \rangle = a(j, j') \underbrace{\langle j, m | Q, K; j', m' \rangle}_{C-G}$$

Use CG to write

$$T_{Q,K} |j', m'\rangle = \sum_J N_J |J, M\rangle \langle J, M | Q, K; j', m'\rangle$$

$$T_{Q,K} |j', m'\rangle = \sum_J |J, M\rangle \langle J, M | T_{QK} |j', m'\rangle$$

These two equations are proportional in each  $J, j', Q$  sector. Because rotation of coordinate systems will change  $M, K, m'$  in exactly the same way in both equations. So the proportionality constant  $N_J$  cannot depend on  $M$ .

As a special case consider

$$T_{QQ} |j', j'\rangle = a(Q + j', j') |Q + j', Q + j'\rangle$$

Let

$$T_{Q, Q-1} |j', j'\rangle = \sqrt{\frac{Q}{Q+j'}} a_1 |Q+j', Q+j'-1\rangle - \sqrt{\frac{j'}{Q+j'}} b_1 |Q+j'-1, Q+j'-1\rangle$$

Take the matrix element:

$$\langle Q + j', Q + j' - 1 | T_{Q, Q-1} |j', j'\rangle = \sqrt{\frac{Q}{Q+j'}} a_1$$

LHS can be written as

$$\begin{aligned} \frac{1}{\sqrt{2(Q+j')}} \langle Q+j', Q+j' | J_+ T_{Q, Q-1} |j', j'\rangle &= \frac{1}{\sqrt{2(Q+j')}} \langle Q+j', Q+j' | [J_+, T_{Q, Q-1}] |j', j'\rangle \\ &= \sqrt{\frac{Q}{Q+j'}} \langle Q+j', Q+j' | T_{QQ} |j', j'\rangle = \sqrt{\frac{Q}{Q+j'}} a(Q+j', j') \end{aligned}$$

$$a_1 = a(Q + j', j')$$

Similarly for the rest, by recursion. The above calculation implements the idea of rotating the coordinate system.

More general proof (a la Schiff): Want to show that  $T_{KQ} |j, m\rangle = \sum_J |J, M\rangle \langle J, M | Q, m\rangle$ . Here  $\langle J, M | Q, m\rangle$  are the C-G's. The

sum is over all allowed values of  $J$ .  $|J, M \rangle\rangle$  transforms like an angular momentum state, but its normalization depends on  $T$ . Want to show that this normalization cannot depend on  $M$ . So invert the above:

$$|J, M \rangle\rangle = \sum_{Q,m} T_{KQ} |jm \rangle \langle Q, m | J, M \rangle$$

Act with  $J_+$ .

RHS gives:

$$\begin{aligned} & \sum_{Q,m} \sqrt{K(K+1) - Q(Q+1)} T_{KQ+1} |j, m \rangle \langle Q, m | J, M \rangle \\ & + \sqrt{j(j+1) - m(m+1)} T_{KQ} |j, m+1 \rangle \langle Q, m | J, M \rangle \end{aligned}$$

Let  $Q' = Q + 1$  in the first term and  $m' = m + 1$  in the second term.

$$\begin{aligned} & = \sum_{Q',m} \sqrt{K(K+1) - Q'(Q'-1)} T_{KQ'} |j, m \rangle \langle Q' - 1, m | J, M \rangle \\ & + \sum_{Q,m'} \sqrt{j(j+1) - m'(m'-1)} T_{KQ} |j, m \rangle \langle Q, m' - 1 | J, M \rangle \end{aligned}$$

Note that the range of  $Q', m'$  is the same as  $Q, m$  because the extra term vanishes anyway. Drop the primes.

If you use the recursion relation RHS becomes

$$\begin{aligned} & \sqrt{J(J+1) - M(M+1)} \sum_{Q,m} T_{KQ} |j, m \rangle \langle Q, m | J, M + 1 \rangle \\ & = \sqrt{J(J+1) - M(M+1)} |J, M + 1 \rangle\rangle \end{aligned}$$

The last equality implies that the proportionality between  $|J, M \rangle$  and  $|J, M \rangle\rangle$  is the same for all  $M$ . In particular if we know one  $\langle j', m' | T_{KQ} |j, m \rangle$  we know all the rest (i.e. other values of  $m, m', Q$  and same  $j, j', K$ ) by using C-G relations. This is the Wigner Eckart Theorem.



#### 4.4 P,T,C

Motivate by asking the question “ How does one communicate the concept of left-handed to a Martian?” This is the idea of symmetry. Ans.  $W^-$  decay. It decays into **left** handed electrons!

**Parity:**

1.

$$\mathcal{P}\vec{r} = -\vec{r}$$

On the ket:

$$P|r \rangle = |-r \rangle .$$

i) As a matrix P has  $\det = -1$ . Not a rotation

ii) Mirror Reflection ( $z \rightarrow -z$ ) followed by rotation about z-axis by 180 gives parity.

2.

$$\psi'(r') = w\psi(r)$$

Allowed as parity is discrete.

$$P\psi(r) = w\psi(-r)$$

However for integer spin can require that  $P^2 = 1$  So  $w^2 = 1$  and  $w = \pm 1$ .

Thus for the *operator*  $r$

3.  $PrP^{-1} = -r$ ,  $PpP^{-1} = -p$  but  $PLP^{-1} = L$  same for  $S$  and  $J$ .

In polar coordinates  $\theta \rightarrow \pi - \theta$  and  $\phi \rightarrow \phi + \pi$ .  $Y_{lm} \rightarrow (-1)^l Y_{l,m}$ . Check.

Current:  $\vec{j} \rightarrow -\vec{j}$  and  $\rho \rightarrow \rho$ .

So  $\phi(x) \rightarrow \phi(-x)$ ,  $\vec{A} \rightarrow -\vec{A}$  Thus photon has intrinsic parity -1.  $E \rightarrow -E$ ,  $B \rightarrow B$  (Axial vectors)

4. If parity is conserved  $PHP^{-1} = H$ . This implies  $PSP^{-1} = S$ .

eg  $\pi^0 \rightarrow 2\gamma$ . What is the intrinsic parity of  $\pi^0$  Does it have defn parity?

If yes :  $J=0$  means the final state wave fn must be a scalar depending on  $\vec{\epsilon}_1, \vec{\epsilon}_2, k$ .

$$\vec{\epsilon}_1 \cdot \vec{\epsilon}_2$$

or

$$(\vec{\epsilon}_1 \times \vec{\epsilon}_2) \cdot k$$

It is found that  $\pi^0$  has  $P=-1$  - **pseudoscalar**.

In terms of helicities  $\psi_{RR} \pm \psi_{LL}$  are the two photon states with defn parity.

5. Parity is violated. eg when a  $W$  decays ( $e^-, \bar{\nu}$ ) the electron coming out is always left helicity.

### Charge Conjugation

Suppose the Martian doesn't know what is +ve and -ve charge. Then how would he distinguish between the  $W^-$  decaying into left handed electron and  $W^+$  decaying into right handed positrons? He can't!

- $e^- \rightarrow e^+$

$CH = HC$  and so  $CS = SC$ . Unitary.

- 

$$\phi \rightarrow -\phi$$

$$\vec{A} \rightarrow -\vec{A}$$

$\Rightarrow$  photon has intrinsic C of -1. Does nothing to  $r, t$ .

examples: 3.  $\pi^0 \rightarrow 2\gamma$  2 photons state has C = +1. So the pion has C = +1. Which means  $\pi \rightarrow 3\gamma$  is not allowed!

4. Furry's theorem: No. of external photons must be even.  $(-1)^n = (-1)^m \Rightarrow n + m$  is even.

5. Positronium:  $e^+e^-$ . The electron has  $r, S, C$  quantum nos and we interchange electron and positron. Fermions, so overall sign has to be negative.

$$(-1)^l (-1)^{s+1} C = -1$$

So  $C = (-1)^{l+s}$ . Thus

$${}^1S_0 \rightarrow 2\gamma$$

(spin = 0, l=0)

$${}^3S_1 \rightarrow 3\gamma$$

(spin 1, l=0) but not  $2\gamma$ .

#### 6. CP

$$K^0 = s\bar{d} \text{ and } \bar{K}^0 = \bar{s}d.$$

$$\frac{K^0 - \bar{K}^0}{\sqrt{2}}$$

has C=-1 and P=-1 so CP=1

$$\frac{K^0 + \bar{K}^0}{\sqrt{2}}$$

has C=1 and P=-1 so CP=-1

$2\pi^0$  has P=1 (S-wave), C=1 So CP=1.  $3\pi^0$  has P=-1 (S-wave) and C=1 so CP=-1. (It has to be S-wave because the K's are J=0)

The K-Kbar goes into  $2\pi$  and is faster decay - hence  $K_S$  and the other one is called  $K_L$  CP odd and longer lived. These are also the mass eigenstates.

But in fact occasionally  $K_L$  decays into  $2\pi$ : violates CP.

So in fact there may be a difference between  $W^+$  decay and  $W^-$  decay! So the Martian will be able to distinguish between left and right after all!

Unless he doesn't know the difference between time going forwards and backwards!

**Time Reversal:**

1.  $T\psi(x, t) = c\psi(x, -t)$  Schroedinger eqn doesn't have this symmetry! Because it is first order. Assume T is unitary. If we take a state at  $t=0$  and propagate to  $t$  and then time reverse, or time reverse and then propagate to  $-t$ , we should get the same answer.

$$Te^{-iEt}u = e^{-iEt}Tu$$

other way

$$e^{iEt}Tu$$

. Want anti linear:  $T(a\psi(x, t)) = a^*T(\psi(x, -t))$

This will solve the problem. So

$$T = UK$$

where U is unitary and K is antilinear - "complex conjugation" - i.e  $K\psi = \psi^*$ .

$$\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^* = \langle T\psi | T\phi \rangle$$

But in general  $U, K$  will depend on the representation.

2.

$$rT = Tr$$

$$pT = -Tp$$

$$TL = -LT$$

$$TY_{lm} = Y_{lm}^*$$

(T does nothing to  $\theta, \phi$ )

$$\rho \rightarrow \rho$$

$$j \rightarrow -j$$

$$\phi \rightarrow \phi$$

$$A(x, t) \rightarrow -A(x, -t)$$

$$E \rightarrow E$$

$$B \rightarrow -B$$

3. Spin is like L. Want to reverse.  $\sigma_y$  is imaginary so K does the job.  $\sigma_x, \sigma_z$  need to be reversed:  $e^{-i\pi S_y}$  will do that. So

$$T = e^{-i\pi S_y} K$$

. This argument works for any spin.  $S_y$  can always be chosen imaginary.

For spin 1/2  $T = -i\sigma_y K$ .

$T^2 = e^{-i2\pi S_y}$  which is +1 on integer spin and -1 on half integer.

4. Application Kramer's degeneracy. Can electric field lift degeneracy?

Suppose there is no degeneracy due to T. Then  $Tu_k = cu_k$  must be true for c a number.  $T^2u_k = |c|^2 u_k$ . Now if we are talking of a half integer then  $|c|^2 = -1$  is a contradiction. So there must be a degeneracy! Regardless how complicated the electric field.

B breaks the symmetry.

$TY_{lm} = cY_{lm}$  is possible only for m=0 or for states like  $Y_{lm} \pm Y_{l-m}$ . Thus m is not a good quantum no.

## 5 Harmonic Oscillator

### 5.1 Review

1. Importance of harmonic oscillator: Leading Aproximation.
2. Hamiltonian and Lagrandgian.

$$H = \frac{P^2}{2m} + \frac{m\omega^2}{2} X^2$$

Rescaling variables.

Let  $X' = \sqrt{m}X$  and  $P' = \frac{P}{\sqrt{m}}$ .  $[X', P'] = i\hbar$ .

$$H = \frac{1}{2}(P'^2 + \omega^2 X'^2)$$

Rescale again:  $\hat{X} = \frac{1}{\sqrt{\omega}}X'$  and  $\hat{P} = \sqrt{\omega}P'$ .

$$H = \frac{\omega}{2}(\hat{P}^2 + \hat{X}^2)$$

Thus  $\hat{x} = \sqrt{\omega}x' = \sqrt{m\omega}x$ . Drop hats from now on.

Creation operator  $a^\dagger = (X - iP)/\sqrt{2\hbar}$  and  $[a, a^\dagger] = i$ .

3. Eigenstates:  $|n\rangle : a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$  Number operator  $N = a^\dagger a$ ,  $H = \hbar\omega(N + 1/2)$ .

4. Wave fns.

$$(x + \frac{\partial}{\partial x})\psi = 0 \Rightarrow d(\ln \psi) = -\frac{1}{2}d(x^2)$$

$$\psi(x) \approx e^{-\frac{x^2}{2}} \approx e^{-\frac{m\omega x^2}{2}}$$

We have rescaled from hat variables to ordinary variables.

$$\phi_0 = (\frac{m\omega}{\pi\hbar})^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \text{ X Hermite polynomials.}$$

## 5.2 Path Integral Treatment

1. Doing Gaussian integrals:

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t)))$$

with  $L = T - V(x)$  where  $V$  is quadratic.

Let  $x(t) = x_c(t) + y(t)$ . Then  $X_c$  satisfies bc. So  $y$  is 0 at both ends. So we get

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t))) = F(t_a, t_b) e^{\frac{i}{\hbar} S_{cl}}$$

where

$$F(t_a, t_b) = \int_{y(t_a)=y(t_b)=0} \mathcal{D}y(t) e^{i \int_{t_a}^{t_b} dt L(y, \dot{y}, t)}$$

and of course  $L$  is quadratic.

Time independent implies  $F(t_a - t_b)$

2. Do the calc for SHO. First  $S_c$ , then  $F$ . Done before.

3. Evaluate  $\phi_0(x)$  and  $\phi_1(x)$  by expanding kernel.

$$2 \cos \omega t = e^{i\omega t} (1 + e^{-2i\omega t})$$

$$2i \sin \omega t = e^{i\omega t} (1 - e^{-2i\omega t})$$

### 5.3 1-dim crystal and field theory

1. Want to solve:

$$L = \sum_{j=1}^N 1/2 \dot{q}_j^2 - \nu^2/2 (q_{j+1} - q_j)^2$$

2. Special case of coupled oscillators:

$$L = \frac{1}{2} [(\dot{q}_1^2 + \dot{q}_2^2) + q_1^2 + q_2^2 + \alpha q_1 q_2]$$

If we define  $Q = \frac{q_1+q_2}{\sqrt{2}}$  and  $q = \frac{q_1-q_2}{\sqrt{2}}$ , then

$$L = \frac{1}{2} [(\dot{Q}^2 + (1+\alpha)Q^2 + \dot{q}^2 + (1-\alpha)q^2)].$$

Gives a decoupled system.

Can get  $q_1(t) = \frac{Q(t)+q(t)}{\sqrt{2}}$  and  $q_2(t) = \frac{Q(t)-q(t)}{\sqrt{2}}$ .

If  $\alpha = -1$ , then we have diatomic molecule - centre of mass is free.

The crystal is a generalization of this.

Now general case:

3. Periodic bc  $q_{N+1} = q_0$ .
4. Eqn of motion.

$$\frac{d^2 q_n}{dt^2} = \nu^2 (q_{n+1} - q_n) + (q_{n-1} - q_n)$$

Solns. Use translation inv. to get the normal modes.

$$q_n = e^{i\beta n}$$

are the form of normal modes with  $\beta = \frac{2\pi k}{N}$

$$e^{i\beta n - \omega t} = e^{i\frac{\beta}{a}(x - avt)}$$

vel is

$$c = a\nu$$

$$w^2 = \nu^2 (4 \sin^2 \frac{\beta}{2})$$

5. Show that normal modes are decoupled oscillators.

$$q_n = \frac{1}{\sqrt{N}} \sum_k a_k e^{i\beta_k n}$$

$$L = 1/2 \sum_k [\dot{a}_k \dot{a}_{-k} - 4\nu^2 \sin^2 \beta_k / 2 a_k a_{-k}]$$

Also need to divide by  $\sqrt{N}$  to get finite limit.

Reality of  $q_n(t)$  implies  $a_k^*(t) = a_{-k}(t)$  But  $a_{-k} = a_{N-k}$ . So  $a_k^* = a_{N-k}$ . Define

$$b_k = 1/2(a_k + a_k^*) = 1/2(a_k + a_{N-k})$$

and

$$c_k = 1/2i(a_k - a_{N-k})$$

The index on b,c clearly go only to  $N/2$ . In terms of b,c:

$$L = 1/2 \sum_{k=1}^{\frac{N}{2}} [(\dot{b}_k)^2 - 4\nu^2 \sin^2 \frac{\beta_k}{2} b_k^2] + \text{same for } c$$

With time dep

$$\begin{aligned} q_n(t) &= a_k e^{i\beta_k n - i w_k t} + a_k^* e^{-i\beta_k n + i w_k t} \\ &= b_k \cos(\beta_k n - w_k t) - c_k \sin(\beta_k n - w_k t) \end{aligned}$$

What happened to waves in the opp direction: by changing  $\beta_k \rightarrow \beta_k - 2\pi = \beta_{k-N}$  we get waves moving the opposite way! So if we want we can change all the indices on the  $c$  to negative. Thus  $N - k \equiv -k$ . Whichever way you count there are  $N$  oscillators.

6. Continuum limit. "Free Field Theory". The velocity of light emerges.  $q_n(t) \rightarrow q(x, t)$ .

$$\begin{aligned} L &= 1/2 \int dx \left[ \frac{\dot{q}^2}{a} - \nu^2 a (q')^2 \right] \\ &= 1/2 \int dx [\dot{Q}^2 - c^2 Q'^2] \end{aligned}$$

where  $q = Q\sqrt{a}$

In terms of oscillators

$$\sum_k \dot{b}_k^2 - 4\nu^2 \sin^2\left(\frac{\beta_k}{2}\right) b_k^2$$

In cont. limit  $4\nu^2 \sin^2 \dots = \left(\frac{2\pi k\nu}{N}\right)^2 = w_k^2$ . Thus we have harmonic osc with energy quanta =

$$\hbar w = \frac{\hbar 2\pi k\nu}{N} = \frac{\hbar 2\pi k}{L} c = pc$$

**phonons / photons ...**

## 5.4 Coherent States

1. Rescale

$$\begin{aligned} \sqrt{m\omega} X &= \hat{x} \\ \frac{P}{\sqrt{m\omega}} &= \hat{p} \end{aligned}$$

2. Classical eqns  $\dot{x} = \omega p$  and  $\dot{p} = -\omega x$ . Can be written as

$$\dot{\alpha} = -i\omega\alpha$$

Want same eqns qm. for  $\langle a \rangle$

$$i\hbar d/dt \langle a \rangle = \langle [a, H] \rangle = \omega \langle a \rangle (t)$$

3. Find a state such that  $\langle a \rangle = \alpha_0$  and also  $\langle H \rangle = \hbar\omega |\alpha_0|^2 =$  classical.

Let

$$a |\alpha\rangle = \alpha |\alpha\rangle$$

This will solve the problem.

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |\phi_n\rangle$$



4. Props: i) closure

$$\frac{1}{\pi} \int d\{Re \alpha\} d\{Im \alpha\} |\alpha\rangle \langle \alpha| = \sum_n |n\rangle \langle n| = 1.$$

Note that the measure is  $dx \frac{dp}{2\pi}$ .

ii) not ortho. They are over complete:

$$\begin{aligned} \langle \alpha | \alpha' \rangle &= e^{-\frac{|\alpha|^2}{2}} e^{-\frac{|\alpha'|^2}{2}} \sum_n \frac{(\alpha^*)^n}{\sqrt{n!}} \frac{(\alpha')^n}{\sqrt{n!}} \\ &= e^{-\frac{|\alpha|^2}{2}} e^{-\frac{|\alpha'|^2}{2}} e^{\alpha^* \alpha'} \end{aligned}$$

Thus  $|\langle \alpha | \alpha' \rangle|^2 = e^{-|\alpha - \alpha'|^2} \neq 0$ .

5.

$$\begin{aligned} \langle H \rangle_\alpha &= \hbar w [|\alpha|^2 + 1/2] \\ \langle H^2 \rangle_\alpha &= \hbar w [|\alpha|^4 + 2|\alpha|^2 + 1/4] \\ \Delta H &= \alpha w \\ \frac{\Delta H}{H} &= 1/\alpha \approx 0 \end{aligned}$$

Same for X,P

$$\begin{aligned} \langle X \rangle, \langle P \rangle &= Re, Im(\alpha)\sqrt{2} \\ \langle X^2 \rangle - \langle X \rangle^2 &= 1/2 \end{aligned}$$

Find

$$\Delta X \Delta P = 1/2$$

Minimum uncertainty.

6. Unitary operator  $D(\alpha) |0\rangle = |\alpha\rangle$

$$D = e^{\alpha a^\dagger - \alpha^* a}. \quad DD^\dagger = 1.$$

$$\begin{aligned} \langle x | \alpha \rangle &= \langle x | D | 0 \rangle \\ \alpha a^\dagger - \alpha^* a &= (\alpha - \alpha^*)x/\sqrt{2} - i(\alpha + \alpha^*)P/\sqrt{2} \end{aligned}$$

Using  $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$ ,

$$D = e^{\frac{\alpha^{*2} - \alpha^2}{4}} e^{\frac{(\alpha - \alpha^*)x}{\sqrt{2}}} e^{\frac{-i(\alpha + \alpha^*)p}{\sqrt{2}}}$$

It follows that

$$\psi(x, 0) = e^{i\theta} e^{i\langle P \rangle x} \phi_0(x - \langle X \rangle)$$

$\phi_0$  is the ground state wave fn. Width of gaussian is  $1/\sqrt{2}$  for  $\hat{x}$  or  $\sqrt{\frac{\hbar}{2m\omega}}$  for  $x$ .

7. Time dependences of everything. Coherent states remain coherent.

$$|\alpha(t)\rangle = e^{-i\omega t/2} |\alpha(0)\rangle e^{-i\omega t}$$

Wave packet remains a wave packet. So at later times also we get same wave fn except that  $\langle x \rangle$  and  $\langle p \rangle$  change with time as  $\cos \omega t$ ,  $\sin \omega t$  etc. and also we get an overall phase.

## 6 Perturbation Theory

### 6.1 Stationary Perturbation Theory

1.

$$H = H_0 + V$$

Matrix elements of  $V$  are assumed to be smaller than  $E_n^0 - E_p^0$ . Let  $V = \lambda W$  where  $\lambda$  is a small number and matrix elements of  $W$  are not small.

2.

$$H(\lambda) |\psi(\lambda)\rangle = E(\lambda) |\psi(\lambda)\rangle$$

Let

$$E(\lambda) = \epsilon_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \dots$$

$$|\psi(\lambda)\rangle = |0\rangle + \lambda|1\rangle + \lambda^2|2\rangle + \dots$$

We get

$$H_0 |0\rangle = \epsilon_0 |0\rangle$$

$$(H_0 - \epsilon_0) |1\rangle + (W - \epsilon_1) |0\rangle = 0$$

$$(H_0 - \epsilon_0) |2\rangle + (W - \epsilon_1) |1\rangle - \epsilon_2 |0\rangle = 0$$

Assume  $\langle \psi | \psi \rangle = 1$  and phase convention  $\langle \psi | 0 \rangle$  is real.

$\Rightarrow \langle 0 | 0 \rangle + \lambda \langle 0 | 1 \rangle$  is real. So  $\langle 0 | 1 \rangle$  is real.

Also  $\langle 0 | 0 \rangle + \lambda \langle 0 | 1 \rangle + \langle 1 | 0 \rangle = 1$ . Plugging in lowest order solution which is  $\langle 0 | 0 \rangle = 1$  and using reality get  $\langle 1 | 0 \rangle = 0$ .

Solution:

**Zeroth** order gives

$$| 0 \rangle = | \phi_n \rangle$$

**1st order** Applying  $\langle \phi_n |$

$$\epsilon_1 = \langle \phi_n | W | \phi_n \rangle$$

Applying  $\langle \phi_p |$  gives

$$| 1 \rangle = \sum_{p, p \neq n} \frac{\langle \phi_p | W | \phi_n \rangle}{E_n - E_p} | \phi_p \rangle$$

**2nd order** Apply  $\langle \phi_n |$  to second order equation:

$$\epsilon_2 = \sum_{p, p \neq n} \frac{\langle \phi_n | W | \phi_p \rangle \langle \phi_p | W | \phi_n \rangle}{E_n - E_p}$$

Note sign: decided by  $E_n - E_p$ . eigen value repulsion.

## 2. Degenerate Perturbation theory

Let  $| \phi_n^i \rangle : i = 1, \dots, g_n$  be states degenerate in energy.

first order eqn is modified: get a matrix eqn insted of a single eqn:

Apply  $\langle \phi_n^i |$  to get

$$\langle \phi_n^i | W | 0 \rangle = \epsilon_1 \langle \phi_n^i | 0 \rangle$$

Insert complete set of states and use orthogonality to restrict sum to sub-space.

$$\sum_j \underbrace{\langle \phi_n^i | W | \phi_n^j \rangle}_{g_n \times g_n \text{ matrix}} \langle \phi_n^j | 0 \rangle = \epsilon_1 \langle \phi_n^i | 0 \rangle$$

This may or may not split degeneracy. But W has been diagonalized so need not fear infinite denominators.

Degeneracy is important because it is qualitative and not quantitative. If due to symmetry, higher orders will not resolve it.

## 6.2 Applications

### 1. Anharmonic oscillator

$$H_0 = 1/2\hbar\omega(P^2 + X^2)$$

$$V = \lambda\hbar\omega X^3$$

Non zero matrix elements of pert:

$$\langle \phi_{n+3} | V | \phi_n \rangle = \frac{\hbar\omega}{2\sqrt{2}} \sqrt{(n+1)(n+2)(n+3)}$$

$$\langle \phi_{n-3} | V | \phi_n \rangle = \frac{\hbar\omega}{2\sqrt{2}} \sqrt{n(n-1)(n-2)}$$

$$\langle \phi_{n+1} | V | \phi_n \rangle = \frac{3\hbar\omega}{2\sqrt{2}} \sqrt{(n+1)^3}$$

$$\langle \phi_{n-1} | V | \phi_n \rangle = \frac{3\hbar\omega}{2\sqrt{2}} \sqrt{n^3}$$

$$\epsilon_1 = \langle \phi_n | V | \phi_n \rangle = 0$$

2nd order

$$\frac{|\langle \phi_{n+3} | V | \phi_n \rangle|^2}{-3\hbar\omega} = -\frac{\hbar\omega}{3} \frac{(n+1)(n+2)(n+3)}{8}$$

$$\frac{|\langle \phi_{n-3} | V | \phi_n \rangle|^2}{+3\hbar\omega} = \frac{\hbar\omega}{3} \frac{n(n-1)(n-2)}{8}$$

$$\frac{|\langle \phi_{n+1} | V | \phi_n \rangle|^2}{-\hbar\omega} = -9\hbar\omega \frac{(n+1)^3}{8}$$

$$\frac{\hbar\omega}{-24} (n+1)(n+2)(n+3) + \frac{\hbar\omega}{24} n(n-1)(n-2) + \bar{w}9/8n^4 - \hbar\omega 9/8(n+1)^3$$

$$= -15/4(n+1/2)^2\hbar\omega - 15/2n\hbar\omega$$

$\times \lambda^2$ .

Note  $E_n - E_{n-1} = \hbar\omega - 15/2n\lambda\hbar\omega$ . The energy difference is not constant.

Eigenstate is of the form

$$|\psi_n\rangle = |\phi_n\rangle + O(\lambda)(|\phi_{n+3}\rangle, |\phi_{n-3}\rangle, |\phi_{n+1}\rangle, |\phi_{n-1}\rangle)$$

2. Applications : Oscillating dipole normally radiates only Bohr frequencies  $w$ . But the anharmonic  $X$  connects  $n$  with  $n+2$  and also  $n-2$ .

This is because  $\langle \psi_2 | X | \psi_0 \rangle \approx \lambda \langle \phi_1 | X | \phi_0 \rangle + O(\lambda^2) \neq 0$ . So we get frequencies corresponding to  $E_2 - E_0 \approx 2\omega$ . So we get  $2\omega$  also.

Even  $\langle \psi_n | X | \psi_n \rangle \neq 0, \approx O(-\lambda n^{3/2})$ . This implies at higher  $n$  the dipole stretches. When  $\lambda$  is negative it is easier to move to the right (+ve  $x$ ) than to the left. Vice versa when  $\lambda$  is positive. So at higher energy levels expect that average  $x$  will change in the direction which is easier. This explains the sign in the equation and also explains why materials expand on heating.

### Van der Waal's force

1. **Potential** due to a charge =  $\phi(r) = \frac{q}{r}$ . Potential due to a dipole

$$\phi(r) = \frac{q}{r} - \frac{q}{r + \delta r} = \frac{q\delta r}{r^2} = \frac{q\vec{r}_D \cdot \hat{r}}{r^2} = \frac{\vec{p} \cdot \hat{r}}{r^2} = \frac{\vec{p} \cdot \vec{r}}{r^3}$$

**Electric field** due to dipole:

$$\begin{aligned} E^i &= -\partial_i \phi(r) = -\left(\frac{p^i}{r^3} + \vec{p} \cdot \vec{r} \frac{\partial}{\partial_i} \left(\frac{1}{r^3}\right)\right) \\ &= -\left(\frac{p^i}{r^3} + \vec{p} \cdot \vec{r} \left(\frac{-3r^i}{r^5}\right)\right) \\ E^i &= -p^j \left[\frac{\delta_{ij}}{r^3} - \frac{3r^i r^j}{r^5}\right] \end{aligned}$$

**Energy**  $-\vec{E}_1 \cdot \vec{p}_2$ :

$$W = p_1^i p_2^j \left[\frac{\delta_{ij}}{r^3} - \frac{3r^i r^j}{r^5}\right]$$

2. We are considering force between two neutral atoms, that have no dipole moments. Say, hydrogen atoms in their ground states. The state is  $|\psi_0\rangle = |1\rangle \otimes |2\rangle$  or  $\psi_0(r_1)\psi_0(r_2)$ . We are given that  $\langle 1|p_1|1\rangle = \langle 2|p_2|2\rangle = 0$ . Therefore  $\langle \psi | W | \psi \rangle = 0$ .

No first order correction.

3. Second order:

$$\frac{\sum_{n \neq 0} \langle \psi_n | W | \psi_0 \rangle^2}{E_0 - E_n}$$

Note the sign: it is negative ( $E_0 < E_n$ ) :  $\Rightarrow$  attractive.

Since  $W \approx \frac{1}{r^3}$ , the van der Waal correction is  $\approx \frac{1}{r^6}$ .  $\Delta E = -\frac{c}{r^6}$ . Let us estimate  $c$ .

4.  $E_0 = E_0^1 + E_0^2$ . For each atom,  $|E_n| = |\frac{E_0}{n^2}| \ll |E_0|$ . So we drop  $E_n$ . Then

$$\begin{aligned} \Delta E &= \sum_n \frac{|\langle n | W | 0 \rangle|^2}{E_0} \\ &= \frac{\langle 0 | W^2 | 0 \rangle}{E_0} \end{aligned}$$

Choose the direction between the atoms to be  $\hat{z}$ . So we get

$$W \approx p_{1x}p_{2x} + p_{1y}p_{2y} - 2p_{1z}p_{2z}$$

$$W^2 = e^4(x_1x_2 + y_1y_2 - 2z_1z_2)^2$$

We need  $\langle 0 | W^2 | 0 \rangle$  so all cross terms can be dropped.

$$\langle W \rangle = \langle x_1x_1 \rangle \langle x_2x_2 \rangle + \langle y_1y_1 \rangle \langle y_2y_2 \rangle + 4 \langle z_1z_1 \rangle \langle z_2z_2 \rangle$$

By symmetry they are all equal to  $\langle \frac{r^2}{3} \rangle \langle \frac{r^2}{3} \rangle$ . For the hydrogen atom  $\langle \frac{r^2}{3} \rangle = a_0^2$ . Also  $E_0 = 2 \frac{e^2}{2a_0^2}$  - the factor of 2 because there are two atoms. Thus we get  $c = 6e^2a_0^3$ .

5. Physical mechanism: QMec fluctuation produces a dipole moment in one atom, which induces a dipole in the second atom and they attract. These two dipoles are correlated because one is induced by the other. The uncorrelated fluctuations average out.

Because one dipole induces the other there is a time lag. So when the time taken for influence is of the order of Bohr frequency, this approx breaks down. Thus  $r < \frac{c}{\nu} = \lambda$ . Also  $R$  should be large enough that the independent wave function approx holds. So  $r \gg a_0$ .

### 6.3 Time dependent pert theory

We ask for transition prob from some initial state  $i$  to some final state  $f$  usually during the perturbation or after. Usually  $i$  and  $f$  are eigenstates of unperturbed  $H$ . Special case 1) Adiabatic 2) Sudden.

Otherwise do pert in  $\lambda$  as before.

$$i\hbar d/dt |\psi(t)\rangle = (H_0 + \lambda V) |\psi(t)\rangle$$

$$|\psi(0)\rangle = |\phi_i\rangle$$

$$\text{Reqd: } P_{fi}(t) = |\langle \phi_f | \psi(t) \rangle|^2$$

$$|\psi(t)\rangle = \sum_k c_k(t) |\phi_k\rangle$$

$c_k(0) = \delta_{ki}$  Project  $\langle \phi_n |$  to get

$$i\hbar \dot{c}_n = \langle \phi_n | H_0 + \lambda W | \sum_k c_k | \phi_k \rangle$$

Insert complete set of states:

$$= \sum_m (E_n \delta_{nm} + \lambda W_{nm}) c_m(t)$$

Redefine  $c_n(t) = b_n(t) e^{-iE_n t}$  to get

$$i\hbar d/dt b_n(t) = \lambda \sum W_{nm} e^{i\omega_{nm} t} b_m$$

Now expand

$$b_n = b_n^0 + \lambda b_n^1 + ..$$

Soln

$$b_n^0 = \text{const} = \delta_{ni}$$

$$b_n^1(t) = \frac{1}{i\hbar} \int_0^t dt W_{ni} e^{i\omega_{ni} t} dt$$

$$P_{fi}(t) = 1/\hbar^2 \left| \int_0^t dt W_{ni} e^{i\omega_{ni} t} dt \right|^2$$

**special case** i) harmonic perturbation  $W(t) = W \sin \omega t$  or  $W \cos \omega t$ . If  $\omega = 0$  use cos to get:

$$\frac{|W_{fi}|^2}{\hbar^2} \left[ \frac{\sin w_{fi}t/2}{w_{fi}/2} \right]^2$$

If  $w \neq 0$  use  $2\sin wt$  and get same formula with  $w_{fi} \rightarrow w_{fi} - w$ .

**Coupling to continuum:**

Use  $(\sin wt/2/w/2)^2 = 2\pi t \hbar \delta(E_f - E_i)$ .

Derivation:

$$\begin{aligned} & \int_{-\infty}^{\infty} e^{ixt} dt = 2\pi\delta(x) \\ & = \lim_{T \rightarrow \infty} \int_{-T}^T e^{ixt} dt = \frac{2i \sin xT}{ix} \\ & \Rightarrow \lim_{T \rightarrow \infty} \frac{\sin xT}{x} = \pi\delta(x) \end{aligned}$$

$$\lim_{T \rightarrow \infty} \left( \frac{\sin xT}{x} \right)^2 = \pi\delta(x) \frac{\sin xT}{x} = \pi T \delta(x).$$

For the case  $\omega = 0$ ,

$$dP_{fi}/\text{unittime}/d\beta = \frac{2\pi}{\hbar} |\langle \beta, E | W | \phi_i \rangle|^2 \rho(\beta, E = E_f = E_i)$$

Here  $\beta$  represents any other continuous parameter (eg. angle).  $\rho(\beta, E)$  is the no. of states per unit  $\Delta E$ , per unit  $\Delta\beta$ . ("number density of states").

This is **Fermi Golden Rule**

2. Prove Born scattering formula: Take initial state to be  $|p_i\rangle$  and final state to be  $|p_f\rangle$ . Note:  $\langle x|p\rangle = e^{ip \cdot r}$  This is different from that in some books where  $\langle x|p\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{ip \cdot r}$ .

Calculate  $\rho(E)$ .

$$\int \frac{d^3p}{(2\pi\hbar)^3} = \int d\Omega dE \rho(E)$$

(In the other normalization there would be no factors of  $2\pi$ .)

$$\int \frac{p^2 dp d\Omega}{(2\pi\hbar)^3} = \int \frac{pm}{(2\pi\hbar)^3} dE d\Omega = \int \frac{\sqrt{2mE}m}{(2\pi\hbar)^3} dE d\Omega$$

Thus  $\rho(E) = \frac{m\sqrt{2mE}}{(2\pi\hbar)^3}$ .



Divide final probability/unit time by flux ( $=\frac{p}{m}$ ) to get prob /unit flux/unit time.

$$\frac{m^2}{4\pi^2\hbar^4} \left| \int d^3r e^{i(p_f - p_i) \cdot r} W(r) \right|^2$$

[If we use the other normalization we also get same. But  $\rho(E) = m\sqrt{2mE}$ . The factors of  $2\pi$  are in the matrix element.]

This is called the “differential scattering cross section”.

The total scattering cross section will now involve integration over  $d\Omega$ .

## 6.4 Scattering

1.

$$dn = \sigma(\theta, \phi) F_i d\Omega$$

where  $F_i$  is the incident flux and  $\sigma(\theta, \phi)$  is the differential scattering cross section. It is no. of scattered particles per unit incident particle per unit solid angle.

$$\int d\Omega \sigma(\theta, \phi) = \sigma$$

is total scattering cross section.

2. Calculation of  $\sigma$ .

Look for *stationary* states:

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

Let  $2mV/\hbar^2 = U$  and let  $\hbar^2 k^2 = 2mE$ , then

$$[\Delta + k^2] \phi(\vec{r}) = U(r) \phi(\vec{r})$$

Now the soln we want has the asymptotic form

$$\phi(r) \approx e^{ikz} + f(\theta, \phi) e^{ikr}/r$$

Because it has the form of incident wave plus outgoing scattered wave. and  $e^{ikr}/r$  is also a soln to the homogeneous eqn as long as  $r > 0$ . To see that:

$$\Delta(1/r) = 4\pi\delta(\vec{r})$$

- from electrostatics. Note that this is the *three-dimensional* delta function. Can check that  $-\frac{e^{\pm ikr}}{4\pi r} = G_{\pm}(r)$  is the **Green fn** [Do they know what it is?] for Scattering eqn above. [Use  $\Delta = \frac{\partial^2}{\partial r^2} + \frac{2\partial}{r\partial r}$ ]

The incident flux is  $\frac{\hbar k}{m}$  and scattered flux is  $\frac{|f|^2 \hbar k}{r^2 m}$ . This is flux per unit area. Multiply by  $r^2 d\Omega$  to get : no. of particles per unit time  $dn = |f|^2 d\Omega \frac{\hbar k}{m}$ . Thus from the definition of  $\sigma$ ,  $\sigma(\theta, \phi) = |f|^2$ . So we need  $f$ .

3. There will be **interference** in forward direction between scattered and incident flux. This follows from unitarity - conservation of particles. Thus we can expect total scattering probability ( $\propto |f|^2$ ) to be related to this interference term ( $\propto f$ ). This is the content of the **optical theorem** -which is done later.
4. Actually the interference should not be *only* in the forward direction, because we have an infinite plane wave front. Resolution: The infinite front is an idealization. Actually it is a narrow beam. So we really should be taking a superposition of several  $\vec{k}_i$  with small amounts of  $k_x, k_y$ . Rotated  $k_i$  has the effect of changing  $\theta, \phi$  in  $f$ . Thus it is as if one has to take  $f$  and average over a small range of  $\theta, \phi$ . However if  $f$  is a **smooth** function (which it is) this makes very little difference. So we can pretend there is only one  $\vec{k}_i = k_z \hat{z}$  and inspite of having an infinite wave front, pretend there is a small beam, and therefore ignore interference in all but the forward direction. It is like having the cake and eating it too! The idealization should be such that it simplifies the calculation but doesn't change the answer.
5. So we get soln

$$\phi(r) = \phi_0(r) + \int d^3 r' G_+(r-r') U(r') \phi(r')$$

where  $\phi_0$  solves the hom eqn.

Iterate by plugging in for  $\phi$  back into the eqn:

$$\phi(r) = \phi_0(r) + \int d^3 r' G_+(r-r') U(r') \phi_0(r') + \int d^3 r' \int d^3 r'' G_+(r-r') U(r') G_+(r'-r'') U(r'') \phi(r'')$$

Hopefully each term is smaller than the other. Keep leading term and get "Born approx" with  $\phi_0 = e^{ikz}$

Using (for large  $r$ )  $|\vec{r} - \vec{r}'| \approx r - \hat{u} \cdot \vec{r}'$  where  $\hat{u}$  is the unit vector in the direction of  $\vec{r}$  which is also the direction of scattered particle. Thus  $\hat{u}k = \vec{k}_f$

we get

$$\phi(r) \approx e^{ikz} - e^{ikr}/4\pi r \int d^3r' e^{-ik\hat{u}\vec{r}'} U(r') e^{i\vec{k}_i \cdot \vec{r}'}$$

for large  $r$ .

So

$$f(\theta, \phi) = -1/4\pi \int d^3r' e^{-i\vec{k}_f \vec{r}'} U(r') e^{i\vec{k}_i \cdot \vec{r}'}$$

.

$$= -\frac{2m}{\hbar^2 4\pi} \int d^3r' e^{-i\vec{k}_f \vec{r}'} V(r') e^{i\vec{k}_i \cdot \vec{r}'}$$

And so we get  $\sigma$  also. This is Born (differential) scattering cross section.

## 6. Path integral approach

$$K(b, a) = K(x_f, t_f; x_i, t_i) = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t)))$$

$L=T-V$ . So expand in powers of  $V$ :

$$\begin{aligned} K(b, a) &= \int_{x(t_i)=x_i}^{x(t_f)=x_f} \underbrace{\mathcal{D}x(t)}_{\text{sum over paths}} \exp(+\frac{i}{\hbar} \int_{t_i}^{t_f} dt T(x(t), \dot{x}(t))) [1 - \frac{i}{\hbar} \int_{t_i}^{t_f} dt' V(x(t')) + \\ &\quad + \frac{1}{2!} \frac{i}{\hbar} \int_{t_i}^{t_f} dt' V(x(t')) \frac{i}{\hbar} \int_{t_i}^{t_f} dt'' V(x(t'')) + \dots] \\ &= K_0(b, a) - \frac{i}{\hbar} \int \int K_0(b, c) V(x(t_c)) K_0(c, a) dt_c dx(t_c) + \dots \end{aligned}$$

Only diff with other series: This has  $t$  - the other is in energy variable.

So do FT. Thus ( $T = t_f - t_i$ )

$$\int_{-\infty}^{\infty} dt e^{i\omega t} K(x, t; x', 0) = -iG(x - x', \omega)$$

where  $G$  satisfies  $(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \omega)G(x - x', E) = \delta(x - x')$ .

(Note that  $K$  is zero if  $t_f < t_i$ ). To see this

$$\begin{aligned} \int_0^\infty dt e^{i\omega t} K(x, t; x', 0) &= \sum_n \psi_n(x) \psi_n^*(x') \int_0^\infty dt e^{-iE_n t + i\omega t} \\ &= \sum_n \frac{\psi_n(x) \psi_n^*(x')}{i(E_n - \omega)} \end{aligned}$$

Thus acting with Schroedinger equation cancels  $E_n - \omega$  and we get  $-i\delta(x - x')$ .

If we let  $\hbar k = p$  and  $\hbar\omega = E$  in  $G_+$  defined earlier we get  $\frac{G}{2m}$ .

Also multiply by  $\phi(x, 0)$  to get in terms of wave fns.

$$\begin{aligned} -iG &= \int_0^\infty dt e^{i\omega t} \int \frac{d^3 p}{(2\pi)^3} e^{-i\frac{p^2}{2m}t} e^{i\vec{p}\cdot\vec{r}} \\ &= - \int_0^\infty \frac{p^2 dp}{8\pi^3} \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta e^{ipr \cos\theta} \frac{1}{i(\frac{p^2}{2m} - \frac{k^2}{2m})} \end{aligned}$$

(Note the sign from :  $d \cos\theta = -d \sin \theta d\theta$ )

$$= -\frac{2\pi}{8\pi^3 i r} \int_0^\infty p dp \frac{e^{ipr}}{i(\frac{p^2}{2m} - \frac{k^2}{2m})} - cc$$

We have set  $\omega = \frac{k^2}{2m}$ . Extend range  $-\infty$  to  $+\infty$  by combining cc. and do contour int. The  $i\epsilon$  prescription is  $\omega + i\epsilon$ . So  $(p - k - i\epsilon)(p + k + i\epsilon)$ . Pick  $p = +k$  since  $r > 0$ , to get  $\frac{2m e^{+ikr}}{i4\pi r} = i2mG_+$ . Thus  $G = -2mG_+$ .

This is a series for  $K$ . Act on initial state  $\psi_i(x', t)$ :

$$\psi_f(x, t) = \int d^3 x' K(x, t; x', t') \psi_i(x', t')$$

Take  $t' \rightarrow -\infty$  so that  $\psi_i$  is a plane wave state  $=\psi_0(x) = e^{ikz}$ . It has definite energy  $E_k = \frac{\hbar^2 k^2}{2m}$ . The integral over  $t_c$  from  $-\infty, +\infty$  guarantees energy conservation in all interacting terms.

7. **Eikonal approx** Instead of  $e^{ikz}$  for  $\phi(r)$  use  $e^{iS_0(r)}$ . whose eqn is

$$(\nabla S_0)^2 = 2m(E - V(r))$$

If  $\frac{\partial S_0}{\partial z}$  is much larger than other variations then,

$$\frac{\partial S_0}{\partial z} \approx \hbar k - \frac{V(x, y, z)}{v}$$

Approx soln is

$$S_0 = \hbar k z - 1/v \int_{-\infty}^z V(x, y, z') dz'$$

Thus momentum depends on V - better approx.

$$F(\theta, \phi) = -\frac{1}{4\pi} \int e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}'} U(r') \underbrace{e^{[-\frac{i}{\hbar v} \int_{-\infty}^z V(x, y, z') dz']}}_{\text{extra factor}} d^3 r'$$

Clearly when velocity is very small or  $\int V dz'$  is large (not V) this term cannot be neglected. Better than Born. Born requires large vel and weak potentials.

8. **Yukawa**

$$\int e^{i(k_i - k_f) \cdot r} V_0 \frac{e^{-\alpha r}}{r} d^3 r$$

Straightforward integration (and multiplication by  $\frac{2m}{\hbar^2 4\pi}$ ) gives:

$$f = V_0 \frac{2m}{\hbar^2 (k^2 + \alpha^2)}$$

where  $k = |\vec{k}_i - \vec{k}_f| = 2k_i \sin \theta / 2$

Also set  $\alpha = 0$  to get Rutherford scatterin:

$$\frac{Z_1^2 Z_2^2 e^4}{\hbar^2 16 E^2 \sin^4 \theta / 2}$$

9. **Partial Wave method**

This is for **central potentials**, where  $\vec{L}$  is conserved.

i) Expand  $e^{ikz}$  in partial waves  $\phi_{kl}^0(r, \theta, \phi)$  which are solns of free eqn.

$$\phi_{klm}^0 = R_{k,l,m} Y_{lm}(r)(\theta, \phi)$$

where

$$\frac{\hbar^2}{2m} \underbrace{\left(-d^2/dr^2 + \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2}\right)}_{\frac{1}{r} \frac{d^2}{dr^2} r} R_{kl}(r) = E_{k,l} R_{kl}(r)$$

Set  $rR_{kl}(r) = u_{kl}(r)$ . For large  $r$ :  $u = \frac{e^{\pm ikr}}{r}$ . For general  $r$

$$\phi_{klm}(r, \theta, \phi) = \sqrt{2k^2/\pi} j_l(kr) Y_{lm}(\theta, \phi)$$

The boundary condition used is that  $u(0) = 0$ .

$j_l(\rho) \approx \rho^l/(2l+1)!!$  for small  $\rho$ . So the fn is negligible for  $\rho < l$ .  
 $\Rightarrow kr > l$  or if the range of the potential is small only very small  $l$ 's will contribute.  $r = l/k$  is the analog of the classical impact parameter.

Without any potential we have incoming plane waves, which can be decomposed as:

$$e^{ikz} = \sum_{l=0}^{\infty} e^{il\pi/2} \sqrt{4\pi(2l+1)} j_l(kr) Y_{l0}(\theta)$$

Note:  $m=0$  because  $e^{ikz} = e^{ikr \cos \theta}$  has no  $\phi$  dependence.

For large  $r$

$$j_l(kr) \approx \sin(kr - l\pi/2)/kr = (e^{ikr} e^{-il\pi/2} - e^{-ikr} e^{il\pi/2})/2ikr$$

ii) Now turn on the potential. The only effect can be to change the relative phase of the ingoing and outgoing waves. Magnitudes cannot change because ingoing flux has to equal outgoing flux. Also since Hamiltonian does not mix different values of  $l$ , the magnitude of each  $l$ - component must not change - it is unitary evolution.

$$\left[\frac{\hbar^2}{2m} \left(-d^2/dr^2 + \frac{l(l+1)}{r^2}\right) + V(r)\right] u_{kl}(r) = E_{k,l} u_{kl}(r)$$

For large  $r$ :

$$u = \frac{Ae^{ikr} + Be^{-ikr}}{r} \approx C \sin(kr - \beta_l)$$

(Since  $|A| = |B|$ ) Thus when  $V = 0$ ,  $\beta_l = \frac{l\pi}{2}$ . We can thus assume that phase changes by an amount  $\delta_l$  ( $\beta \rightarrow \beta + \delta$ ), when  $V \neq 0$ . Total change is  $2\delta_l$ . Thus we try

$$- \sum_l i^l \sqrt{4\pi(2l+1)} Y_{l0}(\theta) \frac{(e^{-ikr} e^{\frac{i\pi}{2}} - e^{ikr} e^{-\frac{i\pi}{2}}) e^{2i\delta_l}}{2ikr}$$

. [Note: When  $\delta = 0$  it reduces to  $e^{ikz}$ .] So  $e^{2i\delta_l} - 1 = 2i \sin \delta_l e^{i\delta_l}$  is the effect of scattering and will produce the  $f$  term. If  $|\eta_l| = |e^{2i\delta_l}| < 1$  then we have lost some particles. This is **inelastic scattering**.

The rest of it will give  $e^{ikz}$ . So

$$f_k(\theta, \phi) = \frac{1}{k} \sum_l \sin \delta_l e^{i\delta_l} \sqrt{4\pi(2l+1)} Y_{l0}(\theta)$$

$$\sigma_{elastic} = \int d\Omega |f|^2 = \frac{4\pi}{k^2} \sum_l \sin^2 \delta_l (2l+1)$$

Note also that:

$$f(0) = \frac{1}{k} \sum_l \sin \delta_l e^{i\delta_l} \sqrt{4\pi(2l+1)} Y_l(0)$$

$$\begin{aligned} \text{Im} f(0) &= \frac{1}{k} \sum_l \sin^2 \delta_l \sqrt{4\pi(2l+1)} Y_l(0) \\ &= \frac{1}{k} \sum_l \sin^2 \delta_l (2l+1) \end{aligned}$$

(Using  $Y_l(0) = \sqrt{\frac{2l+1}{4\pi}}$ ).

$$\frac{4\pi}{k} \text{Im} f(0) = \sigma_{el}.$$

This is the **Optical theorem**.

Do hard sphere. s-wave gives  $4\pi \sin^2(kr_0)/k^2 \approx 4\pi r_0^2$

$$f_k = 1/k \sin \delta_0 e^{i\delta_0}$$

$$\sigma(\theta) = 1/k^2 \sin^2 \delta_0$$

Eqn for large  $r$  is

$$\left(\frac{d^2}{dr^2} + k^2\right)u = 0$$

The soln is

$$\approx \sin k(r - r_0)$$

(Using b.c. that  $u(r_0) = 0$ ).  $\beta_0 = 0$  for  $l = 0$ .

$$\Rightarrow \delta_0 = kr_0$$

Q.E.D.

#### 10. Absorption.

$|\eta_l| = |e^{2i\delta_l}| < 1 \Rightarrow$  absorption. Calculate probability current into target (outgoing - ingoing).  $\int r^2 d\Omega [Re v(r) \frac{\hbar}{im} \partial_r v^*(r)] \propto (1 - |\eta_l|^2)$ .  $\sigma$  is  $\propto |\eta_l - 1|^2$ . Add the two to get  $Re(\eta_l - 1)$ . But  $Im f \propto Im(1/ik(\eta_l - 1)) \propto$  this also. Get

$$\frac{4\pi}{k} Im f(0) = \sigma_{total}$$

Optical theorem.

**Landau-Lifshitz** define S-matrix and optical theorem in terms of that.

Simplified analysis:

Define  $S$  matrix as evolution operator for scattering problem. Thus  $\langle f|S|i \rangle$  is amplitude that at  $t = -\infty$  a particle with momentum  $k_i$  scatters into the state  $k_f$  at  $t = +\infty$ .

Let  $S = I + iT$ . Then if no potential  $T = 0$ . Thus scattering probability (due to potential) is  $\langle f|T|i \rangle$ .  $S^\dagger S = I \Rightarrow i(T - T^\dagger) = T^\dagger T$ . Thus  $\langle i|i(T - T^\dagger)|i \rangle = \langle i|T^\dagger T|i \rangle = \sum_n |\langle n|T|i \rangle|^2$ . LHS is Im part of forward scattering amplitude. RHS is total probability of scattering (into any state).

## 7 Identical Particles

1. In classical mechanics there is never any ambiguity about which particle is which because one can always track the trajectory. In QM when wavefunctions overlap, this is not possible. Thus  $|+, - \rangle$  and



$|-, + \rangle$  are both acceptable descriptions for a state with one up and one down spin. So are  $\alpha|+, - \rangle + \beta|-, + \rangle$ . Need a prescription for  $\alpha, \beta$ . **Symmetrization Postulate** resolves this.

2. Permutations: Let  $|1, u_i; 2, u_j \rangle$  be basis states of two particles.  $|u_i \rangle$  is a basis for one particle states. Then define

$$P_{21}|1, u_i; 2, u_j \rangle = |2, u_i; 1, u_j \rangle$$

( $P_{nq}$  means replace 1 by  $n$  and 2 by  $q$ .) Note that  $|1, u_i; 2, u_j \rangle = |2, u_j; 1, u_i \rangle$ .

3. Action on wave function:

$$|\psi \rangle = \sum_{\epsilon, \epsilon'} \int d^3r \int d^3r' \psi_{\epsilon, \epsilon'}(r, r') |1, r, \epsilon; 2, r', \epsilon' \rangle .$$

$$\begin{aligned} P_{21}|\psi \rangle &= \sum_{\epsilon, \epsilon'} \int d^3r \int d^3r' \psi_{\epsilon, \epsilon'}(r, r') P_{21}|1, r, \epsilon; 2, r', \epsilon' \rangle . \\ &= \sum_{\epsilon, \epsilon'} \int d^3r \int d^3r' \psi_{\epsilon, \epsilon'}(r, r') |2, r, \epsilon; 1, r', \epsilon' \rangle . \\ &= \sum_{\epsilon, \epsilon'} \int d^3r \int d^3r' \psi_{\epsilon, \epsilon'}(r, r') |1, r', \epsilon'; 2, r, \epsilon \rangle . \\ &= \sum_{\epsilon, \epsilon'} \int d^3r \int d^3r' \psi_{\epsilon', \epsilon}(r', r) |1, r, \epsilon; 2, r', \epsilon' \rangle . \end{aligned}$$

We have exchanged the primed and unprimed variables - being dummy variables. Thus we can define the action of  $P_{21}$  on the wave function:  $P_{21}\psi_{\epsilon, \epsilon'}(r, r') = \psi_{\epsilon', \epsilon}(r', r)$ .

4. Obviously  $P_{21}^2 = I$ . Also  $P_{21}^\dagger = P_{21}$  Thus  $P^\dagger P = I$  thus it is unitary.
5. If  $P_{21}|\psi \rangle = |\psi \rangle$  then it is a symmetric state. If  $P_{21}|\psi \rangle = -|\psi \rangle$  then it is antisymmetric.
6. Define projection operators  $S = \frac{1+P_{21}}{2}$  and  $A = \frac{1-P_{21}}{2}$ .  
 $S^2 = S$ ,  $A^2 = A$ ,  $SA = 0$ ,  $A + S = 1$ . Also  $P_{21}S|\psi \rangle = |\psi \rangle$   
 $P_{21}A|\psi \rangle = -A|\psi \rangle$

7. Action of  $P$  on observables.  $P_{21}O(1)P_{21}^\dagger = O(2)$ . Check by acting on a state. Assume that  $|u_i\rangle$  has ev  $o_i$  for observable  $O$ . Similarly  $P_{21}O(1,2)P_{21}^\dagger = O(2,1)$ .

Observables can be symmetric or not. Hamiltonian for identical particles should be symmetric.

8. For three particles:  $P_{npq}|1, u_i; 2, u_j; 3, u_k\rangle = |n, u_i; p, u_j; q, u_k\rangle$ .

There are  $3!$  such permutations. For  $N$ -particles  $N!$  permutations.

They form a group: i) Identity= $P_{123}$  ii) product of two is a perm iii) Inverse also exists. eg  $P_{312}^{-1} = P_{231}$ .

9. Any permutation can be expressed as a product of **transpositions** which are perms that interchange two only. This decomposition is not unique. However the **parity** - which is whether it involves even no. or odd number of transpositions - is. Define  $\epsilon_\alpha$  - parity of perm  $P_\alpha = +1$  if even and  $= -1$  if odd.

Then  $S = \frac{1}{N!} \sum_\alpha P_\alpha$  and  $A = \frac{1}{N!} \sum_\alpha \epsilon_\alpha P_\alpha$

are the projection operators for  $N$ -particle wave functions..

$P_{\alpha_0}A = \epsilon_{\alpha_0}A$ . (Proof: Let  $P_{\alpha_0}P_\alpha = P_\beta$ . Then  $\epsilon_{\alpha_0}\epsilon_\alpha = \epsilon_\beta$ . Thus

$$\begin{aligned} P_{\alpha_0} \sum_\alpha \epsilon_\alpha P_\alpha &= \sum_\alpha \epsilon_\alpha P_{\alpha_0} P_\alpha \\ &= \sum_\alpha \epsilon_{\alpha_0} \epsilon_\beta P_\beta = \epsilon_{\alpha_0} \sum_\beta \epsilon_\beta P_\beta \end{aligned}$$

Summation over  $\alpha$  has ben changed to  $\beta$ .)

10. For bosons we get a symmetric state classified by occupation numbers  $N_1, N_2, \dots, N_k$  with  $N_1 + N_2 + \dots + N_k = N$ .

$S|1, u_1; 2, u_1, N_1, u_1; N_1 + 1, u_2; N_1 + 2, u_2; \dots; N_1 + N_2, u_2; \dots, N, u_k\rangle$

The number of permutations are now  $\frac{N!}{N_1!N_2!\dots N_k!}$ . The normalization constant will be inverse of the square root of this.

For fermions we get the Slater determinant.  $\frac{1}{\sqrt{N!}} \det|i, u_j\rangle$ . Note that if  $u_i = u_j$  the determinant vanishes - **Pauli exclusion**.

11. Amplitude for transition/scattering:

Let initial states be  $|\phi\rangle$  and  $|\chi\rangle$ . Then the symmetrized state is  $\frac{1}{\sqrt{2}}(|1, \phi; 2, \chi\rangle \pm |2, \phi; 1, \chi\rangle)$ . Let final state be  $|u_i\rangle$  and  $|u_j\rangle$ . Then the symmetrized state is  $\frac{1}{\sqrt{2}}(|1, u_i; 2, u_j\rangle \pm |2, u_i; 1, u_j\rangle)$ . Thus amplitude is

$A = \langle u_i | \phi \rangle \langle u_j | \chi \rangle \pm \langle u_j | \phi \rangle \langle u_i | \chi \rangle$ . The first term is the direct term and the second is the exchange term.

Note that when  $u_i = u_j$  for fermions the amplitude vanishes. For bosons the final state is then  $|1, u_i; 2, u_i\rangle$ .  $A = \sqrt{2} \langle u_i | \phi \rangle \langle u_i | \chi \rangle$ .  $Prob = |A|^2$ .

Classically we would just add the probabilities for the two. So we would have  $|\langle u_i | \phi \rangle \langle u_j | \chi \rangle|^2 + |\langle u_j | \phi \rangle \langle u_i | \chi \rangle|^2$ . If they are identical then  $|\langle u_i | \phi \rangle \langle u_i | \chi \rangle|^2$  - which is less than the quantum one by a factor of 2.

12. When can the effect of symmetrization be neglected: If for some reason the exchange term is very small. eg if the two one particle states are spatially very far apart. eg an electron on earth need not be symmetrized with the electron on the moon.

## 8 Applications of QM

### 8.1 Hydrogen atom

#### 1. Pauli's solution.

$$H = P^2/2m - c/r$$

has  $\vec{L}$  and also  $\vec{M} = (\vec{P} \times \vec{L} - \vec{L} \times \vec{P})/2m - c\vec{r}/r$  Runge Lenz vector as conserved quantities. Commutation relns

$$[M, H] = [L, H] = 0 \quad L.M = M.L = 0$$

$$M^2 = \frac{2H}{m}(L^2 + \hbar^2) + c^2$$

$$[M_i, L_j] = i\epsilon_{ijk}M_k$$

obviously - being a vector.

$$[M_i, M_j] = -\frac{2i}{m}H\epsilon_{ijk}L_k$$

Working on energy eigenfn's can redefine  $M' = (-m/2E)^{1/2}M$

$$[M'_i, M'_j] = i\epsilon_{ijk}L_k$$

and it is clear that M,L form SO(4) algebra. Split into SU(2)XSU(2):  $I = L + M'$  and  $K = L - M'$ .

In SO(4) notation

$$[L_{ij}, L_{kl}] = i\delta_{ik}L_{jl} + i\delta_{jl}L_{ik} - i\delta_{il}L_{jk} - i\delta_{jk}L_{il}$$

where  $L_{i4} = M'_i$  Also  $I^2 = K^2$  (from L.M=0). And  $I^2 + K^2 = 2k(k+1)$   
Also

$$M'^2 + L^2 = -\hbar^2 - c^2m/2E$$

So

$$\hbar^2 E = \frac{-c^2m}{4k(k+1)+1} = \frac{-e^4m}{n^2}$$

2. **Fine structure and Hyperfine structure** (Students work it out on the board)

## 8.2 Interaction of an atom with plane waves

1. To calculate transition rate we use Golden rule:  $\frac{dP}{d\beta} = \frac{2\pi}{\hbar} |W_{fi}|^2 \rho(E_f, \beta)$  (with energy conservation).
2.  $W = \frac{e(p \cdot A + A \cdot p)}{2m}$ .  $e$  is charge of electron. We will use semiclassical treatment whereby  $A = a\hat{e}e^{ikX - i\omega t}$
3. Normalization : Energy in em fld =  $\frac{1}{2}\epsilon_0 E^2 + \frac{B^2}{2\mu_0}$ .  $E = -\frac{\partial A}{\partial t} \approx \omega A$   
Thus  $1/2\epsilon_0\omega^2 a^2 \times 2(B - fld) \times 1/2(\text{time average})$  is the energy density. This must be equal to  $\hbar\omega$  (1 photon per unit volume) Thus  $a^2 = \frac{2\hbar}{\epsilon_0\omega}$ . We have assumed that  $A(t) = a\cos \omega t$ . The normalization of one photon per unit volume is arbitrary. That fixes the overall scale only. If there are two, we get twice the absorption or induced emission rate. For  $N$  photons we get a factor of  $N$ . When we include spontaneous emission,  $N \rightarrow N + 1$ .

Thus  $a = \sqrt{\frac{2\hbar}{\epsilon_0\omega}}$ . If we want the coefficient of  $e^{i\omega t}$  rather than  $\cos$  then we get a factor of  $1/2$ :  $a = \sqrt{\frac{\hbar}{2\epsilon_0\omega}}$ .

4. **Dipole Approximation:** Let  $e^{ikX} \approx 1$ . Thus  $W = \frac{a\hat{e} \cdot \vec{p}}{m}$ .

5.

$$W_{fi} = \frac{e}{m} \langle f | \vec{p} | i \rangle \cdot \hat{e} a = e \omega_{fi} \vec{X}_{fi} \cdot \hat{e}$$

6. phase space :

$$\frac{d^3 p}{(2\pi\hbar)^3} \delta(E_f - E_i - \omega).$$

Also  $pc = E$ .

$$\begin{aligned} &= \frac{E^2 d\Omega}{(2\pi\hbar c)^3} \\ &= \frac{\omega^2 d\Omega}{(2\pi c)^3 \hbar} \end{aligned}$$

We have used up the energy delta fn to do dE.

7. Put everything together:

$$a^2 e^2 \omega^2 |\vec{X}_{fi} \cdot \hat{e}|^2 d\Omega \frac{\omega^2}{(2\pi c)^3 \hbar} \frac{2\pi}{\hbar}$$

$$dP = \frac{e^2}{2\epsilon_0} \frac{\omega^3}{(2\pi c)^3} \frac{2\pi}{\hbar} |\vec{X}_{fi} \cdot \hat{e}|^2 d\Omega$$

8. Do the angular integral: Choose  $z$  axis along  $\vec{X}_{fi}$ . Then  $\theta$  is angle made by  $\vec{k}$  the direction of the photon.  $\hat{e}$  is perpendicular to  $\vec{k}$ . Thus  $\vec{X}_{fi} \cdot \hat{e} = |\vec{X}_{fi}| \sin \theta$ . Thus we have to do  $\int_{-1}^1 d\cos \theta \sin^2 \theta \int d\phi = 2\pi \frac{4}{3}$ .

$$P = \frac{e^2}{4\pi\epsilon_0 \hbar c} \frac{4}{3} \frac{\omega^3}{c^2} |\vec{X}_{fi}|^2$$

where

$$\vec{X}_{fi} = \langle f | \vec{X} | i \rangle = \int d^3 x \psi_f^*(x) \vec{x} \psi_i(x).$$

If we have  $n$  photons then the answer is  $nP$ . Actually if we include spontaneous emission the answer is  $(n+1)P$ . We can also express  $n$  in terms of Intensity of the plane wave.

### 8.3 Charge particle in a magnetic field

#### 1. Classical

$\frac{mv^2}{r}(-\hat{r}) = q\vec{v} \times \vec{B}$ . Thus  $\omega = \frac{qB}{m}$ . Direction of motion: Current induced opposes build up of  $B$ .

#### 2. Quantum Mechanically

$$\begin{aligned} \frac{1}{2m}(p - eA)^2\Psi &= E\Psi \\ \Rightarrow \frac{1}{2m}[\Pi_x^2 + \Pi_y^2]\Psi &= E\Psi \end{aligned}$$

$\Pi_x = (-i\hbar\frac{\partial}{\partial x} - eA_x)$  etc.

$$[\Pi_x, \Pi_y] = i\hbar e\left[\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right] = i\hbar eB_z$$

Define  $\tilde{\Pi}_x = \frac{\Pi_x}{\sqrt{eB}}$ ,  $\tilde{\Pi}_y = \frac{\Pi_y}{\sqrt{eB}}$  Then  $[\tilde{\Pi}_x, \tilde{\Pi}_y] = i\hbar$  and

$$\begin{aligned} H &= \frac{eB}{2m}(\tilde{\Pi}_x^2 + \tilde{\Pi}_y^2) = \frac{1}{2}\omega(\hat{P}^2 + \hat{X}^2) \\ &= (N + \frac{1}{2})\hbar\omega \end{aligned}$$

Thus we have the energy levels and in principle a wave fn. What about degeneracy? Classically the centre of the orbit can be anywhere.

#### 3. Simple solution: Choose gauge that separates $x, y$ : $A_x = -By$

$$\begin{aligned} H &= (-i\partial_x + eBy)^2 + (-i\partial_y)^2 \\ &= -(\partial_x^2 + \partial_y^2) + e^2B^2y^2 - 2ieyB\partial_x \end{aligned}$$

Choose  $x$ -dependence  $e^{ik_x X}$  where  $k_x = \frac{2\pi n}{L_x}$ .

Then

$$\begin{aligned} H &= -\partial_y^2 + \hbar^2 k_x^2 + e^2 B^2 y^2 + 2eB\hbar k_x y \\ &= -\partial_y^2 + e^2 B^2 \left(y + \frac{B\hbar k_x}{eB^2}\right)^2 \end{aligned}$$

Thus the  $y$  dependence is that of a harmonic oscillator with center  $\frac{\hbar k_x}{eB}$ . Note when  $\frac{\hbar k_x}{eB} = L_y$  we cannot shift any further. Thus we get  $2\pi n_{max}\hbar = L_y L_x B e$  Thus  $n_{max} = \frac{\Phi}{2\pi\hbar} = \frac{\Phi}{\Phi_0}$

Thus we have a degeneracy of  $N_\phi = \frac{\Phi}{\Phi_0}$ .

4. More elegant methods:

Choose circular gauge:  $A_x = -\frac{By}{2}$  and  $A_y = \frac{Bx}{2}$ . Define  $K_x = -i\hbar\partial_x + eA_x$  and  $K_y = -i\hbar\partial_y + eA_y$

Check that the following are true:

$$[K_x, \Pi_x] = [K_x, \Pi_y] = [K_y, \Pi_y] = [K_y, \Pi_x] = 0$$

$$[K_x, K_y] = -ieB\hbar$$

Thus

$$[H, K_x] = [H, K_y] = 0$$

.  $K_x, K_y$  are symmetry generators. They are like translation operators : call them “magnetic translation operators”.

If we define  $T_x = e^{i\frac{L_x}{N\phi}K_x}$   $T_y = e^{i\frac{L_y}{N\phi}K_y}$  then

$$\begin{aligned} T_x T_y &= T_y T_x e^{\frac{i^2 L_x L_y}{N^2 \phi} [K_x, K_y]} \\ &= T_y T_x e^{\frac{i2\pi}{N\phi}} \end{aligned}$$

This means  $T_x, T_y$  can be written as  $N_\phi \times N_\phi$  matrices. We can diagonalize one of them.

Thus let  $T_x \Psi_{n,0} = e^{i\lambda_0} \Psi_{n,0}$  and  $H \Psi_{n,0} = (n + \frac{1}{2})\hbar\omega \psi_{n,0}$ .

Then it is easy to see that  $T_y^m \Psi_{n,0} \equiv \Psi_{n,m}$  satisfies  $T_x \Psi_{n,m} = e^{i(\frac{2\pi m}{N\phi} + \lambda_0)} \Psi_{n,m}$ .

Thus clearly  $m = 0, 1, \dots, N_\phi$ .

5. Even more elegant (!): Choose complex notation:

Define

$$\frac{(\Pi_x + i\Pi_y)}{2} = P \quad ; \quad \frac{(\Pi_x - i\Pi_y)}{2} = \bar{P}$$

The following can be checked:

$$P = (\partial_{\bar{z}} + \frac{eBz}{4})$$

$$\bar{P} = (\partial_z - \frac{eB\bar{z}}{4})$$

$$K = \left( \partial_{\bar{z}} - \frac{eBz}{4} \right)$$

$$\bar{K} = \left( \partial_z + \frac{eB\bar{z}}{4} \right)$$

where  $K, \bar{K}$  are defined analogously. and  $z = x + iy$ .

Define  $T = e^{\frac{iL}{N\phi} K}$   $\bar{T} = e^{\frac{iL}{N\phi} \bar{K}}$

$\Psi_{n,0} = \bar{z}^n e^{-\frac{eB}{4\hbar}|z|^2}$  satisfies  $H\Psi_{n,0} = (n + \frac{1}{2})\hbar\omega\Psi_{n,0}$ .

Elegant way to check this: Find action of  $P, \bar{P}$ :

$$\bar{P}\Psi_{n,0} = -\frac{eB}{2}\Psi_{n+1,0}$$

$$P\Psi_{n,0} = \hbar n\Psi_{n-1,0}$$

and  $H = -\frac{P\bar{P} + \bar{P}P}{m}$ .

Also  $\bar{K}\Psi_{n,0} = 0$ . Thus  $\bar{T}\Psi_{n,0} = \Psi_{n,0}$ .

Now act on it with  $T^m$  to get  $\Psi_{n,m}$ .

## 8.4 Bohm-Aharanov Effect, Monopole etc

1.  $A^\mu = (\phi, \vec{A})$ ,  $A_\mu = (-\phi, \vec{A})$

$$F_{ij} = \partial_i A_j - \partial_j A_i = \epsilon_{ijk} B^k$$

$$F^{0i} = -F_{0i} = E_i$$

### 2. Bohm-Aharanov Effect

Can associate a phase  $e^{\frac{i}{\hbar} \int_0^x A \cdot dx}$  in the Feynman sum over paths. The phase depends on the path. However if  $B = 0$  the phase does not depend on path. If we have a solenoid of flux, and electron is not allowed to see solenoid, then the propagator will have such a factor for each path in the sum. Depending on whether the path is on one side of the solenoid or the other there will be a phase difference  $e^{\frac{ie}{\hbar} \oint B \cdot ds} = e^{\frac{ie\Phi}{\hbar}}$ . Thus there can be destructive or constructive interference depending on  $\Phi$  even if electron never actually sees the magnetic field. Note: if  $e\Phi = 2\pi n\hbar$  the flux tube has no effect!



### 3. monopole

Dirac said: Have an infinitely thin tube of flux coming out of the monopole to satisfy  $\text{div of } \mathbf{B} = 0$ . If the flux satisfies  $e\phi = 2n\pi\hbar$ , we see from the discussion of Bohm-Aharonov effect that the tube is invisible. So if  $g = \phi = \frac{2n\pi}{\hbar}$  monopoles can exist!

### 8.5 Semi-classical techniques (see Landau-Lifshitz)

1. When system is almost classical, we can assume a form  $e^{\frac{i}{\hbar}S_{cl}}$  for the particle propagator. Motivated by this try a solution of the form  $\psi(x) = e^{\frac{i}{\hbar}S}$  and expand  $S$  in a power series in  $\hbar$ :

$$S = S_0 + \left(\frac{\hbar}{i}\right)S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + \dots$$

2. Schrodinger's eqn is

$$\begin{aligned} -\frac{\hbar^2}{2m}\partial_x^2\psi + V(x)\psi &= E\psi \\ \Rightarrow -\frac{\hbar^2}{2m}\left[\frac{i}{\hbar}S'' + \left(\frac{iS'}{\hbar}\right)^2\right] + V(x) &= E \\ \frac{1}{2m}(S')^2 - \frac{i\hbar}{2m}S'' &= E - V \end{aligned}$$

This is non-linear in  $S$ . Substitute above series:

$$\frac{1}{2m}[(S'_0)^2 + \left(\frac{\hbar}{i}\right)^2(S'_1)^2 + 2\frac{\hbar}{i}S'_0S'_1] - \frac{i\hbar}{2m}S''_0 - \frac{\hbar^2}{2m}S''_1 = E - V$$

$O(\hbar^0)$

$$\begin{aligned} S_0'^2 &= 2m(E - V) = p^2 \\ S_0(x) &= \pm \int_a^x \sqrt{2m(E - V(x))} dx + S_0(a) = \pm \int^x p dx \end{aligned}$$

$O(\hbar)$

$$S'_0S'_1 + \frac{1}{2}S''_0 = 0$$

$$\Rightarrow S'_1 = -\frac{p'}{2p}$$

$$S_1 = -\frac{1}{2} \ln p$$

$$\psi = \frac{1}{\sqrt{p}} (C_1 e^{\frac{i}{\hbar} \int_a^x p \, dx} + C_2 e^{-\frac{i}{\hbar} \int_a^x p \, dx})$$

This is the leading non-trivial part of semiclassical (WKB) approximation for the wave function.

3. Normalization:  $\frac{1}{p} \approx (\text{velocity})^{-1}$ . This is expected since the prob of finding a particle between  $x$  and  $x + dx$  is prop to time it spends there, which is inversely prop to velocity.
4. Taking the exponent  $\int p \, dx$  would be exact if  $\hbar S'' \ll S'^2$ .

$$\hbar \left| \frac{d(1/S')}{dx} \right| \ll 1$$

$$\lambda \frac{d\lambda}{dx} \ll \lambda$$

The change in de-Broglie wavelength over a wavelength should be less than the wavelength itself. In particular when  $p \rightarrow 0$  this cannot be true. These are the classical turning points.

5. If  $p$  is imaginary then we have a rising exponential and falling exp. Can keep the falling one only if rising one is strictly zero. This has to be imposed as a boundary condition.
6. Thus for a rising potential with  $x = a$  as the turning point:

$$\psi = \frac{1}{\sqrt{p}} (C_1 e^{\frac{i}{\hbar} \int_a^x p \, dx} + C_2 e^{-\frac{i}{\hbar} \int_a^x p \, dx})$$

for  $x \ll a$

and

$$\frac{1}{\sqrt{p}} C e^{-\frac{1}{\hbar} \int_a^x |p| \, dx}$$

for  $x \gg a$ .

To find the relation between the coefficients do an analytic continuation of  $p$  in a semi circle around  $x = a$ . In this region we assume  $V(x) - E = V'(a)(x - a)$ .

So  $p = \sqrt{2mV'(a)(a-x)}$ .

Let  $x - a = \rho e^{i\theta}$ . When  $\theta = 0$ ,  $x$  is to the right of  $a$ . Here the exponentially falling solution is assumed. Now let  $\theta$  increase to  $\pi$ . Start with  $x > a$  and  $\theta = 0$ ,

$$\begin{aligned} \int_a^x |p| dx &= \int_a^x \sqrt{(x-a)} dx = \int \rho i d\theta e^{i\theta} \sqrt{\rho} e^{i\theta/2} \\ &= \frac{2}{3} \rho^{\frac{3}{2}} e^{\frac{3i\theta}{2}} \\ &= -i \frac{2}{3} \rho^{\frac{3}{2}} \quad \text{at } \theta = \pi \end{aligned}$$

So

$$e^{-\frac{1}{\hbar} \int_a^x \sqrt{x-a} dx} \rightarrow e^{+i\phi}$$

Where  $\phi$  is a positive real number.

Thus we conclude that

$$e^{-\frac{1}{\hbar} \int_a^x |p| dx} \rightarrow e^{-\frac{i}{\hbar} \int_a^x |p| dx}$$

when we go to the classically allowed region  $x < a$ . Note that because  $x < a$  the integral is -ve and so phase is positive as required.

Another way is to see that  $(x-a)^{\frac{1}{2}} \rightarrow (a-x)^{\frac{1}{2}}(+i)$  when we go on the upper semi circle. Thus we get exponent of  $C_2$  term.

This is the  $C_2$  term in the wave function. Also  $\sqrt{|p|} = (x-a)^{\frac{1}{4}} \rightarrow (a-x)^{\frac{1}{4}} e^{\frac{i\pi}{4}}$  Thus  $C_2 = C e^{-\frac{i\pi}{4}}$

Similarly we get  $C_1$  piece by going on the lower semi circle.  $C_1 = C e^{\frac{i\pi}{4}}$ .

Thus

$$\begin{aligned} \psi &= \frac{C}{\sqrt{|p|}} e^{-\frac{1}{\hbar} \int_a^x |p| dx} \quad \text{when } x > a \\ &= \frac{1}{\sqrt{p}} (C e^{\frac{i\pi}{4}} e^{\frac{i}{\hbar} \int_a^x |p| dx} + C e^{-\frac{i\pi}{4}} e^{-\frac{i}{\hbar} \int_a^x |p| dx}) \quad \text{when } x < a \end{aligned}$$

This is the main result. Rest are applications.

## 7. Barrier tunneling

Three regions:

$x < a$  : I to left of barrier where we have incoming and reflected wave.

$a < x < b$ : II - inside barrier, where we have a falling exponential.

$x > b$ : III - to right of barrier where we have only right moving wave.

- Start with right moving soln in III. Analytically continue over a semi circle to make sure that in II we get a falling exponential. Now we again analytically continue as in the previous para to get the  $C_{1,2}$  terms in region I.

- Assume that in region II, we have  $\frac{D}{\sqrt{|p|}} e^{\frac{i}{\hbar} \int_b^x |p| dx + \frac{i\pi}{4}}$ . which is a wave travelling to right.

Analytically continue as before.  $x - b = \rho e^{i\theta}$ . We have to go from  $\theta = 0$  to  $\theta = \pm\pi$  depending on whether we go along upper semi circle or lower one.

$$\theta = \pi \text{ gives : } \sqrt{x-b} = \sqrt{\rho} e^{\frac{i\theta}{2}} \rightarrow \sqrt{\rho} i$$

$$\theta = -\pi \text{ gives : } \sqrt{x-b} = \sqrt{\rho} e^{\frac{i\theta}{2}} \rightarrow \sqrt{\rho} (-i)$$

$$i \int_b^x |p| dx \rightarrow - \int_b^x |p| dx \quad \text{for } \theta = \pi$$

This is positive because  $x < b$  and becomes zero at  $b$ . So it is a falling exponential, which is what we want. Also since  $(x-b)^{\frac{1}{4}} \rightarrow \rho^{\frac{1}{4}} e^{\frac{i\pi}{4}}$  we get

$$\frac{D}{\sqrt{|p|}} e^{-\frac{1}{\hbar} \int_b^x |p| dx} \text{ for } x < b.$$

(Note: Exponent is 0 at  $x = b$  and +ve for  $x < b$  so it is a falling exp as reqd.)

$$= \frac{D}{\sqrt{|p|}} e^{+\frac{1}{\hbar} \int_a^b |p| dx - \int_a^x |p| dx}$$

Thus comparing with the WKB expression we get  $C = D e^{\int_a^b |p| dx}$ .

Thus tunnelling probability is  $|D/C|^2 = e^{-2 \int_a^b |p| dx}$ .

## 8. Energy Splitting due to tunneling

Given a double well with a barrier. In lowest order approx there are two degenerate eigenstates: If  $x = 0$  is the symmetric point ( $V(x) = V(-x)$ ) then  $\psi_0(x)$  is a wave fn mainly in well I, the  $\psi_0(-x)$  is the solution in the other well, II.

$$\psi_1(x) = \frac{1}{\sqrt{2}}[\psi_0(x) + \psi_0(-x)]$$

$$\psi_2(x) = \frac{1}{\sqrt{2}}[\psi_0(x) - \psi_0(-x)]$$

Thus, to lowest order these have same energy as  $\psi_0$ , but in next order they don't.

Assume that  $\psi_0(x)\psi_0(-x) \ll 1$  because the wave fns are strongly damped outside the well.

$$\psi_0'' + 2m(E_0 - V)\psi_0 = 0$$

$$\psi_1'' + 2m(E_1 - V)\psi_1 = 0$$

Multiply first by  $\psi_1$  and second by  $\psi_0$  and subtract and integrate from  $0 - \infty$ :

$$\int_0^\infty (\psi_1\psi_0'' - \psi_0\psi_1'') dx + \frac{2m}{\hbar^2}(E_0 - E_1) \int_0^\infty dx \psi_0\psi_1$$

Integrate by parts: first term is  $\psi_1\psi_0'|_0^\infty - \psi_0\psi_1'|_0^\infty$  At  $x = \infty$ ,  $\psi_1 = \psi_0 = 0$ . At  $x = 0$ ,  $\psi_1' = 0$ . Thus we get  $-\psi_1\psi_0'(0) = -\sqrt{2}\psi_0\psi_0'(0)$ .

Second term:  $\int_0^\infty dx \psi_0\psi_1 = \int dx \frac{\psi_0^2}{\sqrt{2}} = \frac{1}{\sqrt{2}}$  So eqn becomes

$$-\sqrt{2}\psi_0\psi_0'(0) + \frac{\sqrt{2}m}{\hbar^2}(E_0 - E_1) = 0$$

$$\Rightarrow E_1 - E_0 = -\frac{\hbar^2}{m}\psi_0\psi_0'(0)$$

Similarly  $E_2 - E_0$  is the opposite sign. Thus

$$E_2 - E_1 = \frac{2\hbar^2}{m}\psi_0\psi_0'(0)$$

Using  $\psi_0(x) = \frac{C}{\sqrt{|p|}} e^{\int_a^x |p| dx}$  for  $x < a$

$$\psi_0(0) = \frac{C}{\sqrt{|p|}} e^{-\frac{1}{\hbar} \int_0^a |p| dx}$$

and

$$\psi'_0(0) = \frac{p}{\hbar} \psi_0(0)$$

Thus

$$E_2 - E_1 = \frac{2\hbar p}{m} \psi_0(0)^2.$$

The normalization  $C$  is fixed by assuming the cosine soln ( $\frac{2C}{\sqrt{p}} \cos..$ ) inside the well:  $\int dx \frac{4C^2}{2p} = 1$  (Average of cos is 1/2). Using  $p = m \frac{dx}{dt}$  we get  $\int \frac{dx}{p} = \int_a^b \frac{dt}{m} = \frac{T}{2m}$  where  $T$  is time period  $T = \frac{2\pi}{\omega}$ . Thus  $\frac{C^2 2\pi}{m\omega} = 1$ .  $C^2 = \frac{m\omega}{2\pi} \cdot \frac{C}{\sqrt{p}} = \sqrt{\frac{\omega}{2\pi v}}$ .

$$\text{Thus } \Delta E = \frac{\hbar\omega}{\pi} e^{-2 \int_0^a |p| dx} = \frac{\hbar\omega}{\pi} e^{-\int_{-a}^a |p| dx}.$$

## 8.6 Dirac Equation

We want a Lorentz covariant version of Schrodinger equation to describe relativistic quantum particles. Klein Gordon eqn has problems with square root etc. Try for an equation linear in derivatives.

1.

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar \alpha^i \frac{\partial \psi}{\partial x^i} + m\beta\psi$$

Or better still

$$i\hbar \gamma^\mu \frac{\partial \psi}{\partial x^\mu} = m\psi$$

Conventions:  $\eta^{\mu\nu} = (-, +, +, +)$ .  $x^\mu = (t, \vec{x})$ .  $p^0 = E = -p_0, p^i = \vec{p}$ .  
 $p^\mu p_\mu = -p^0 p^0 + p^i p^i = -E^2 + \vec{p} \cdot \vec{p} = -m^2$

$$p_\mu = -i\hbar \frac{\partial}{\partial x^\mu} = -i\hbar \left( \frac{\partial}{\partial t}, \frac{\partial}{\partial x^i} \right) \quad E = p^0 = -p_0 = i\hbar \frac{\partial}{\partial t}$$

If we act again with  $i\hbar \gamma^\mu p_\mu$  we get

$$-\hbar^2 \gamma^\mu \gamma^\nu \frac{\partial^2}{\partial x^\mu \partial x^\nu} \psi = m^2 \psi$$

If we require  $\{\gamma^\mu, \gamma^\nu\} = -2\eta^{\mu\nu}$  then the above equation will become

$$\hbar^2 \left[ -\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^{i^2}} \right] \psi = m^2 \psi$$

So  $(\gamma^0)^2 = 1$  and the eigenvalues are  $\pm 1$ .  $\gamma^0$  is Hermitian.  $(\gamma^i)^2 = -1$  and  $\gamma^i$  are anti Hermitian, with eigenvalues  $\pm i$ .

Explicitly

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \quad (17)$$

Note  $\gamma^0 \gamma^i$  is Hermitian.

Thus

$$i\hbar \frac{\partial \psi}{\partial t} + i\hbar \gamma^0 \gamma^i \frac{\partial \psi}{\partial x^i} = m \gamma^0 \psi$$

is Dirac equation in its original form, with  $\alpha, \beta$  matrices.

2. Solutions in the rest frame:

$$i\hbar \frac{\partial \psi}{\partial t} = m \gamma^0 \psi$$

$$\psi = \begin{bmatrix} e^{-imt} \psi_1(0) \\ e^{-imt} \psi_2(0) \\ e^{+imt} \psi_3(0) \\ e^{+imt} \psi_4(0) \end{bmatrix}$$

Why shouldn't a positive energy particle fall into the negative energy state with emission of photon? Dirac postulated a "sea" of filled negative energy states. Pauli exclusion ensures that positive energy electron will not fall into these states. Also this means that a photon can knock an electron from a filled negative energy state to a higher energy positive state. Effectively creating an electron and a hole (positron). This was the theoretical discovery of anti-particle.

3. Reduction to nrSE with spin (Pauli eqn):

Couple to em :  $p^\mu \rightarrow p^\mu - eA^\mu$ .  $A^0 = \Phi$ ,  $A^i = \vec{A}$

$$-i\hbar \gamma^0 \frac{\partial \psi}{\partial t} - i\hbar \gamma^i \frac{\partial \psi}{\partial x^i} + e \gamma^0 \Phi - e \gamma^i A_i \psi = -m \psi$$

Negative energy solutions need an interpretation. For the moment assume  $\psi_{3,4} = 0$ .

Assume:

$$\psi = \begin{bmatrix} \phi \\ \chi \end{bmatrix}$$

$$\gamma^0 \psi = \begin{bmatrix} \phi \\ -\chi \end{bmatrix}$$

$$\gamma^i \psi = \begin{bmatrix} \sigma^i \chi \\ -\sigma^i \phi \end{bmatrix}$$

$$-i\hbar \frac{\partial \phi}{\partial t} - i\hbar \sigma^i \frac{\partial \chi}{\partial x^i} + e\Phi \phi - e\sigma^i A_i \chi = -m\phi$$

$$+i\hbar \frac{\partial \chi}{\partial t} + i\hbar \sigma^i \frac{\partial \phi}{\partial x^i} - e\Phi \chi + e\sigma^i A_i \phi = -m\chi$$

Set  $\phi = e^{-imt} \phi$  and  $\chi = e^{-imt} \chi$  - take out the main time dependence.

$$-m\phi - i\hbar \frac{\partial \phi}{\partial t} - i\hbar \sigma^i \frac{\partial \chi}{\partial x^i} + e\Phi \phi - e\sigma^i A_i \chi = -m\phi$$

$$+m\chi + i\hbar \frac{\partial \chi}{\partial t} + i\hbar \sigma^i \frac{\partial \phi}{\partial x^i} - e\Phi \chi + e\sigma^i A_i \phi = -m\chi$$

$$-i\hbar \frac{\partial \phi}{\partial t} = i\hbar \sigma^i \frac{\partial \chi}{\partial x^i} - e\Phi \phi + e\sigma^i A_i \chi$$

$$+i\hbar \frac{\partial \chi}{\partial t} = -i\hbar \sigma^i \frac{\partial \phi}{\partial x^i} + e\Phi \chi - e\sigma^i A_i \phi - 2m\chi$$

The dominant term involving  $\chi$  is  $-2m\chi$ . Thus

$$i\hbar \sigma^i \frac{\partial \phi}{\partial x^i} + e\sigma^i A_i \phi = -2m\chi$$

$$\chi = \frac{(i\hbar \sigma^i \frac{\partial}{\partial x^i} + eA_i) \phi}{-2m} = \frac{\Pi_i \phi}{2m}$$

Thus  $\chi \ll \phi$  is called the small component and  $\phi$  is the large component. Eqn for  $\phi$ :



$$i\hbar \frac{\partial \phi}{\partial t} = \frac{\sigma^i \sigma^j \Pi_i \Pi_j \phi}{2m} + e\Phi \phi$$

where  $\Pi = p - eA$ .

Using  $\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk} \sigma^k$  we get

$$\frac{\Pi^2}{2m} \phi - e\hbar \epsilon^{ijk} \frac{\partial A_j}{\partial x^i} \phi + e\Phi \phi = \left( \frac{\Pi^2}{2m} - \frac{e\hbar \sigma^k B_k}{2m} + e\Phi \right) \phi$$

Thus we get the Pauli equation. Using  $\sigma \hbar = 2S$  we get  $\frac{e\hbar \vec{S} \cdot \vec{B}}{m}$ . This is the correct gyromagnetic ratio: because  $e(p \cdot A + A \cdot p) \rightarrow eL \cdot B$  in a uniform magnetic field. So we get the expected  $-\frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}$  coupling.

#### 4. Lorentz Covariance:

Want  $\psi'(x') = S\psi(x)$  or  $\psi'(x) = S\psi(\mathcal{R}^{-1}x)$ .  $S$  represents spin.

$$(\gamma^\mu p_\mu + m)\psi(x) = 0 \Rightarrow (\gamma^\mu p'_\mu + m)\psi'(x') = (-i\hbar \gamma^\mu \frac{\partial}{\partial x'^\mu} + m)\psi'(x') = 0$$

$$(-i\hbar \gamma^\mu \frac{\partial}{\partial x^\mu} + m)\psi(x) = (-i\hbar \frac{\partial x'^\nu}{\partial x^\mu} \frac{\partial}{\partial x'^\nu} + m) \underbrace{\psi(\mathcal{R}^{-1}x')}_{S^{-1}\psi'(x')} = 0$$

$$x'^\mu = \mathcal{R}^\mu_\nu x^\nu$$

$$\Rightarrow (-i\hbar \gamma^\mu \mathcal{R}^\nu_\mu \frac{\partial}{\partial x'^\nu} + m)S^{-1}\psi'(x') = 0$$

Thus we want  $S\gamma^\mu S^{-1}\mathcal{R}^\nu_\mu = \gamma^\nu$ .

$$\mathcal{R}^\mu_\nu = \delta^\mu_\nu + \epsilon^\mu_\nu \text{ with } \epsilon^{\mu\nu} = -\epsilon^{\nu\mu}.$$

$$\text{Let } S = 1 + i\epsilon^{\mu\nu} \sigma_{\mu\nu}$$

We find:

$$S^{-1}\gamma^\mu S = \gamma^\mu + \epsilon^\mu_\nu \gamma^\nu$$

$$-i\epsilon^{\rho\sigma} [\sigma_{\rho\sigma}, \gamma^\mu] = \epsilon^\mu_\nu \gamma^\nu$$

$$\text{Find } \sigma_{\rho\sigma} = \frac{i}{8} [\gamma_\rho, \gamma_\sigma].$$

Note:  $[\gamma_0, \gamma_1]$  is Hermitian.  $[\gamma_2, \gamma_1]$  is Anti-Hermitian.  $S_{rot}$  is Unitary. But  $S_{boost}^\dagger = S_{boost}$ .

We can check that all  $S$  satisfy:  $\gamma_0 S^\dagger \gamma_0 = S^{-1}$

Using this can show that  $\psi^\dagger \gamma^0 \gamma^\mu \psi$  is a 4-vector.

Define  $\bar{\psi} = \psi^\dagger \gamma^0$ . Then the four vector is  $\bar{\psi} \gamma^\mu \psi$ . Clearly  $\bar{\psi} \psi$  is a scalar.

5. Can define various tensors...HW. Need  $\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3$ .  $\gamma^{5^2} = 1$ .

Under parity  $:\gamma^i \rightarrow -\gamma^i$ . So  $\gamma^5 \rightarrow -\gamma^5$ . Thus  $\bar{\psi} \gamma^5 \psi$  is a **pseudoscalar**. Check that it is a scalar under LT.

6. **Parity:**  $P^{-1} \gamma^\mu P = \mathcal{R}^\mu_\nu \gamma^\nu$ . Where  $\mathcal{R}$  is the diagonal matrix:  $(1, -1, -1, -1)$ .  $\gamma^0$  satisfies this property. Thus  $\psi'(x') = \gamma^0 \psi(x)$  where  $x' = \mathcal{R}x$ . Thus we can check that  $\bar{\psi} \gamma^5 \psi$  is a pseudoscalar.

7. **current:**

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial x^0} &= -i\hbar \gamma^0 \gamma^i \frac{\partial \psi}{\partial x^i} + m \gamma^0 \psi \\ i\hbar \psi^\dagger \frac{\partial \psi}{\partial x^0} &= -i\hbar \psi^\dagger \gamma^0 \gamma^i \frac{\partial \psi}{\partial x^i} + m \psi^\dagger \gamma^0 \psi \\ -i\hbar \frac{\partial \psi^\dagger}{\partial x^0} &= +i\hbar \frac{\partial \psi^\dagger}{\partial x^i} (\gamma^0 \gamma^i)^\dagger + m \psi^\dagger \gamma^0 \\ -i\hbar \frac{\partial \psi^\dagger}{\partial x^0} \psi &= +i\hbar \frac{\partial \psi^\dagger}{\partial x^i} \gamma^0 \gamma^i \psi + m \psi^\dagger \gamma^0 \psi \end{aligned}$$

Subtracting,

$$\Rightarrow i\hbar \frac{\partial}{\partial t} (\psi^\dagger \psi) = -i\hbar \frac{\partial}{\partial x^i} (\psi^\dagger \gamma^0 \gamma^i \psi)$$

Thus  $j^0 = \psi^\dagger \psi$  and  $j^i = \psi^\dagger \gamma^0 \gamma^i \psi$ . Thus  $j^\mu = \bar{\psi} \gamma^\mu \psi$  is a conserved current.

8. **Spin 4-vector:** Define  $s^\mu = (0, \vec{s})$  in the rest frame of the particle. This is the usual spin. Then the general 4-vector is defined by LT of this:  $s'^\mu = a^\mu_\nu s^\nu$ . Another way (more formal) Define  $W^\mu = \epsilon^{\mu\nu\sigma\rho} P_\nu J_{\sigma\rho}$ . For a massive particle this is  $m_0 s^\mu$  where  $s$  is a  $s$  defined above. (Note:  $\epsilon^{ijk} J_{jk} = J^i$ ).

Note that  $p_\mu s^\mu = 0$  in the rest frame and hence in all frames. It is also manifest that  $p_\mu W^\mu = 0$ .

9. Can construct explicit solutions of Dirac equation corresponding to moving particles by boosting the rest frame solutions.

Finite  $S = e^{i\omega^{\mu\nu}\sigma_{\mu\nu}}$ . We use  $\omega = \omega^{01}$  for finite LT. What is this parameter physically? Try on 4-vectors

$$e^{i\omega M} = \begin{bmatrix} \cosh \omega & -\sinh \omega & 0 & 0 \\ -\sinh \omega & \cosh \omega & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

This is obtained by exponentiating  $M$  defined by  $\delta x^0 = \epsilon M x = -\epsilon x^1$  and  $\delta x^1 = -\epsilon x^0$ .

$$M = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Thus  $\tanh \omega = \beta = \frac{v}{c}$  and  $\cosh \omega = \gamma = \frac{1}{\sqrt{1-\beta^2}}$ . Also

$$\sigma_{01} = \frac{i}{4} \begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}$$

$S = e^{2i\omega\sigma_{01}}$ . Note:  $\sigma_{01}^2 = I$  Thus

$$S = \cosh \frac{\omega}{2} \begin{bmatrix} 1 & 0 & 0 & -\tanh \frac{\omega}{2} \\ 0 & 1 & -\tanh \frac{\omega}{2} & 0 \\ 0 & -\tanh \frac{\omega}{2} & 1 & 0 \\ -\tanh \frac{\omega}{2} & 0 & 0 & 1 \end{bmatrix}$$

10. Express in terms of  $p, E$  etc: (Note:  $\sin i\theta = i\sinh \theta$ ,  $\cos i\theta = \cosh \theta$ ) Use  $\tanh x = \frac{2\tanh \frac{x}{2}}{\tanh^2 \frac{x}{2} + 1}$  and invert to get  $\tanh \frac{\omega}{2} = \frac{\tanh \omega}{1 + \sqrt{1 - \tanh^2 \omega}} = \frac{\beta}{1 + \frac{1}{\gamma}} = \frac{p}{E + m_0}$ . and  $\cosh \frac{\omega}{2} = \sqrt{\frac{E + m_0}{2m_0}}$ .

Use this in the matrix and get

$$\psi(x, t) = \sqrt{\frac{E + m_0}{2m_0}} \begin{bmatrix} 1 & 0 & 0 & \frac{-p}{E + m_0} \\ 0 & 1 & \frac{-p}{E + m_0} & 0 \\ 0 & \frac{-p}{E + m_0} & 1 & 0 \\ \frac{-p}{E + m_0} & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} e^{-i(Et - px)}$$

$$= \sqrt{\frac{E + m_0}{2m_0}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ \frac{-p}{E+m_0} \end{bmatrix} e^{-i(Et-px)}$$

Note the presence of large and small components of the spinor. Similarly we get three other solutions including 2 negative energy ones.