12.1.2011

• Quantum Field Theory :-

→ It is a technique to deal with a system of many particles.

- In particular, this technique is essential when, the number of particles, is not conserved.
  - For example in a photon gas, the number of photons is not conserved.
  - For example, the number of electrons, is <u>not conserved</u> in high energy. $e^{(-)}$, $e^{(+)}$ pairs are created. Then, we need quantum field theory.
- It is also a convenient tool, when the, number of particles is large, but <u>conserved</u>.

- We begin with a system, where the, number of particles, is conserved.
  - Let us first consider the simplest possible system :-
    A single (3-D) particle moving in some potential $V(\vec{r})$.

The Schrödinger equation is :-

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{h}\psi \text{ ; where } \hat{h} \text{ is the Hamiltonian operator and } \hat{h} \equiv -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}).$$

Suppose, we want to find a general solution.
We want to find the eigenstates of $\hat{h}$ and then put in the time-evolution.

- Eigenstates of $\hat{h}$:-

The eigenvalue equation is :-

$\hat{h}\, u_n(\vec{r}) = e_n u_n(\vec{r})$; where $u_n(\vec{r})$ are the eigenfunctions and 'e_n' are the eigenvalues.

$\{u_n(\vec{r})\}$ forms a complete basis of states.

It comes out that, we can write a general solution of the Schrödinger equation as:-

$$\psi(\vec{r},t) = \sum_n a_n(t)\, u_n(\vec{r}) \text{ ; where } a_n(t) = a_n(0) e^{-i e_n t/\hbar}$$

Thus, $\psi(\vec{r},t)$ is written as a linear combination of the basis states, only with the coefficients having a certain time dependence.

- Now, let us take, instead of one-particle, 'N'- identical bosonic (non-interacting) particles, moving under the same potential.

Let us denote the i^{th} particle's coordinates by :-

$\vec{r}_i \equiv (x_i, y_i, z_i)$

and $\vec{\nabla}_i \equiv \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i}\right)$ being the gradient operator for the i^{th} particle's coordinates.

Then, a generic wave function will be described by N- of these coordinates, viz.,

$\psi(\vec{r}_1, \vec{r}_2, \ldots\ldots, \vec{r}_N, t)$, and this follows the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N, t) = \hat{h}_{(N)}\psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N, t),$$

where $\hat{h}_{(N)} = \sum_{i=1}^{N} \hat{h}_i$ and $\hat{h}_i = -\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{r}_i)$

• Now, if the particles are identical, the wave function should be symmetric for bosons and antisymmetric for fermions under the exchange of two particles.

So, here, $\psi(\vec{r}_1, \cdots, \vec{r}_N, t)$ is symmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

We are now to introduce a basis of N-particle states which will be suitable for the evolution of a wave-function like this.

We write the basis of states as:-

$$u_{\{m_1, \cdots, m_N\}}(\vec{r}_1, \cdots, \vec{r}_N) = u_{m_1}(\vec{r}_1)\, u_{m_2}(\vec{r}_2) \cdots u_{m_N}(\vec{r}_N).$$

But this is not a proper choice of a basis, as, we want a function which should be symmetric under the exchange of any two particles → clearly the above function does not satisfy this.

The basis should, therefore, be also symmetric under the exchange of particles.

Thus, we add to this all terms with permutations of $\vec{r}_1, \cdots, \vec{r}_N$, and we write:-

$$u_{\{m_1, \cdots, m_N\}}(\vec{r}_1, \cdots, \vec{r}_N) = \frac{1}{\sqrt{N!}}\{u_{m_1}(\vec{r}_1)\, u_{m_2}(\vec{r}_2) \cdots u_{m_N}(\vec{r}_N) + u_{m_1}(\vec{r}_2)\, u_{m_2}(\vec{r}_1) \cdots u_{m_N}(\vec{r}_N) + \cdots \cdots (N! - \text{factorial terms})\}.$$

We have also made it automatically symmetric under the exchange of n_i's instead of just the $\vec{\pi}_i$'s.

For example, $U_{\{1,2\}} = U_{\{2,1\}}$. We should not count them separately.

- We want to check the normalisation of this function:-

Now, $\int d^3\pi_1 \ldots d^3\pi_N \, U^*_{\{n_1,\ldots,n_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N) U_{\{n_1,\ldots,n_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N)$.

We will assume that the single particle wave functions are normalised to 1, i.e.

$$\int d^3\pi \, U^*_m(\vec{\pi}) U_n(\vec{\pi}) = \delta_{mn}$$

[orthonormal basis states].

- Let us first consider that $\{n_1,\ldots,n_N\}$ are all different.

Then the value of the integral will be:-

$\frac{1}{\sqrt{N!}} \cdot \frac{1}{\sqrt{N!}} \times N! = 1$ [The cross terms like,

$U^*_{n_1}(\vec{\pi}_1) U^*_{n_2}(\vec{\pi}_2) \cdots U^*_{n_N}(\vec{\pi}_N)$

$\times U_{n_1}(\vec{\pi}_2) U_{n_2}(\vec{\pi}_1) \cdots U_{n_N}(\vec{\pi}_N)$

will be zeroes].

- Now, suppose, some of the indices (n_i's) are the same. We use something called an Occupation Number Representation.

To see how many n_i's are 1, i.e. how many U_1's, then we see how many n_i's are 2, then how many n_i's are 3 and so on.

Let, "m_1" of the n_i's be 1.
Let, "m_2" of the n_i's be 2.
and so on.....

We have, $\sum_i m_i = N$.

Example:- $m_1 = 1$, $m_2 = 0$, $m_3 = 1$, all others are zeroes.

$$\text{Then, } u(\vec{\pi}_1, \vec{\pi}_2) = \frac{1}{\sqrt{2!}} [u_1(\vec{\pi}_1) u_3(\vec{\pi}_2) + u_1(\vec{\pi}_2) u_3(\vec{\pi}_1)]$$

Here $n_1 = 1$
$n_2 = 3$

The function is normalised.

Example:- $m_1 = 2$, $m_2 = m_3 = \cdots = 0$.

$$\text{Then, } u(\vec{\pi}_1, \vec{\pi}_2) = \frac{1}{\sqrt{2!}} [u_1(\vec{\pi}_1) u_1(\vec{\pi}_2) + u_1(\vec{\pi}_2) u_1(\vec{\pi}_1)]$$

$$= \sqrt{2}\, u_1(\vec{\pi}_1) u_1(\vec{\pi}_2)$$

This state is clearly not normalised.

We will try to find the norm of a state like this by using the occupation number representation.

If some of the m_i's are > 1, then some of the terms are identical in $\{\ \}$.

There will be $(m_1!\, m_2! \cdots)$ identical terms.
If we permute these (m_1) times, we get the same term.
So, altogether, there are $\frac{N!}{m_1! m_2! \cdots}$ different terms.

So, the structure of,

$$U_{\{m_1,\ldots,m_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N) = \frac{1}{\sqrt{N!}}(m_1!\,m_2!\cdots)[T_1+T_2+\cdots+T_p],$$

where $p = \dfrac{N!}{m_1!\,m_2!\cdots}$,

$$T_1 = \{u_1(\vec{\pi}_1)\,u_1(\vec{\pi}_2)\cdots u_1(\vec{\pi}_{m_1}) \times u_2(\vec{\pi}_{m_1+1})\cdots u_2(\vec{\pi}_{m_1+m_2}) \times u_3(\vec{\pi}_{m_1+m_2+1})\cdots\}$$

$T_2, T_3, \ldots$ are obtained from "T_1" by inequivalent permutations of $(\vec{\pi}_1,\ldots,\vec{\pi}_N)$.

If, we permute any of the $\vec{\pi}_1$ to $\vec{\pi}_m$ terms, we get the same term. There are thus $(m_1!)$ of such terms.

If we permute $\vec{\pi}_1$ with $\vec{\pi}_{m+1}$, we will get a separate term.

In our example, $m_1 = 2$, $m_2 = m_3 = \cdots = 0$,

then $p = \dfrac{2!}{2!} = 1$

$m_1! = 2!$

and we get our previous result.

It is now easy to calculate the norm,

$T_1^* T_1 = 1$; $T_2^* T_2 = 1$,

$T_1^* T_2 = 0$ [for one of the $\vec{\pi}_i$'s, at least, the $u(\vec{\pi}_i)$ will be different].

$$\therefore \int d^3\pi_1 \cdots d^3\pi_N\, U^*_{\{n_1,\ldots,n_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N)\, U_{\{n_1,\ldots,n_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N)$$

$$= \frac{1}{N!}(m_1!\,m_2!\cdots)^2\left[1+1+\cdots\left[\frac{N!}{m_1!\,m_2!\cdots}\text{ terms}\right]\right]$$

$$= \frac{1}{N!}(m_1! m_2! \cdots)^2 \cdot \frac{N!}{(m_1! m_2! \cdots)}$$

$$= (m_1! m_2! \cdots)$$

We do not choose a normalised state for this. For the previous case, we had the norm = 1.

- How does the Hamiltonian act on these basis states ?

The 'N'- particle Hamiltonian is given by :-

$$\hat{h}_{(N)} = \sum_{i=1}^{N} \hat{h}_i \; ; \text{ where } \hat{h}_i = -\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{\pi}_i)$$

Now, $\hat{h}_N u_{\{m_1, m_2, \cdots, m_N\}}(\vec{\pi}_1, \cdots, \vec{\pi}_N)$

$$= \left(\sum_{i=1}^{N} e_{m_i}\right) u_{\{m_1, \cdots, m_N\}}(\vec{\pi}_1, \cdots, \vec{\pi}_N)$$

[$\because$ $\hat{h}_{(N)} u_{m_1}(\vec{\pi}_1) u_{m_2}(\vec{\pi}_2) \cdots u_{m_N}(\vec{\pi}_N)$

$= (e_{m_1} + e_{m_2} + \cdots + e_{m_N}) u_{m_1}(\vec{\pi}_1) \cdots u_{m_N}(\vec{\pi}_N)$

$\hat{h}_{(N)} u_{m_1}(\vec{\pi}_2) u_{m_2}(\vec{\pi}_1) \cdots u_{m_N}(\vec{\pi}_N)$

$= (e_{m_2} + e_{m_1} + \cdots + e_{m_N}) u_{m_1}(\vec{\pi}_2) \cdots u_{m_N}(\vec{\pi}_N)$

So, we take out $\left(\sum_{i=1}^{N} e_{m_i}\right)$ common].

Now, if we use the occupation number representation, then, $\hat{h}_{(N)} u_{\{m_1, \cdots, m_N\}}(\vec{\pi}_1, \cdots, \vec{\pi}_N)$

$$= (m_1 e_1 + m_2 e_2 + \cdots) u_{\{m_1, \cdots, m_N\}}(\vec{\pi}_1, \cdots, \vec{\pi}_N)$$

$$= \left(\sum_{K=1}^{\infty} m_K e_K\right) u_{\{m_1, \cdots, m_N\}}(\vec{\pi}_1, \cdots, \vec{\pi}_N)$$

[$\because$ $\hat{h}_{(N)} u_{m_1}(\vec{\pi}_1) u_{m_2}(\vec{\pi}_2) \cdots u_{m_1}(\vec{\pi}_{m_1}) u_{m_2}(\vec{\pi}_{m_1+1}) \cdots$

$= [e_{1 \cdots (m_1 \text{ times})} + e_{2 \cdots (m_2 \text{ times})} + \cdots]$].

- Let us now consider a different system (leaving aside this system) :-

For every single energy eigenstate, we consider a harmonic oscillator.

Let, for every "u_κ", we introduce a pair of operators $(a_\kappa, a_\kappa^\dagger)$, such that :-

$$[a_\kappa, a_{\kappa'}^\dagger] = \delta_{\kappa\kappa'}$$

$$[a_\kappa, a_{\kappa'}] = [a_\kappa^\dagger, a_{\kappa'}^\dagger] = 0$$

The index "κ" labels the single particle eigenstates.

We also write the Hamiltonian as :-

$$\hat{H} = \sum_\kappa e_\kappa a_\kappa^\dagger a_\kappa$$ [actually, $\sum_\kappa e_\kappa [a_\kappa^\dagger a_\kappa + \frac{1}{2}]$, but we subtract this constant ground state energy].

a_κ, $a_\kappa^\dagger$ are like the annihilation and creation operators.

It is as if the κ^{th} harmonic oscillator has $\hbar\omega_\kappa = e_\kappa$ with ground state energy, $\frac{1}{2}\hbar\omega_\kappa$ removed (subtracted).

Let us consider an electron in a coulombic potential and we introduce a harmonic oscillator with a frequency such that $e_\kappa = \hbar\omega_\kappa$.

- Goal :- Show that this system is equivalent to the earlier system, if we identify :-

$$u_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N) \leftrightarrow a_{n_1}^{\dagger}\ldots a_{n_N}^{\dagger}|0\rangle,$$

where $|0\rangle$ is the direct product of the ground states of the (∞) number of harmonic oscillators.

$|0\rangle$ satisfies,

$$a_k|0\rangle = 0 \text{ for each "k".}$$

All the matrix elements in both the quantum systems should be the same.

① [Here one particle with many frequencies is being mapped to many particles in the previous system].

We can also use the occupation number representation. For this case, it will be:-

$$(a_1^{\dagger})^{m_1}(a_2^{\dagger})^{m_2}\ldots|0\rangle$$

It does not matter in which order they appear as they commute.

• We need to check that the energy eigenvalues must match.

To find:- $\hat{H}\, a_{n_1}^{\dagger} a_{n_2}^{\dagger} \ldots a_{n_N}^{\dagger}|0\rangle$

Now, $[\hat{H}, a_s^{\dagger}] = \left[\sum_k e_k a_k^{\dagger} a_k, a_s^{\dagger}\right]$

$$= [e_s a_s^{\dagger} a_s, a_s^{\dagger}]$$

$$= e_s a_s^{\dagger}$$

$$\therefore \hat{H} a_s^{\dagger} = e_s a_s^{\dagger} + a_s^{\dagger}\hat{H}$$

$$\therefore \hat{H}\, a_{n_1}^{\dagger} a_{n_2}^{\dagger} \ldots a_{n_N}^{\dagger}|0\rangle$$

$$= (e_{n_1} a_{n_1}^{\dagger} + a_{n_1}^{\dagger}\hat{H}) a_{n_2}^{\dagger}\ldots a_{n_N}^{\dagger}|0\rangle$$

$$= e_{n_1} a_{n_1}^{\dagger} a_{n_2}^{\dagger}\ldots a_{n_N}^{\dagger}|0\rangle + a_{n_1}^{\dagger}(e_{n_2} a_{n_2}^{\dagger} + a_{n_2}^{\dagger}\hat{H}) a_{n_3}^{\dagger} \ldots a_{n_N}^{\dagger}|0\rangle$$

$$= (e_{n_1} + e_{n_2} + \ldots + e_{n_N})\, a_{n_1}^{\dagger} a_{n_2}^{\dagger}\ldots a_{n_N}^{\dagger}|0\rangle.$$

If there is $(a_{m_1}^\dagger)^3$, it will count the state 3 times etc. so, the energy eigenvalues match with our previous case.

- We need to check the normalisation, i.e. it has the exact same norm as "U".

Now, we calculate the norm of this state (in either of the two representations).

Let us take the occupation number representation:-

Norm of $(a_1^\dagger)^{m_1} (a_2^\dagger)^{m_2} \cdots |0\rangle$ is:-

$$\langle 0| \cdots (a_2)^{m_2} (a_1)^{m_1} (a_1^\dagger)^{m_1} (a_2^\dagger)^{m_2} \cdots |0\rangle$$

Now, $(a_1)^{m_1} = \underbrace{a_1 \cdots a_1}_{m_1 \text{ times}}$

$$(a_1^\dagger)^{m_1} = \overbrace{a_1^\dagger \cdots a_1^\dagger}$$

$$\therefore (a_1)^{m_1} \cdot (a_1^\dagger)^{m_1} = (a_1)^{m_1-1} a_1 a_1^\dagger (a_1^\dagger)^{m_1-1}$$

Again, $[a_1, a_1^\dagger] = 1$

$$\therefore a_1 a_1^\dagger = 1 + a_1^\dagger a_1$$

Now, $\langle 0| a_1^2 (a_1^\dagger)^2 |0\rangle$

$$= \langle 0| a_1 \cdot a_1 \cdot a_1^\dagger \cdot a_1^\dagger |0\rangle$$

$$= \langle 0| a_1 \cdot (1 + a_1^\dagger a_1) a_1^\dagger |0\rangle$$

$$= \langle 0| a_1 a_1^\dagger |0\rangle + \langle 0| a_1 a_1^\dagger a_1 a_1^\dagger |0\rangle$$

$$= \langle 0| a_1 a_1^\dagger |0\rangle + \langle 0| a_1 a_1^\dagger (1 + a_1^\dagger a_1) |0\rangle$$

$$= \langle 0| a_1 a_1^\dagger |0\rangle + \langle 0| a_1 a_1^\dagger |0\rangle + \langle 0| a_1 a_1^\dagger a_1^\dagger a_1 |0\rangle$$

[Again $a_1|0\rangle = 0$].

$$= 2 \langle 0| a_1 a_1^\dagger |0\rangle = 2 \langle 1|1\rangle = 2$$

In the same way, $(a_1)^{m_1} \cdot (a_1^\dagger)^{m_1}$ gives $m_1(m_1-1) \cdots 1 = m_1!$

Similarly, for $(a_2)^{m_2}(a_2^\dagger)^{m_2}$

gives $m_2!$

Thus, we will get, $m_1! m_2! \cdots$ which is the final result.

check :- $\langle 0|(a_2)^2 (a_1)(a_1^\dagger)(a_2^\dagger)^2|0\rangle$

$= \langle 0|(a_2)(a_2)[1 + a_1^\dagger a_1](a_2^\dagger)(a_2^\dagger)|0\rangle$

$= \langle 0| a_2 \cdot a_2 \cdot a_2^\dagger \cdot a_2^\dagger |0\rangle$

$+ \langle 0| a_2 \cdot a_2 \cdot a_2^\dagger \cdot a_2^\dagger \cdot a_1^\dagger \cdot a_1 |0\rangle$ → 0

[$\because [a_2, a_1^\dagger] = 0$ etc.].

$= \langle 0| a_2 (1 + a_2^\dagger a_2) a_2^\dagger |0\rangle$

$= \langle 0| a_2 a_2^\dagger |0\rangle + \langle 0| a_2 a_2^\dagger a_2 a_2^\dagger |0\rangle$

$= \langle 0| a_2 a_2^\dagger |0\rangle + \langle 0| a_2 a_2^\dagger (1 + a_2^\dagger a_2)|0\rangle$

$= 2\langle 0| a_2 a_2^\dagger |0\rangle + \langle 0| a_2 a_2^\dagger a_2^\dagger a_2 |0\rangle$ → 0

$= 2$.

- Thus, here we do not have to worry about symmetrising the wave functions, as there are no $\vec{r}_i$'s.

The above formalism only works for bosons (& is distinguishable).

Here, in this system, the eigenvalues and the norm shows us that the particles are indistinguishable.

In this system, the total number of particles were nowhere specified.

The total number of particles is the sum of m_i's.

The ground state will map to a zero-particle state, total $m_i = 0$.

For the first excited state, total $m_i = 1$.

$(a_1^\dagger)^2 \approx u_1(\vec{\pi}_1')\, u_1(\vec{\pi}_2')$ (with the normalisation constant $\sqrt{2}$).

In the original system, we have to fix "N", here we do not have to.

If our quantum system is such that the particle number is not conserved, it goes through.

For example:-

Photon gas:- The total energy is conserved but the number of particles may change.

In the original system, we can not have a transition of a system of N-particles to a system of (N-1) particles. It will then move us from one Hilbert space to another.

But, in the present system, the Hilbert space allows all such systems.

In the original system, the position operator is an observable. It needs to be seen, how we calculate it in the new system.

$a_1^\dagger |N\text{-particle state}\rangle \approx |(N+1)\text{-particle state}\rangle$.

The number of harmonic oscillators have to do with the number of energy eigenstates (in general ∞).

Let $\hat{H} = \sum_k e_k a_k^\dagger a_k$.

If we add a small perturbation which takes a 2-particle state to a 3-particle state, for example:-

$$\hat{H}' = \sum_k e_k a_k^\dagger a_k + \underbrace{(\lambda a_1^\dagger + \lambda^* a_1)}_{\text{Hermitian.}}$$

it can take a 2-particle state to a 3-particle state or vice versa.

We may as well take the perturbation to be:-
$(a_1^\dagger a_2 + a_3^\dagger a_4 + h.c.)$; where h.c. ≡ Hermitian conjugate. What perturbation we add, depends on the experiment we are performing.

13.1.2011

● **Recap:-**

• A particle in a potential is described by:-

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{h}\psi(\vec{r},t); \text{ where } \hat{h} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})$$

We denoted the eigenstates of this operator by $u_n(\vec{r})$, such that:-

$$\hat{h}u_n(\vec{r}) = e_n u_n(\vec{r})$$

The set $\{u_n(\vec{r})\}$ forms a basis.

• We then considered N- mutually non-interacting identical bosons, each moving in the same potential $V(\vec{r})$.

For this system, the Schrödinger equation takes the form:-

$$i\hbar \frac{\partial \psi(\vec{r}_1, \ldots, \vec{r}_N, t)}{\partial t} = \hat{h}_{(N)}\psi(\vec{r}_1, \ldots, \vec{r}_N, t); \text{ where}$$

$$\hat{h}_{(N)} = \sum_i h_i \text{ and } h_i = -\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{r}_i).$$

The suitable basis of this state can be obtained by taking the direct product of the individual bases and then symmetrising.

We have :-

$$U_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N) = \frac{1}{\sqrt{N!}}\left[u_{n_1}(\vec{r}_1)\ldots u_{n_N}(\vec{r}_N) + \text{all permutations of } \vec{r}_1,\ldots,\vec{r}_N\right].$$

We claimed that this system is equivalent to another system (of infinitely many S.H.O.'s) each corresponding to an energy eigenstate, where the frequency "ω_k" was related to the energy eigenvalue of the previous system by :-

$$e_k = \hbar\omega_k .$$

- claim :- This quantum system is equivalent to another quantum system of infinite number of harmonic oscillators with $\omega_n = \frac{e_n}{\hbar}$ and the Hamiltonian of this system is :-

$$\hat{H} = \sum_{n=1}^{\infty} e_n a_n^{\dagger} a_n ;$$ where $a_n^{\dagger}$ is the creation operator and a_n is the annihilation operator of the n^{th} harmonic oscillator.

These follow the commutator relations as follows :-

$$[a_m, a_n^{\dagger}] = \delta_{mn},$$
$$[a_m, a_n] = 0,$$
$$[a_m^{\dagger}, a_n^{\dagger}] = 0.$$

Even for degenerate eigenstates, we introduce those many harmonic oscillators.

If $V(x) = \frac{1}{2}Kx^2$, then all the e_n's will be different.

This system does not have a knowledge about "N" aforehand.

e_n's are obtained by solving single particle quantum mechanics → they have no knowledge about the n_i's. They only depend on what state we use.

- If two quantum systems have all their matrix elements same, if all the observables have a one-to-one map in the two systems, then the two systems are equivalent.

The Simple Harmonic Oscillators are associated with the u_k's → one simple harmonic oscillator to every energy eigenstate.

The $\hat{x}$ and $\hat{p}$ of this new system created by the combination of $(a, a^\dagger)$ has nothing to do with the $\hat{x}$ and $\hat{p}$ operators of our original system.

[N.B.:- Later, we will think of the wave function as a dynamical variable and obtain $(a, a^\dagger)$ from it.].

We made the claim that:-

$$u_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N) \longleftrightarrow a_{n_1}^\dagger \cdots a_{n_N}^\dagger |0\rangle \equiv |n_1 n_2 \cdots n_N\rangle;$$

where $a_k|0\rangle = 0$ for every "k".

The fact that we have N-creation operators corresponds to the fact that we have an N-particle system.

Let m_1 of the n_i's are 1,
m_2 of the n_i's are 2, and so on.

Those m_i's have nothing (well not really) to do with the new formulation.

The Hamiltonian as such knows nothing about the n_i's as :-

$$\hat{H} = \sum_{n=1}^{\infty} e_n a_n^{\dagger} a_n .$$

We checked that the eigenvalue of $\hat{h}_{(N)}$ and $\hat{H}$ are the same and that is :-

$$\sum_{n=1}^{\infty} e_{n_i}$$

We also checked that :-

$$\int d^3 r_1 \ldots d^3 r_N \, u^{(\vec{r}_1, \ldots, \vec{r}_N)}_{\{n_1, \ldots, n_N\}} \, u^{*}_{\{m_1, \ldots, m_N\}} = \langle m_1 \ldots m_N | n_1 \ldots n_N \rangle .$$

If two quantum systems are the same, they must have the same inner product.

How many particles in the new formulation, we have, depends on the number of $a^{\dagger}$'s we use, while in our original problem, it is there in the hamiltonian.

- The Number operator :-

  It is defined as :-

$$\hat{N} = \sum_{k=1}^{\infty} a_k^{\dagger} a_k$$

Now, $\hat{N} | n_1, n_2 \ldots n_N \rangle$

$$= \sum_k a_k^{\dagger} a_k a_{n_1}^{\dagger} a_{n_2}^{\dagger} \ldots a_{n_N}^{\dagger} | 0 \rangle$$

$$= \sum_k a_k^\dagger [\delta_{k,n_1} + a_{n_1}^\dagger a_k] a_{n_2}^\dagger \cdots a_{n_N}^\dagger |0\rangle$$

$$= \sum_k a_k^\dagger \delta_{k,n_1} a_{n_2}^\dagger \cdots a_{n_N}^\dagger |0\rangle$$

$$+ \sum_k a_k^\dagger a_{n_1}^\dagger [\delta_{k,n_2} + a_{n_2}^\dagger a_k] a_{n_3}^\dagger \cdots a_{n_N}^\dagger |0\rangle$$

$$= a_{n_1}^\dagger \cdots a_{n_N}^\dagger |0\rangle$$
$$+ a_{n_2}^\dagger a_{n_1}^\dagger a_{n_3}^\dagger \cdots a_{n_N}^\dagger |0\rangle$$
$$+ \cdots \text{(N times)}$$
$$= N |n_1 n_2 \cdots n_N\rangle \quad [\because a_{n_2}^\dagger a_{n_1}^\dagger = a_{n_1}^\dagger a_{n_2}^\dagger \ (\because n_1 \neq n_2)].$$

[We had similarly,

$$\sum_{k=1}^{\infty} e_k a_k^\dagger a_k |n_1 \cdots n_N\rangle = \left(\sum_{i=1}^{N} e_{n_i}\right) |n_1 \cdots n_N\rangle$$ [refer page 9.].

- **Other Observables :-**

→ Hermitian operators.

N- particle quantum mechanics.

We have $(\hat{x}_1, \hat{y}_1, \hat{z}_1)$, $(\hat{x}_2, \hat{y}_2, \hat{z}_2)$, $\vdots$, $(\hat{x}_n, \hat{y}_n, \hat{z}_n)$ } as the position operators.

Let us consider the position operator $\hat{x}_1$.

Q:- Does this make a good quantum observable?

Ans:- No. The first particle does not make any sense as the particles are indistinguishable.

But, on the other hand, $\sum_i \hat{x}_i$ is a good quantum observable. This ($\sum_i \hat{x}_i$) is a special case of what is known as a one-body operator, and a general one-body operator (though for an N-particle system), has the following form:-

$$\hat{b}_{(N)} = \sum_{i=1}^{N} \hat{b}_i \quad ; \text{ where } \hat{b}_i = \hat{b}_i(\hat{x}_i, \hat{y}_i, \hat{z}_i, \hat{p}_{x_i}, \hat{p}_{y_i}, \hat{p}_{z_i});$$

where $\hat{p}_{x_i} = -i\hbar \frac{\partial}{\partial x_i}$; $\hat{p}_{y_i} = -i\hbar \frac{\partial}{\partial y_i}$ and $\hat{p}_{z_i} = -i\hbar \frac{\partial}{\partial z_i}$.

These are not particularly general, but, they are of a certain class (each element in the sum depends on the coordinates and momenta of one particle).

Thus, $\sum_{i=1}^{N} \sum_{j=1}^{N} \hat{p}_i \hat{p}_j$ is not a one-body operator.

We want to calculate,

(L.H.S.) $\int d^3r_1 \cdots d^3r_N \, U_{\{n_1, \ldots, n_N\}}^{(\vec{r}_1, \ldots, \vec{r}_N)*} \hat{b}_{(N)} U_{\{n_1', \ldots, n_N'\}}^{(\vec{r}_1, \ldots, \vec{r}_N)}$

If we say that there is an exact map with the new formulation, the matrix elements must match.

- Problem:- Find an operator $\hat{B}$, such that the matrix element of this is equal to :-

(R.H.S.) $\langle n_1, \ldots, n_N | \hat{B} | n_1', \ldots, n_N' \rangle$.

We define, $\hat{B} = \sum_k \sum_l b_{kl} \, a_k^\dagger a_l$;

where $b_{kl} = \int d^3r_1 \, u_k^*(\vec{r}_1) \, b_1 \, u_l(\vec{r}_1)$

We just have to calculate the 3D-integrals.

We can do them by manipulating the u_k's and the u_k^*'s by combinations of $a, a^\dagger$'s.

We will try to establish that the :-

L.H.S. = R.H.S.

Now, $R.H.S. = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} b_{kl} \langle 0 | a_{n_1} \cdots a_{n_N} a_k^\dagger a_l a_{n_1'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$= \sum_{k,l=1}^{\infty} b_{kl} \langle 0 | a_{n_1} \cdots [\delta_{n_N,k} + a_k^\dagger a_{n_N}] \cdot [\delta_{n_1',l} + a_{n_1'}^\dagger a_l] a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$= \sum_{k,l=1}^{\infty} b_{kl} \delta_{k,n_N} \delta_{l,n_1'} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \delta_{k,n_N} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_1'}^\dagger a_l a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \delta_{l,n_1'} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_k^\dagger a_{n_N} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_k^\dagger a_{n_N} a_{n_1'}^\dagger a_l a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$= \sum_{k,l=1}^{\infty} b_{kl} \delta_{k,n_N} \delta_{l,n_1'} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \delta_{k,n_N} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_1'}^\dagger [\delta_{l,n_2'} + a_{n_2'}^\dagger a_l] a_{n_3'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \delta_{l,n_1'} \langle 0 | a_{n_1} \cdots [\delta_{k,n_{N-1}} + a_k^\dagger a_{n_{N-1}}] a_{n_N} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$+ \sum_{k,l=1}^{\infty} b_{kl} \langle 0 | a_{n_1} \cdots a_{n_{N-2}} [\delta_{k,n_{N-1}} + a_k^\dagger a_{n_{N-1}}] a_{n_N} a_{n_1'}^\dagger [\delta_{l,n_2'} + a_{n_2'}^\dagger a_l] \cdot a_{n_3'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$= \sum_{k,l=1}^{\infty} \sum_{i=1}^{N} \sum_{j=1}^{N} b_{kl} \delta_{k,n_i} \delta_{l,n_j'} \boxed{\langle 0 | a_{n_1} \cdots \not{a}_{n_i} \cdots a_{n_N} a_{n_1'}^\dagger \cdots \not{a}_{n_j'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle}$

Where $\not{a}_{n_i}$ means a_{n_i} is missing and $\not{a}_{n_j'}^\dagger$ means $a_{n_j'}^\dagger$ is missing.

Here we have used the fact that $[a_{n_i}, a_k^\dagger] = \delta_{n_i,k}$

Thus, R.H.S. $= \sum_{i=1}^{N}\sum_{j=1}^{N} b_{n_i,n_j} \langle 0 | a_{n_1} \cdots \not{a}_{n_i} \cdots a_{n_N} a^\dagger_{n_1} \cdots \not{a}^\dagger_{n_j} \cdots a^\dagger_{n_N} | 0 \rangle$

• We define in general, the kronecker delta as:-

$$\delta(p_1, \ldots, p_n; \alpha_1, \ldots, \alpha_n) \equiv \delta_{p_1\alpha_1}\delta_{p_2\alpha_2}\cdots\delta_{p_n\alpha_n} + \text{all permutations of } \alpha_1, \ldots, \alpha_n.$$

• For example, $\delta(p_1, \alpha_1; p_2, \alpha_2) = \delta_{p_1\alpha_1}\delta_{p_2\alpha_2} + \delta_{p_1\alpha_2}\delta_{p_2\alpha_1}$.
We can, very well, generalise this to higher terms.

So, in terms of this, the matrix element (the part in the box), can be given by a simple expression:-

$$\delta(\alpha_1, \ldots, \not{\alpha}_i, \ldots, \alpha_N; n_1', \ldots, \not{n}_j', \ldots n_N').$$

Let us consider:-

$\langle 0 | a_{p_1} \cdots a_{p_n} a_{\alpha_1}^\dagger \cdots a_{\alpha_n}^\dagger | 0 \rangle$

We start pushing the a's towards the right.

First, we push a_{p_n}. This will pick up a commutator with $a_{\alpha_n}^\dagger$, and then we push $a_{p_{n-1}}$ which picks up a commutator with $a_{\alpha_{n-1}}^\dagger$. But, a_{p_n} could have picked up a commutator with any other $a_{\alpha_i}^\dagger$.

• For example:- $\langle 0 | a_{p_1} a_{p_2} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger | 0 \rangle$

$$= \langle 0 | a_{p_1} [\delta_{p_2,\alpha_1} + a_{\alpha_1}^\dagger a_{p_2}] a_{\alpha_2}^\dagger | 0 \rangle$$

$$= \langle 0 | a_{p_1} \delta_{p_2,\alpha_1} a_{\alpha_2}^\dagger | 0 \rangle + \langle 0 | a_{p_1} a_{\alpha_1}^\dagger a_{p_2} a_{\alpha_2}^\dagger | 0 \rangle$$

$$= \delta_{p_2,\alpha_1} \langle 0 | a_{p_1} a_{\alpha_2}^\dagger | 0 \rangle + \langle 0 | a_{p_1} a_{\alpha_1}^\dagger [\delta_{p_2,\alpha_2} + a_{\alpha_2}^\dagger a_{p_2}] | 0 \rangle$$

$$= \delta_{p_2,\alpha_1} \langle 0 | [\delta_{p_1,\alpha_2} + a_{\alpha_2}^\dagger a_{p_1}] | 0 \rangle + \langle 0 | [\delta_{p_1,\alpha_1} + a_{\alpha_1}^\dagger a_{p_1}] | 0 \rangle \delta_{p_2,\alpha_2} + \langle 0 | a_{p_1} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \not{a}_{p_2}^{\,0} | 0 \rangle$$

$= \delta_{p_2,q_1}\delta_{p_1,q_2} + \delta_{p_1,q_1}\delta_{p_2,q_2}$

$\therefore$ our claim is that :-

$$\langle 0 | a_{p_1} \cdots a_{p_N} a_{q_1}^\dagger \cdots a_{q_N}^\dagger | 0 \rangle = \delta_{(p_1,\ldots,p_N),(q_1,\ldots,q_N)}$$

$\therefore$ We write, the R.H.S. matrix element $= \sum_{i=1}^{N}\sum_{j=1}^{N} b_{n_i,n_j'}\, \delta_{(n_1,\ldots,\not{n_i},\ldots,n_N;\, n_1',\ldots,\not{n_j'},\ldots,n_N')}$

Now, L.H.S. $= \int d^3r_1 \cdots d^3r_N\, u^{*}_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N)\, \hat{b}_{(N)}\, u_{\{n_1',\ldots,n_N'\}}(\vec{r}_1,\ldots,\vec{r}_N)$

Now, $u_{\{n_1',\ldots,n_N'\}}(\vec{r}_1,\ldots,\vec{r}_N)$ is a function which by construction is completely symmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j"). Again, $\hat{b}_{(N)}$ is also symmetric under the exchange of any two particles.

So, $\hat{b}_{(N)}\, u_{\{n_1',\ldots,n_N'\}}(\vec{r}_1,\ldots,\vec{r}_N)$ is completely symmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

Again, $u_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N) = \frac{1}{\sqrt{N!}}\{ u_{n_1}(\vec{r}_1)\cdots u_{n_N}(\vec{r}_N)$ + all permutations of $\vec{r}_i$'s$\}$

This term is also symmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

So instead of calculating the $(N!)$ integrals separately, we perform only the first and multiply the whole by $(N!)$ as each of these integrals gives us the same value because of symmetry under $\vec{r}_i \leftrightarrow \vec{r}_j$.

So, we write the L.H.S. $=$

$$\int d^3r_1 \cdots d^3r_N \times N! \cdot \frac{1}{\sqrt{N!}} u_{m_1}(\vec{r}_1)^* \cdots u_{m_N}(\vec{r}_N)^* \Big(\sum_{i=1}^{N} \hat{b}_i\Big) \cdot \frac{1}{\sqrt{N!}} \sum_P u_{m_{P(1)}'}(\vec{r}_1)\cdots u_{m_{P(N)}'}(\vec{r}_N);$$

where $\sum_P$ is the sum over all permutations of $1,\ldots,N$.

$P(i)$ is the i^{th} entry in the i^{th} position of the permutation.

• For example:- $N = 3$

1	2	3
1	3	2
2	3	1
2	1	3
3	1	2
3	2	1

For the first term, $P(1) = 1 \quad P(2) = 2, \; P(3) = 3$

For the second term, $P(1) = 1, \; P(2) = 3, \; P(3) = 1$

and so on.

So, we get:-

$$u_{n_1'}(\vec{\pi}_1)\, u_{n_2'}(\vec{\pi}_2)\, u_{n_3'}(\vec{\pi}_3) + u_{n_1'}(\vec{\pi}_1)\, u_{n_3'}(\vec{\pi}_2)\, u_{n_2'}(\vec{\pi}_3) + \cdots$$

Now, we first, pull the sums outside the integrals and write the

$$\text{L.H.S.} = \sum_{i=1}^{N} \sum_{P} \int d^3\pi_i \, u^*_{n_i}(\vec{\pi}_i) \hat{b}_i \, u_{n'_{P(i)}}(\vec{\pi}_i) \prod_{k \neq i} \left(\int d^3\pi_k \, u_{n_k}(\vec{\pi}_k)^* \, u_{n'_{P(k)}}(\vec{\pi}_k) \right)$$

$$= \sum_{i=1}^{N} \sum_{P} b_{n_i, n'_{P(i)}} \prod_{k \neq i} \delta_{n_k, n'_{P(k)}}$$

Now, the R.H.S. $= \sum_{i=1}^{N} \sum_{j=1}^{N} b_{n_i, n_j'} \, \delta_{(n_1, \ldots, \not{n_i}, \ldots, n_N;\, n_1', \ldots, \not{n_j'}, \ldots, n_N')}$

$$\therefore \text{L.H.S.} = \sum_{i=1}^{N} \sum_{j=1}^{N} b_{n_i, n_j'} \left(\sum_{P} \delta_{j, P(i)} \right) \prod_{k \neq i} \delta_{n_k, n'_{P(k)}}$$

Now, $\sum_P \delta_{j,P(i)}$ has $N!$ terms but not all are non-zeroes. They are non-zero only when $j = P(i)$.

Now, when $P(i) = j$, the remaining $(N-1)$ terms can permute in $(N-1)!$ ways. So, there are $(N-1)!$ terms.

$$\left[\sum_{j=1}^{N} b_{n_i, n_j'} \sum_{P} \delta_{j, P(i)} = \sum_{P} b_{n_i, n'_{P(i)}} \right].$$

In the product, there is no n_i (as $k \neq i$), again $n_k = n'_{P(k)}$ and $k \neq i$; thus, $n'_{P(i)} = n_j'$ never appears.

So, $\sum_P \delta_{j,P(i)} \prod_{k \neq i} \delta_{n_k, n'_{P(k)}} = \delta_{(n_1, \ldots, \not{n_i}, \ldots, n_N;\, n_1', \ldots, \not{n_j'}, \ldots, n_N')}$

[This also has $(N-1)!$ terms].

This is how, we map a one-body operator in our original system, to a one-body operator in the harmonic oscillator problem.

- Two-body operator.

$$\hat{V}_N^{(2)} = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v_{i,j}\left(\hat{\vec{r}}_i, \hat{\vec{r}}_j, \hat{\vec{p}}_i, \hat{\vec{p}}_j\right)$$

- Problem:- To find an appropriate operator $\hat{V}$ in the harmonic oscillator problem which corresponds to this.

It will involve two creation and two annihilation operators.

N.B. $u_{\{n_1, \ldots, n_N\}}(\vec{r}_1, \ldots, \vec{r}_N) \leftrightarrow a_{n_1}^{\dagger} \ldots a_{n_N}^{\dagger} |0\rangle$

Now, let $n_1 = 1$, $n_3 = 1$, $n_2 = 2$, $n_4 = 3$, then we write it as:-

$a_1^{\dagger} a_2^{\dagger} a_1^{\dagger} a_3^{\dagger} \ldots |0\rangle$.

- coming back to the two-body operator, we define $\hat{V}$ in the second description as:-

$$\hat{V} = \sum_{k,l,p,q=1}^{\infty} v_{kl,pq}\, a_k^{\dagger} a_l^{\dagger} a_p a_q ;$$

where $v_{kl,pq} = \int d^3r_1 d^3r_2\, u_k^*(\vec{r}_1)\, u_l^*(\vec{r}_2)\, v(\hat{\vec{r}}_1, \hat{\vec{r}}_2, \hat{\vec{p}}_1, \hat{\vec{p}}_2)\, u_p(\vec{r}_1) u_q(\vec{r}_2)$

such that, $\langle n_1 \ldots n_N | \hat{V} | n_1' \ldots n_N' \rangle$

$= \int d^3r_1 \ldots d^3r_N\, u^*_{\{n_1, \ldots, n_N\}}(\vec{r}_1, \ldots, \vec{r}_N)\, \hat{V}_N^{(2)}\, u_{\{n_1', \ldots, n_N'\}}(\vec{r}_1, \ldots, \vec{r}_N)$

$$L.H.S. = \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots a_{n_N} | a_k^\dagger a_l^\dagger a_p a_q | a_{n_1'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$= \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots [\delta_{k,n_N} + a_k^\dagger a_{n_N}] a_l^\dagger a_p [\delta_{q,n_1'} + a_{n_1'}^\dagger a_q] a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$= \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_l^\dagger a_p a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle \delta_{k,n_N} \delta_{q,n_1'}$$

$$+ \sum_{k,l,p,q} \nu_{kl,pq} \delta_{k,n_N} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_l^\dagger a_p a_{n_1'}^\dagger a_q a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$+ \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_k^\dagger a_{n_N} a_l^\dagger a_p a_{n_1'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle \delta_{q,n_1'}$$

$$+ \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_k^\dagger a_{n_N} a_l^\dagger a_p a_{n_1'}^\dagger a_q a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$1st\ term = \sum_{k,l,p,q} \nu_{kl,pq} \langle 0 | a_{n_1} \cdots a_{n_{N-2}} [\delta_{l,n_{N-1}} + a_l^\dagger a_{n_{N-1}}] \cdot [\delta_{p,n_2'} + a_{n_2'}^\dagger a_p] \cdots a_{n_N'}^\dagger | 0 \rangle \cdot \delta_{k,n_N} \delta_{q,n_1'}$$

$$= \sum_{k,l,p,q} \nu_{kl,pq} \delta_{k,n_N} \delta_{q,n_1'} \delta_{l,n_{N-1}} \delta_{p,n_2'} \cdot \langle 0 | a_{n_1} \cdots a_{n_{N-2}} a_{n_3'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$+ \cdots \cdots$$

$$\therefore L.H.S. = \sum_{i,j,a,b\ [i \neq j,\ a \neq b]} \nu_{n_i n_j, n_a' n_b'} \langle 0 | a_{n_1} \cdots \not{a}_{n_i} \cdots \not{a}_{n_j} \cdots a_{n_N} \cdot a_{n_1'}^\dagger \cdots \not{a}_{n_a'}^\dagger \cdots \not{a}_{n_b'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$= \sum_{i,j,a,b\ [i \neq j,\ a \neq b]} \nu_{n_i n_j, n_a' n_b'} \delta(n_1, \cdots, \not{n}_i, \cdots, \not{n}_j, \cdots, n_N; n_1', \cdots, \not{n}_a', \cdots, \not{n}_b', \cdots n_N')$$

$$R.H.S. = \int d^3x_1 \cdots d^3x_N \, u^*_{\{n_1,\ldots,n_N\}}(\vec{x}_1,\ldots,\vec{x}_N)\, \hat{v}_N^{(2)}\, u_{\{n'_1,\ldots,n'_N\}}(\vec{x}_1,\ldots,\vec{x}_N)$$

$$= \int d^3x_1 \cdots d^3x_N \times N! \times \frac{1}{\sqrt{N!}} u^*_{n_1}(\vec{x}_1)\cdots u^*_{n_N}(\vec{x}_N) \sum_{i\neq j=1}^{N} v_{ij}(\hat{\vec{x}}_i, \hat{\vec{x}}_j; \hat{\vec{p}}_i, \hat{\vec{p}}_j)\cdot$$

$$\frac{1}{\sqrt{N!}} \sum_P u_{n'_{P(1)}}(\vec{x}_1)\cdots u_{n'_{P(N)}}(\vec{x}_N)$$

[By the same argument as in page 21.];

where $\sum_P$ is the sum over all permutations of $1,\ldots,N$.

$$\therefore R.H.S. = \sum_{i,j=1}^{N} \sum_P \int d^3x_i\, d^3x_j\, u^*_{n_i}(\vec{x}_i)\, u^*_{n_j}(\vec{x}_j)\, v_{ij}\, u_{n'_{P(i)}}(\vec{x}_i)\, u_{n'_{P(j)}}(\vec{x}_j)\cdot$$

$$\prod_{k\neq i,j}\left(\int d^3x_k\, u_{n_k}(\vec{x}_k)^*\, u_{n'_{P(k)}}(\vec{x}_k)\right)$$

$$= \sum_{i,j=1}^{N} \sum_P v_{n_i n_j, n'_{P(i)} n'_{P(j)}} \prod_{k\neq i,j} \delta_{n_k, n'_{P(k)}}$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{a=1}^{N}\sum_{b=1}^{N} v_{n_i n_j, n'_a n'_b}\left(\sum_P \delta_{a,P(i)}\,\delta_{b,P(j)}\right)\cdot \prod_{k\neq i,j}\delta_{n_k, n'_{P(k)}}$$

$[i\neq j]$. $[a\neq b]$.

Now, $\sum_P \delta_{a,P(i)}\,\delta_{b,P(j)}$ has $(N-2)!$ terms because if we fix a, b, then we have $(N-2)$ places which can be filled in $(N-2)!$ ways.

Now, $\prod_{k\neq i,j}^{N} \delta_{n_k, n'_{P(k)}}$, $n_k \neq n_i$ $[\because k\neq i]$.

and $n_k \neq n_j$ $[\because k\neq j]$.

again $[i\neq j]$

$$n'_{P(k)} \neq n'_{P(i)} = n'_a$$

$$\neq n'_{P(j)} = n'_b.$$

$$\therefore \prod_{k\neq i,j}^{N} \delta_{n_k, n'_{P(k)}} = \delta(n_1,\ldots,\not{n}_i,\ldots,\not{n}_j,\ldots,n_N;\, n'_1,\ldots,\not{n}'_a,\ldots,\not{n}'_b,\ldots,n'_N).$$

Hence, L.H.S. = R.H.S. (proved).

14.1.2011

- We distinguish particles by their position wave functions. Electrons inside a certain volume, for example. We are not making any distinction between the "first" electron and the "second" electron.

  Just like we can ask, how many electrons within a certain energy are there, we can very well ask how many electrons with a specific position wave-function there are.

- [The information of the potential in the first description has gone into the ϵ_n's in the Harmonic oscillator formulation. We must note that here we do not mean an infinite number of Harmonic oscillators moving in a 3-D space. Construction of this second system, depends on the ϵ_n's which clearly depend on $V(\vec{r})$. We have, $\epsilon_n = \hbar\omega_n$, where ω_n is the frequency of the Harmonic oscillator with energy 'ϵ_n'.]

- Two-Body operator:-

$$\hat{V}^{(2)}_{(N)} = \sum_{\substack{i,j=1 \\ i\neq j}}^{N} v(\hat{\vec{r}}_i, \hat{\vec{r}}_j, \hat{\vec{p}}_i, \hat{\vec{p}}_j)$$

To symmetrise it, we have to sum over all $i, j (i \neq j)$. If $i = j$, then it becomes like a one-body operator, which we have already dealt with.

Q:- What is the operator $\hat{V}$ in the second description such that the following holds:-

The matrix elements, $\langle n_1, \ldots, n_N | \hat{V} | n_1', \ldots, n_N' \rangle$

$$= \int d^3r_1 \ldots d^3r_N \, u^*_{\{n_1, \ldots, n_N\}}(\vec{r}_1, \ldots, \vec{r}_N) \hat{V}^{(2)}_{(N)} u_{\{n_1', \ldots, n_N'\}}(\vec{r}_1, \ldots, \vec{r}_N) \; ?$$

If this is the case, we say that the two-body operator $\hat{v}$, gets mapped to $\hat{V}$.

Answer :- $\hat{V} = \sum_{K,l,p,q=1}^{\infty} v_{Kl,pq}\, a_K^\dagger a_l^\dagger a_p a_q$;

where $v_{Kl,pq} = \int d^3\pi_1\, d^3\pi_2\, u_K^*(\vec{\pi}_1)\, u_l^*(\vec{\pi}_2)\, v(\hat{\vec{\pi}}_1, \hat{\vec{\pi}}_2, \hat{\vec{r}}_1, \hat{\vec{r}}_2)\, u_p(\vec{\pi}_1)\, u_q(\vec{\pi}_2)$

where $v(\hat{\vec{\pi}}_1, \hat{\vec{\pi}}_2, \hat{\vec{r}}_1, \hat{\vec{r}}_2)$ is a differential operator.

- N.B. :- If we did not choose the u_n's to be eigenstates of $\hat{h}$, then we would have got cross terms for $\hat{H}$ as well.

- If we simultaneously interchange $K \leftrightarrow l$ and $p \leftrightarrow q$, then $v_{Kl,pq}$ and $\hat{V}$ are symmetric.

- Here we did not assume that $i < j$, but only assumed that $i \neq j$, in the sum.

- Possible application of this two-body operator :- Suppose, we have N-particles, each moving under a potential $V(\vec{r})$, and now, suppose further that each of the particles interact with one another via a potential, $\sum_{\substack{i,j=1 \\ i \neq j}}^{N} v(\hat{\vec{\pi}}_i, \hat{\vec{\pi}}_j, \hat{\vec{r}}_i, \hat{\vec{r}}_j)$. These are no more free particles.

Q :- What is an equivalent description with $(a, a^\dagger)$? Is it possible?

Ans :- Now, to our previous Harmonic oscillator Hamiltonian, we add $\hat{V}$, such that now the new effective Hamiltonian is :-

$$\hat{H} = \sum_K e_K a_K^\dagger a_K + \sum_{K,l,p,q=1}^{\infty} v_{Kl,pq}\, a_K^\dagger a_l^\dagger a_p a_q .$$

We now find the eigenstates of the original formulation. We can find the eigenvalues of this new problem.

• Claim :- The eigenvalues in both the representations should be the same.

Here, in the new representation, the number operator,

$$\hat{N} = \sum_k a_k^\dagger a_k.$$

This operator commutes with the Hamiltonian $\hat{H}$, i.e. $[\hat{N}, \hat{H}] = 0$.

Proof :-

$$[\hat{N}, \hat{H}] = \sum_{m,k} e_k [a_m^\dagger a_m, a_k^\dagger a_k] + \sum_{m,k,l,p,q} V_{kl,pq} [a_m^\dagger a_m, a_k^\dagger a_l^\dagger a_p a_q]$$

Now, $[A, BC] = [A, B]C + B[A, C]$

$$\therefore [a_m^\dagger a_m, a_k^\dagger a_k] = [a_m^\dagger a_m, a_k^\dagger] a_k^\dagger + a_k^\dagger [a_m^\dagger a_m, a_k]$$

Again, $[AB, C] = A[B, C] + [A, C]B$

$$\therefore [a_m^\dagger a_m, a_k^\dagger a_k] = \{a_m^\dagger [a_m, a_k^\dagger] + [a_m^\dagger, \overset{\circ}{a_k^\dagger}] a_m\} a_k + a_k^\dagger \{a_m^\dagger [a_m, \overset{\circ}{a_k}] + [a_m^\dagger, a_k] a_m\}$$

$$= a_m^\dagger \delta_{mk} a_k + a_k^\dagger (-\delta_{mk}) a_m$$

$$= a_m^\dagger a_m - a_m^\dagger a_m = 0$$

$$\therefore [a_m^\dagger a_m, a_k^\dagger a_l^\dagger a_p a_q] = [a_m^\dagger a_m, a_k^\dagger] a_l^\dagger a_p a_q + a_k^\dagger [a_m^\dagger a_m, a_l^\dagger a_p a_q]$$

$$= a_m^\dagger \delta_{mk} a_l^\dagger a_p a_q + a_k^\dagger \{[a_m^\dagger a_m, a_l^\dagger] a_p a_q + a_l^\dagger [a_m^\dagger a_m, a_p a_q]\}$$

$$= a_k^\dagger a_l^\dagger a_p a_q + a_k^\dagger a_m^\dagger \delta_{lm} a_p a_q + a_k^\dagger a_l^\dagger \{[a_m^\dagger a_m, a_p] a_q + a_p [a_m^\dagger a_m, a_q]\}$$

$$\therefore [a_m^\dagger a_m, a_\mu^\dagger a_\lambda^\dagger a_\rho a_\sigma] = 2 a_\mu^\dagger a_\lambda^\dagger a_\rho a_\sigma + a_\mu^\dagger a_\lambda^\dagger (-\delta_{m\rho}) a_m a_\sigma + a_\mu^\dagger a_\lambda^\dagger a_\rho (-\delta_{m\sigma}) a_m$$

$$= 2 a_\mu^\dagger a_\lambda^\dagger a_\rho a_\sigma - 2 a_\mu^\dagger a_\lambda^\dagger a_\rho a_\sigma$$

$$= 0$$

But, we must note that $\hat{N}$ does not commute with any arbitrary Hamiltonian $\hat{H}$. Thus, the above statement is in no sense general. If the number of creation and annihilation operators in both the terms are not equal, then $[\hat{N}, \hat{H}] \neq 0$. In this case, in the first term in $\hat{H}$ (inside the sum), there is one creation and one annihilation operator (each), while in the second term, there are two of each.

Thus, we can always find a Hamiltonian which does not commute with $\hat{N}$.

But, here, we can simultaneously diagonalise $\hat{N}$ and $\hat{H}$. The eigenvalue of $\hat{N}$ will be "N" (the number of particles in the original system). Here, in this new formulation, while writing down the Hamiltonian, we did not incorporate "N" explicitly.

- For example:- If we want solutions with N=19, we only write the Hamiltonian with the states whose eigenvalues with $\hat{N}$ are equal to 19.

- We note that this trick till now nowhere deals with fields.

- We now describe a third quantum system which, we will find out is, equivalent two these two systems.

In this third approach, the meaning of Quantum Field Theory

will become clear.

Let us (again) consider the single particle Schrödinger equation, viz.

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{h}\psi(\vec{r},t) \; ; \text{ where } \hat{h} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}).$$

We now forget about the fact that this $\psi(\vec{r},t)$ describes a quantum state. Let us think that this $\psi(\vec{r},t)$ describes a classical field and that the Schrödinger equation satisfies this. A field is supposed to be a function of $(\vec{r},t)$.

Here, we treat $\psi(\vec{r},t)$ as a classical field and quantise it. This is known as Second Quantisation.

- **Quantum Field Theory / Second Quantisation :-**

Q:- How do we quantise a classical system?

Ans:- We find the canonically conjugate coordinates and momenta of the system. We find the Poisson Brackets and then make them quantum (commutator) brackets.

- **Step 1:-** Find a Lagrangian / Action which upon varying, gives the Schrödinger equation as its classical equation of motion.

Answer :-

$$L = \int d^3r \; \psi^*(\vec{r},t)\left(i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} - \hat{h}\psi(\vec{r},t)\right);$$

here $\hat{h}$ is thought of as an ordinary differential operator.

Q :- What does a Lagrangian do?

Ans :- It takes a field configuration and generates a number at time "t".

The action, $S = \int L\,dt = \int dt\, d^3x\, \psi^*(\vec{x},t)\left(i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} - \hat{h}\psi(\vec{x},t)\right)$.

We extremise this action. The first variation of the action should be zero. We change $\psi \to \psi + \delta\psi$.

$$\therefore \delta S = \int dt\, d^3x\, \delta\psi^*(\vec{x},t)\left(i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} - \hat{h}\,\psi(\vec{x},t)\right)$$

$$+ \int dt\, d^3x\, \psi^*(\vec{x},t)\left\{i\hbar \frac{\partial(\delta\psi(\vec{x},t))}{\partial t} - \hat{h}\,\delta\psi(\vec{x},t)\right\} + O(\delta\psi^*\delta\psi)$$

Here $\psi(\vec{x},t)$ is kind of a trajectory which we vary. We vary it with respect to the field itself.

Here $\psi(\vec{x},t)$ at every $\vec{x}$ is a dynamical variable, "$\vec{x}$" is a continuous variable.

$$\therefore \delta S = \int dt\, d^3x\, \delta\psi^*(\vec{x},t)\left(i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} - \hat{h}\,\psi(\vec{x},t)\right)$$

$$+ \int dt\, d^3x \left\{-i\hbar \frac{\partial \psi^*(\vec{x},t)}{\partial t} - \hat{h}\,\psi^*(\vec{x},t)\right\}\delta\psi(\vec{x},t)$$

[neglecting terms of $O(\delta\psi^*.\delta\psi)$].

$$\left[\because \int dt\, d^3x\, \psi^*(\vec{x},t)\frac{\partial \delta\psi(\vec{x},t))}{\partial t}\right. \qquad \left[\because \frac{\partial}{\partial t}(\psi^*\psi)\right.$$

$$= \int dt\, d^3x \frac{\partial}{\partial t}(\psi^*\delta\psi) - \int dt\, d^3x \frac{\partial\psi^*}{\partial t}\delta\psi \qquad \left.= \left(\frac{\partial\psi^*}{\partial t}\right)\psi + \psi^*\frac{\partial\psi}{\partial t}\right].$$

The first term vanishes at the boundary,

again $\hat{h} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})$,

$\oint \vec{p} \cdot \vec{A}\, d\vec{N} =$

$\therefore \int dt \int d^3r\, (\vec{\nabla}^2 \psi^*)\, \delta\psi$ $\left[\int_V dV \left[A\vec{\nabla}^2 B - B\vec{\nabla}^2 A \right] = \oint_S [A\vec{\nabla}B - B\vec{\nabla}A] \cdot d\vec{S} \right]$.

$= \int dt \int d^3r\, \vec{\nabla} \cdot (\vec{\nabla}\psi^*)\, \delta\psi$ $\left[\int_V dV\, \vec{\nabla} \cdot (A\vec{\nabla}B) = \oint_S A\vec{\nabla}B \cdot d\vec{S} \right.$

$= \int dt\, (\vec{\nabla}\psi^*)\, \delta\psi \Big|_{\text{boundary}} - \int dt\, \vec{\nabla}(\delta\psi) \cdot (\vec{\nabla}\psi^*)\, d^3r$ $\Rightarrow \int_V dV [\vec{\nabla}B \cdot \vec{\nabla}A + B\vec{\nabla}^2 A]$

(The first term vanishes at the boundary). $= \oint_S A\vec{\nabla}B \cdot d\vec{S}$

$= -\int dt\, \psi^* \vec{\nabla}(\delta\psi) \Big|_{\text{boundary}} + \int dt \int d^3r\, \vec{\nabla}^2(\delta\psi)\, \psi^*$ and, $\int_V dV [\vec{\nabla}A \cdot \vec{\nabla}B + A\vec{\nabla}^2 B]$

(The first term vanishes at the boundary). $= \oint_S B\vec{\nabla}A \cdot d\vec{S}$

$= +\int dt \int d^3r\, \psi^* \vec{\nabla}^2(\delta\psi)$ (subtract)].

$\therefore \int dt \int d^3r\, \hat{h}\psi^* (\delta\psi) = +\int dt \int d^3r\, \psi^* \hat{h}(\delta\psi)$].

Again V is scalar, $\therefore \int dt \int d^3r\, \psi^*(\vec{r},t)\, V(\vec{r})\, \delta\psi(\vec{r},t) = \int dt \int d^3r\, (V(\vec{r})\psi^*(\vec{r},t))\, \delta\psi(\vec{r},t)$

We want this to vanish for an arbitrary variation of "ψ^*".

- Useful trick:- We can think of the variations of $(\delta\psi)$ and $(\delta\psi^*)$ as independent (though they are not so) variables. Q:- Why can we treat them so?

[Ans:- Imagine that we have a complex variable "z".

Suppose, we have an equation like,

$F\delta z + F^* \delta z^* = 0$.

What is the consequence?

Let $F = F_1 + iF_2$; $z = z_1 + iz_2$; where F_1, F_2, z_1, z_2 are real functions.

$\therefore (F_1 + iF_2)(\delta z_1 + i\delta z_2) + (F_1 - iF_2)(\delta z_1 - i\delta z_2) = 0$

or $2F_1 \delta z_1 - 2F_2 \delta z_2 = 0$

Now, δz_1 and δz_2 are independent. So, if we vary them, we get $F_1 = 0$, $F_2 = 0 \Rightarrow F = F_1 + iF_2 = 0$.

Thus in this problem, we could have treated (δz) and (δz^*) as independent variables and obtained the same result, i.e. $F = 0$.].

Coming back to our problem, if $\delta S = 0$, then varying $(\delta\psi)$ and $(\delta\psi^*)$ separately gives us the equations :-

$$i\hbar \frac{\partial \psi}{\partial t} - \hat{h}\psi = 0$$

and $$-i\hbar \frac{\partial \psi^*}{\partial t} - \hat{h}\psi^* = 0$$

which are nothing but the Schrödinger equation and its conjugate equation.

Alternatively :- We write $\delta\psi = \delta\psi_1 + i\delta\psi_2$; where $(\delta\psi_1), (\delta\psi_2)$ are real.

The above formulation holds as long as the Hamiltonian is Hermitian.

$$\therefore \delta S = \int dt\, d^3x \{ [\delta\psi_1 - i\delta\psi_2][i\hbar \frac{\partial \psi}{\partial t} - \hat{h}\psi] + [\delta\psi_1 + i\delta\psi_2][-i\hbar \frac{\partial \psi^*}{\partial t} - \hat{h}\psi^*] \}$$

[Here we are using, $\int \psi^* \hat{h}\psi = \int (\hat{h}\psi)^* \psi$. This will work as long as $\hat{h}$ is hermitian].

$$\therefore \delta S = \int dt\, d^3x \{ \delta\psi_1 [i\hbar \frac{\partial \psi}{\partial t} - \hat{h}\psi - i\hbar \frac{\partial \psi^*}{\partial t} - \hat{h}\psi^*] + \delta\psi_2 [\hbar \frac{\partial \psi}{\partial t} + i\hat{h}\psi + \hbar \frac{\partial \psi^*}{\partial t} - i\hat{h}\psi^*] \}$$

[We will treat in many cases as if the field and its complex conjugate are independent variables].

Thus, here taking $\delta S = 0$ and varying $(\delta\psi_1)$ and $(\delta\psi_2)$ independently, we get :-

$$i\hbar \frac{\partial \psi}{\partial t} - \hat{h}\psi - i\hbar \frac{\partial \psi^*}{\partial t} - \hat{h}\psi^* = 0$$

and $$\hbar \frac{\partial \psi}{\partial t} + i\hat{h}\psi + \hbar \frac{\partial \psi^*}{\partial t} - i\hat{h}\psi^* = 0$$

Now, multiplying the second equation by $(-i)$ and adding (subtracting) it to (from) the first equation gives us the

Schrödinger equation (and its complex conjugate).

Now, we replace the continuous index "$\vec{x}$" by a discrete index. We replace it, as we do not always have a good intuition of what these continuous variables actually do.

Suppose $\{u_n(\vec{x})\}$ is a complete basis of states. [It is not necessary to choose these as the eigenstates of $\hat{h}$].
But for simplicity, we do take them to be the eigenstates of $\hat{h}$.
Then, we write :-

$$\psi(\vec{x},t) = \sum_n a_n(t)\, u_n(\vec{x}).$$

We note that $\psi(\vec{x},t)$ has exactly the same information as $a_n(t)$ [which incidentally has a discrete index].

• N.B.:- Free particles have continuous index, which we can discretise by putting them in a box.

We regard the $a_1(t), a_2(t), \ldots$ as the various coordinate variables.

i.e., $a_n(t) \equiv$ coordinate variables.

- A map between classical mechanics (whose basic objects are the trajectories, $q(t)$, the action must be extremised under the variation of these trajectories) and quantum field theory (specifying $\psi(\vec{x},t)$ is equivalent to specifying the $a_n(t)$'s).
The analog of these trajectories $q(t)$'s are these $a_1(t), a_2(t), \ldots$
Thus classical field theory is classical mechanics with infinite number of variables.

• $\psi(\vec{r},t)$, because of its continuous variable "$\vec{r}$" may seem to have an uncountable infinity of basis states but the right hand side shows a countable infinity of basis states. We can always do it. We can always use a normalisable basis.

$a_n(t)$'s functional form is yet unknown.

• Here, we have assumed that the Hamiltonian, $\hat{h}_{(N)}$ is not a function of time, i.e.:-

$$\hat{h}_{(N)} \neq \hat{h}_{(N)}(t).$$

• Let us now write the original action in terms of these $a_n(t)$'s.

$$S = \int dt \int d^3r \; \psi^*(\vec{r},t)\left(i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} - \hat{h}\psi(\vec{r},t)\right)$$

$$= \int dt \int d^3r \sum_k a_k^*(t)\,u_k^*(\vec{r})\left[i\hbar\frac{\partial}{\partial t}\left(\sum_k a_k(t)\,u_k(\vec{r})\right) - \hat{h}\left(\sum_k a_k(t)\,u_k(\vec{r})\right)\right]$$

$$= \int dt \int d^3r \sum_k a_k^*(t)\,u_k^*(\vec{r}) \sum_k \left(i\hbar\frac{\partial a_k(t)}{\partial t} - e_k a_k(t)\right) u_k(\vec{r})$$

(must justify, $\because \hat{h}u_k(\vec{r}) = e_k u_k(\vec{r})$).

We now use the orthonormality of the basis: $\int d^3r\, u_k^*(\vec{r})\,u_k(\vec{r}) = \delta_{kk}$ (i.e. same state)

$$\therefore S = \int dt \sum_k a_k^*(t)\left(i\hbar\frac{\partial a_k(t)}{\partial t} - e_k a_k(t)\right)$$

We think this as a classical system with an infinite number of degrees of freedom.

$\therefore \delta S = 0$, we thus get from the Euler-Lagrange's equations:-

$$i\hbar\frac{\partial a_k(t)}{\partial t} - e_k a_k(t) = 0 \quad \text{and its complex conjugate.}$$

$$\text{or} \quad \frac{da_k(t)}{a_k(t)} = \frac{-ie_k}{\hbar}\,dt$$

Integrating, we get :-

$$\ln a_k(t) = -\frac{i}{\hbar} e_k t + \underbrace{\ln a_k(t=0)}_{\text{constant}}$$

$$\text{or } a_k(t) = a_k(t=0)\, e^{-\frac{i}{\hbar} e_k t}$$

This is clearly a consequence of the equations of motion. We did not assume this form for the $a_k(t)$'s at the beginning.

$$\delta S = \sum_k \int dt\, \delta a_k^*(t) \left\{ i\hbar \frac{\partial a_k(t)}{\partial t} - e_k a_k(t) \right\}$$

$$+ \sum_k \int dt\, a_k^*(t) \left\{ i\hbar \frac{\partial (\delta a_k(t))}{\partial t} - e_k \delta a_k(t) \right\}$$

[We write $\delta a_k^* \cdot a_k = \delta(a_k^* a_k) - a_k^* \delta a_k$].

$$= \sum_k \int dt\, \delta a_k^*(t) \left\{ i\hbar \frac{\partial a_k(t)}{\partial t} - e_k a_k(t) \right\}$$

$$+ \sum_k \int dt \left\{ -\frac{\partial a_k^*(t)}{\partial t} i\hbar - e_k a_k^*(t) \right\} \delta a_k(t)$$

[We drop the boundary terms].

Again, independently varying $\delta a_k(t)$ and $\delta a_k^*(t)$ leads us to the same equations.

The Lagrangian, $L = \sum_k a_k^*(t) \left(i\hbar \dot{a}_k(t) - e_k a_k(t) \right)$

[The correct way to arrive at it is to write it in terms of the real coordinates].

Here the coordinates are the "$a_k(t)$"'s.

Thus, the conjugate momentum to "$a_k(t)$" is :-

$$p_k(t) = \frac{\partial L}{\partial \dot{a}_k(t)} = i\hbar\, a_k^*(t) \quad \left[\because L = \sum_l a_l^*(t) \left(i\hbar \dot{a}_l(t) - e_l a_l(t) \right) \right]$$

$$= \left(i\hbar \sum_l a_l^*(t)\, \delta_{lk} \right).$$

We postulate the Poisson-Bracket relation as :-

$$\{ a_k(t), p_l(t) \}_{P.B.} = \delta_{kl}$$

or $i\hbar \{a_\kappa(t), a_\ell^*(t)\} = \delta_{\kappa\ell}$

The Hamiltonian, $H = \sum_\kappa p_\kappa(t)\dot{a}_\kappa(t) - L$

$$= \sum_\kappa i\hbar\, a_\kappa^*(t)\,\dot{a}_\kappa(t) - \sum_\kappa a_\kappa^*(t)(i\hbar\,\dot{a}_\kappa(t) - e_\kappa a_\kappa)$$
$$= \sum_\kappa e_\kappa a_\kappa^*(t)\, a_\kappa(t)$$

● Now, we quantise.

We replace the "*" by the "†" and we also replace the Poisson-Bracket $\{,\}_{P.B.}$ by the quantum commutator bracket (divided by $(i\hbar)$), $\frac{1}{i\hbar}[,]$.

i.e. we do, $* \longrightarrow \dagger$ and

$$\{,\}_{P.B.} \longrightarrow \frac{1}{i\hbar}[,].$$

These are the rules.

∴ We get :- $\frac{i\hbar}{i\hbar}[a_\kappa, a_\ell^\dagger] = \delta_{\kappa\ell}$

$$\Rightarrow [a_\kappa, a_\ell^\dagger] = \delta_{\kappa\ell}$$

and the Hamiltonian,

$$\hat{H} = \sum_\kappa e_\kappa a_\kappa^\dagger a_\kappa .$$

Now, the Poisson-Bracket, $\{a_\kappa, a_\ell\}_{P.B.} = 0$ (as both are coordinates)

again, $\{a_\kappa^*, a_\ell^*\}_{P.B.} = 0$ .....!

Quantising these, we get :-

$[a_\kappa, a_\ell] = 0$ and $[a_\kappa^\dagger, a_\ell^\dagger] = 0$ respectively.

Thus, we have recovered, exactly the system that we found in the multi-particle mechanics.

Here the "a_κ's" are encoding the same information as "ψ". Thus, these "a_κ's" are the oscillation modes of "ψ".

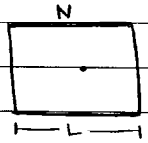
• N.B. :- By construction, this automatically gives us a Bosonic result.

For Fermions, we have to think of another way. At no points the Bosons went into our assumption.

We get multiple Bosons here, not multiple Fermions. Here, in our calculation, we never used any symmetry element.

19.1.2011

• To measure the position of an electron:-



Whatever operator we choose, should be symmetric under the interchange of any two electrons' positions.

Let us choose the heaviside step function,

$$\theta(y) = 0 \quad \text{for } y < 0$$
$$= 1 \quad \text{for } y \geq 0$$

Let us now, consider a function,

$$\theta(x_i)\,\theta(L_x - x_i)\,\theta(y_i)\,\theta(L_y - y_i)\,\theta(z_i)\,\theta(L_z - z_i).$$

This function takes the value 1, when the i^{th} electron lies inside the box with edges L_x, L_y, L_z. Otherwise it gives zero.

Then, we consider the following operator,

$$\sum_{i=1}^{N} \hat{x}_i\,\theta(\hat{x}_i)\,\theta(L_x - \hat{x}_i)\,\theta(\hat{y}_i)\,\theta(L_y - \hat{y}_i)\,\theta(\hat{z}_i)\,\theta(L_z - \hat{z}_i);$$

where now these $\hat{x}_i$, $\hat{y}_i$ and $\hat{z}_i$ are operators.

Let us consider a situation, where there is only one electron in the box, then, if we take the expectation value of this operator in a proper basis, we should get the position eigenvalue.

Let us now consider an array of "N" electrons in space

For simplicity, let us choose the electrons to be having the wave function,

$$\frac{1}{\sqrt{N!}} \{ \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \cdots \psi_N(\vec{r}_N) + \text{all permutations of } \vec{r}_1, \cdots, \vec{r}_N \}.$$

This is an allowed wave function and is completely symmetrical under the interchange of any pair of $\vec{r}_i \leftrightarrow \vec{r}_j$ for any $i, j = 1$ to N.

We, now, introduce a constraint,

$\psi_i(\vec{r}) = 0$ when $\vec{r}$ is inside the box for $i = 2, \cdots, N$.

$\psi_1(\vec{r}) = 0$ when $\vec{r}$ is outside the box

So, let our wave function be of the above form with these above constraints.

The above operator will measure the position.

We want to know what the expectation value of this operator is in this state.

The $i=1$ term (in the operator) will contribute for the first term in the wave function.

The $i=2$ term (i.e. $\vec{r}_2$, associated with ψ_1 now) will contribute for the second term in the wave function, and so on.

We have to chose $\psi_1(\vec{r}_1)$ as the position eigenstate. Till now, we only know that $\psi_1(\vec{r}_1) \neq 0$ when it is inside the box.

We can not ask for it collapsing into the position eigenstate

of the "first" or the "second" electron, etc.

If we take the position eigenstates as $\psi_1(\vec{r}_1)$, $\psi_2(\vec{r}_2)$ etc., then it will remain a position eigenstate.

If the position eigenstate inside the box collapses, it does not mean that the position eigenstates outside the box also collapse.

For each box, we have a different operator as the L's will change.

Here our universe is the whole system. The particle can be anywhere in space, the box (hypothetical) is just a subsystem.

If there are "N" electrons in the system, we have to symmetrise over all the electrons' positions.

We can only restrict a condition on the wave function. We can put a constraint, that to choose a wavefunction where the electrons are inside the box. The wavefunctions outside and inside the box should not overlap. They are either outside or inside. We can distinguish a subsystem by restricting the wave function, not by restricting the identity of the particles.

- Recap:- We took a system of "N" identical, non-interacting bosons, each moving under a potential $V(\vec{r})$.

So, the corresponding Hamiltonian was the sum of the single particle Hamiltonians:-

$$\hat{h}_{(N)} = \sum_{i=1}^{N} \hat{h}_i \quad ; \text{where } \hat{h}_i = -\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{r}_i).$$

We choose the eigenstates as:-

$\hat{h}_{(x)} u_n(\vec{r}) = e_n u_n(\vec{r})$.

Then we found that this system is equivalent to a system of infinite number of harmonic oscillators with a hamiltonian,

$$\hat{H} = \sum_n e_n a_n^\dagger a_n,$$

where $[a_m, a_n^\dagger] = \delta_{mn}$; $[a_m, a_n] = 0$; $[a_m^\dagger, a_n^\dagger] = 0$, are the commutation relations.

We also found that this system allows us to consider different number of particles.

There is a number operator defined as :-

$\hat{N} = \sum_n a_n^\dagger a_n$ and its eigenvalue is "N".

So, this new system can describe quantum mechanical system with multiparticles.

Then we found that this in theory is equivalent to the second quantisation of Schrödinger equation for a single particle.

We take the Schrödinger equation,

$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{h}\psi(\vec{r},t)$; where $\hat{h} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})$ now is an ordinary differential operator.

We now forget what the ψ's are and then treat them as classical fields, functions of $(\vec{r},t)$.

We now write, $\psi(\vec{r},t) = \sum_n a_n(t)\, u_n(\vec{r})$.

The $a_n(t)$'s are like the dynamical coordinate variables.

The equation of motion then takes the form :-

$$i\hbar \frac{da_n(t)}{dt} = e_n a_n(t).$$

Equivalently the Action $= \int dt \left[a_n^* \, i\hbar \frac{da_n(t)}{dt} - \epsilon_n a_n^* a_n \right]$.

We can think these a_n's as an infinite number of variables like the q's.

We have, then, the conjugate momentum,

$$p_n = \frac{\partial L}{\partial \dot{a}_n} = i\hbar a_n^* .$$

We have the classical Poisson-Bracket, $\{ a_m, p_n \}_{P.B.} = 1$, which led (in the quantum theory after quantising) to the commutator relations, $[a_n, a_m^\dagger] = \delta_{mn}$; where these a_n's and $a_n^\dagger$'s are operators in the Heisenberg picture. These would evolve in time.

The equation, $i\hbar \frac{da_n(t)}{dt} = \epsilon_n a_n(t)$ after quantising becomes an operator equation (from the time evolution of the operator).

- Steps for second quantisation:-

(i) Take the Schrödinger equation for a single particle system. [This equation is not invariant under Special Relativity. For relativistic cases it will be replaced by the Klein-Gordon equation. The steps in the quantisation procedure would remain the same though].

(ii) Regard the wave function as a classical field and the Schrödinger equation as the classical equation of motion.

(iii) Then, from here, we construct the Lagrangian and the Hamiltonian which gives us the equation of motion.

(iv) We then quantise this classical field theory (classical system).

This procedure leads to a system which has the ability to describe multiparticle systems which are mutually non-interacting.

If we follow these steps, we get a system for identical bosons, we do not get those for fermions.

- We first traded in the continuous wave functions for the discrete a_n's.
- We now do the manipulations in terms of the functions ψ's itself.
- To see how the different things in the harmonic oscillator formalism look in terms of the wave function formalism.

We have, $[a_n^\dagger(t), a_m^\dagger(t)] = 0 = [a_n(t), a_m(t)]$ and $[a_n, a_m^\dagger] = \delta_{mn}$. These commutation relations are equal time.

- For example, in quantum mechanics, $[q, p] = i\hbar$, where q, p are at the same time "t".

- Now $\psi(\vec{x}, t) = \sum_n a_n(t)\, u_n(\vec{x})$

$\therefore \quad [\psi(\vec{x}, t), \psi(\vec{x}', t)]$

$$= \left[\sum_n a_n(t) u_n(\vec{x}), \sum_m a_m(t) u_m(\vec{x}')\right]$$

$$= \sum_{n,m} [a_n(t), a_m(t)]^{0} u_n(\vec{x}) u_m(\vec{x}') = 0$$

Again, $[\psi^\dagger(\vec{x}, t), \psi^\dagger(\vec{x}', t)]$

$$= \sum_{m,n} [a_m^\dagger(t), a_m^\dagger(t)]^{0} u_n^*(\vec{x}) u_m^*(\vec{x}') = 0$$

Again, $[\psi(\vec{r},t),\ \psi^\dagger(\vec{r}',t)]$

$$= \sum_{m,n} [a_m(t),\ a_m^\dagger(t)]\ u_n(\vec{r})\ u_m^*(\vec{r}')$$

$$= \sum_{m,n} \delta_{mn}\, u_n(\vec{r})\, u_m^*(\vec{r}') = \sum_n u_n(\vec{r})\, u_n^*(\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')$$

[Using completeness of the basis].

We could have considered (before quantising), the $\psi(\vec{r},t)$ as the coordinates, then the $\psi^*(\vec{r},t)$ would be considered as the conjugate momentum.

Now, $\psi(\vec{r},t) = \sum_n a_n(t)\ u_n(\vec{r})$

$$\therefore \int \psi(\vec{r}',t)\, u_n^*(\vec{r}')\, d^3r' = \sum_n a_m(t) \int d^3r'\, u_m(\vec{r}')\, u_m^*(\vec{r}')$$

$$= \int d^3r' \sum_m a_m(t)\, u_m(\vec{r}')\, u_m^*(\vec{r}')$$

$$= \int d^3r'\, \delta_{mn}(\vec{r}-\vec{r}')\, a_m(t)$$

$$= a_n(t)$$

$$\therefore a_n(t) = \int \psi(\vec{r},t)\, u_n^*(\vec{r})\, d^3r'$$

$$\therefore a_n^\dagger(t) = \int u_n(\vec{r}')\, \psi^\dagger(\vec{r}',t)\, d^3r'$$

Now, in terms of a_n's and $a_n^\dagger$'s, the Hamiltonian is:-

$$\hat{H} = \sum_n e_n a_n^\dagger a_n$$

$\therefore$ We now write,

$$\hat{H} = \sum_m e_n \iint d^3r\, d^3r'\, u_n(\vec{r}')\, u_n^*(\vec{r})\, \psi^\dagger(\vec{r}',t)\, \psi(\vec{r},t)$$

$$= \sum_m \iint d^3r\, d^3r'\, u_n(\vec{r}')\, \hat{h}\, u_n^*(\vec{r})\, \psi^\dagger(\vec{r}',t)\, \psi(\vec{r},t)$$

Now, $\hat{h}$ is a Hermitian operator, so integrating by parts twice [$\int \hat{h} u_n^*(\vec{r}) \psi(\vec{r},t) d^3r = \int u_n^*(\vec{r}) \hat{h} \psi(\vec{r},t) d^3r$, with the boundary terms going to zeroes], we get :-

$$\hat{H} = \sum_n \int\int d^3r\, d^3r'\, u_n(\vec{r}')\, u_n^*(\vec{r})\, \psi^\dagger(\vec{r}',t)\, \hat{h}\, \psi(\vec{r},t)$$

[Again, $\sum_n u_n(\vec{r}')\, u_n^*(\vec{r}) = \delta^{(3)}(\vec{r}' - \vec{r})$], we get :-

$$\hat{H} = \int\int d^3r\, d^3r'\, \delta^{(3)}(\vec{r}' - \vec{r})\, \psi^\dagger(\vec{r}',t)\, \hat{h}\, \psi(\vec{r},t)$$

$$\text{or } \hat{H} = \int d^3r\, \psi^\dagger(\vec{r},t)\, \hat{h}\, \psi(\vec{r},t)$$

• N.B. :- 'ψ' is an operator here, so "$\psi^\dagger$" is an operator. In quantum theory, the "ψ's" are the fields. We consider the $a_n(t)$'s and the $a_n^\dagger(t)$'s as the operators while the $u_n(\vec{r})$'s and $u_n^*(\vec{r})$'s are just some functions.

The best way to think of the ψ's is the sum of the linear operators a_n's along with the functions u_n's.

• N.B. :- Here "$\hat{h}$" is a differential operator, not an operator in the quantum theory, these act on the $u_n(\vec{r})$'s in the expansion of $\psi(\vec{r},t) = \sum_n a_n(t)\, u_n(\vec{r})$, the $a_n(t)$'s are the operators, the $u_n(\vec{r})$'s are just ordinary functions.

The Hilbert space operators are the $a_n(t)$'s and the $a_n^\dagger(t)$'s. $\hat{h}$ here is not a Hilbert space operator.

$$\hat{H} = \int d^3r\, \psi^\dagger(\vec{r},t)\, \hat{h}\, \psi(\vec{r},t)$$

Q :- How to interpret this?

Ans :- We first expand the ψ's and then use the completeness of the u_n's using the δ- function and then again land up

to, $\hat{H} = \sum_n e_n a_n^\dagger a_n$ [Here there is no notion of $\hat{n}$, which has become a set of numbers, viz. the e_n's].

- **One-body operator:-**

Q:- Now, if we have a general one-body operator, how to write it in terms of the fields?

Ans:- Let us have a one-body operator in an N-particle Quantum mechanical system, viz.

$\hat{b}(N) = \sum_{i=1}^{N} b(\hat{\vec{\pi}}_i, \hat{\vec{p}}_i)$, where each of the terms in the sum dipend on the coordinates and momentum of one particle.

This operator maps into the harmonic oscillator picture as:-

$\hat{B} = \sum_{m,n} b_{mn} a_m^\dagger a_n$; where $b_{mn} = \int d^3\pi \, u_m^*(\vec{\pi}) b(\hat{\vec{\pi}}, \hat{\vec{p}}) u_n(\vec{\pi})$

Now, we rewrite,

$$\hat{B} = \sum_{m,n} b_{mn} \int\int d^3\pi' d^3\pi'' \, u_m(\vec{\pi}'') u_n^*(\vec{\pi}') \psi^\dagger(\vec{\pi}'', t) \psi(\vec{\pi}', t)$$

$$= \sum_{m,n} \int d^3\pi d^3\pi' d^3\pi'' u_m^*(\vec{\pi}) b(\hat{\vec{\pi}}, \hat{\vec{p}}) u_n(\vec{\pi}) u_m(\vec{\pi}'') u_n^*(\vec{\pi}') \psi^\dagger(\vec{\pi}'', t). \psi(\vec{\pi}', t)$$

$$= \sum_n \int d^3\pi' d^3\pi'' d^3\pi \, b(\hat{\vec{\pi}}, \hat{\vec{p}}) u_n(\vec{\pi}) \left(\sum_m u_m^*(\vec{\pi}) u_m(\vec{\pi}'') \right) u_n^*(\vec{\pi}') \psi^\dagger(\vec{\pi}'', t). \psi(\vec{\pi}', t)$$

$$= \sum_n \int d^3\pi' d^3\pi'' d^3\pi \, b(\hat{\vec{\pi}}, \hat{\vec{p}}) u_n(\vec{\pi}) \delta^{(3)}(\vec{\pi} - \vec{\pi}'') u_n^*(\vec{\pi}') \psi^\dagger(\vec{\pi}'', t) \psi(\vec{\pi}', t)$$

$$= \sum_n \int d^3\pi' d^3\pi \, b(\hat{\vec{\pi}}, \hat{\vec{p}}) u_n(\vec{\pi}) u_n^*(\vec{\pi}') \psi^\dagger(\vec{\pi}', t) \psi(\vec{\pi}'', t)$$

$$= \int d^3\pi' d^3\pi \, b(\hat{\vec{\pi}}, \hat{\vec{p}}) \delta^{(3)}(\vec{\pi} - \vec{\pi}') \psi^\dagger(\vec{\pi}', t) \psi(\vec{\pi}', t)$$

or $\hat{B} = \int d^3x\ \psi^\dagger(\vec{x}, t)\ b(\hat{\vec{x}}, \hat{\vec{p}})\ \psi(\vec{x}, t)$

• N.B. If "ψ" was a Schrödinger wave function, then it is an expectation value of "b" in ψ, ψ^* and we would get :-

$B = \langle \hat{b} \rangle_\psi$.

So the general rule is :- In a quantum expectation value, we replace ψ^* by $\psi^\dagger$, i.e. we change the classical fields to quantum operators and we retrieve our above result.

• Number operator :-

The number operator is given by :-

$\hat{N} = \sum_n a_n^\dagger(t) a_n(t)$ whose eigenvalue is "N".

Now, we replace the a_n's and the $a_n^\dagger$'s.

$\therefore \hat{N} = \sum_n \iint d^3x\, d^3x'\ u_n(\vec{x}')\, u_n^*(\vec{x})\, \psi^\dagger(\vec{x}', t)\, \psi(\vec{x}, t)$

$= \iint d^3x\, d^3x'\ \delta^{(3)}(\vec{x}' - \vec{x})\, \psi^\dagger(\vec{x}', t) \psi(\vec{x}, t)$

$= \int d^3x\ \psi^\dagger(\vec{x}, t)\, \psi(\vec{x}, t)$.

[• N.B. :- Let $|0\rangle$ be the ground state.

Then $a_n|0\rangle = 0$ for all n's.

The states are :-

$(a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \ldots\ldots |0\rangle$ in this harmonic oscillator representation. These are the states in the Hilbert space. These solutions, we do not think as states anymore, these are the explicit functions for the Harmonic oscillator, for

example, we get the Hermite polynomials.

The Hilbert space is spanned by the states of the Harmonic oscillator.

When we write, $\hat{H} = \sum_n e_n a_n^\dagger a_n$, the original Schrödinger equation gives us the e_n's, these are not the Hilbert space states. The Hilbert spaces in both the cases are completely different.

We could have written it as:-

$$\hat{H} = \int \psi^\dagger(\vec{r}, t) \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \psi(\vec{r}, t)\, d^3 r .$$

The original single particle Hilbert space is not the Hilbert space of this system. Here the Hilbert space is much bigger.

If we start with a different basis, the new a_n's will be linear combinations of the old a_n's.

So, instead of using the basis $\{u_n\}$, we could, very well, have used any other basis $\{v_n\}$ or $\{w_n\}$, where

$w_n = \sum_m S_{nm} u_m$, where (S_{nm}) is the $(nm)^{th}$ element of a unitary matrix.

We can still carry out the whole formalism using this basis.

Now, the Hamiltonian in this new basis, will not be diagonal, some other operator might be diagonal in this new basis.

- If, instead of the energy eigenbasis, we use the position eigenbasis, then the a_n's will be replaced by the ψ's.

The relation is :- [$\because \psi(\vec{x}) = \langle \vec{x} | \psi(\vec{x}) \rangle$

$\sum_n u_n^*(\vec{x}) |n\rangle = |\vec{x}\rangle$; where $|n\rangle$ is the energy eigenstate with eigenvalue ϵ_n and $|\vec{x}\rangle$ is the position eigenstate. We think the u_n's as numbers.

So, we can write the $\psi(\vec{x}, t)$ in terms of the position eigenbasis.]

In the classical limit, we obtain our quantum mechanics normalisation, i.e. if we replace the quantum operators by the classical fields, we obtain,

$\int d^3x \; \psi^*(\vec{x}, t) \psi(\vec{x}, t) = 1$ for a single particle quantum system.

For a second quantised system, these ψ's are operators and can have any eigenvalues and can have multiparticle states.

- <u>Two-body operator</u>:-

A two-body operator in the N-particle Hilbert space has the following form:-

$\hat{v}_{(N)} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ i \neq j}}^{N} v(\hat{\vec{x}}_i, \hat{\vec{p}}_i, \hat{\vec{x}}_j, \hat{\vec{p}}_j)$; where each of the terms in the sum depends on the coordinates and momenta of two particles.

In the harmonic oscillator representation, we have:-

$$\hat{V} = \sum_{m,n,p,q} v_{mn,pq}\, a_m^\dagger a_n^\dagger a_p a_q \text{ ; where,}$$

$$v_{mn,pq} = \int d^3\pi_1 d^3\pi_2\; u_m^*(\vec{\pi}_1)\, u_n^*(\vec{\pi}_2)\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, u_p(\vec{\pi}_1)\, u_q(\vec{\pi}_2).$$

So, in terms of the ψ's and $\psi^\dagger$'s,

$$\hat{V} = \int d^3\pi_1 d^3\pi_2\; \psi^\dagger(\vec{\pi}_1, t)\, \psi^\dagger(\vec{\pi}_2, t)\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, \psi(\vec{\pi}_1, t)\, \psi(\vec{\pi}_2, t).$$

Proof:- $\hat{V} = \sum_{m,n,p,q} \int d^3\pi d^3\pi''' d^3\pi_1 d^3\pi_2 d^3\pi' d^3\pi''\; u_m^*(\vec{\pi}_1)\, u_n^*(\vec{\pi}_2)\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, u_p(\vec{\pi}_1)\, u_q(\vec{\pi}_2)\, u_m(\vec{\pi})\, \psi^\dagger(\vec{\pi}, t)\, u_n(\vec{\pi}')\, \psi^\dagger(\vec{\pi}', t)\, u_p^*(\vec{\pi}'')\, \psi(\vec{\pi}'', t)\, u_q^*(\vec{\pi}''')\, \psi(\vec{\pi}''', t)$

$$= \sum_{n,p,q} \int d^3\pi_1 d^3\pi''' d^3\pi_2 d^3\pi' d^3\pi''\; u_n^*(\vec{\pi}_2)\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, u_p(\vec{\pi}_1)\, u_q(\vec{\pi}_2)\, \psi^\dagger(\vec{\pi}_1, t)\, u_n(\vec{\pi}')\, \psi^\dagger(\vec{\pi}', t)\, u_p^*(\vec{\pi}'')\, \psi(\vec{\pi}'', t)\, u_q^*(\vec{\pi}''')\, \psi(\vec{\pi}''', t)$$

$$= \sum_{p,q} \int d^3\pi_1 d^3\pi''' d^3\pi_2 d^3\pi''\; \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, u_p(\vec{\pi}_1)\, u_q(\vec{\pi}_2)\, \psi^\dagger(\vec{\pi}_1, t)\, \psi^\dagger(\vec{\pi}_2, t)\, u_p^*(\vec{\pi}'')\, \psi(\vec{\pi}'', t)\, u_q^*(\vec{\pi}''')\, \psi(\vec{\pi}''', t)$$

$$= \int d^3\pi_1 d^3\pi''' d^3\pi_2 d^3\pi''\; \delta^{(3)}(\vec{\pi}_2 - \vec{\pi}''')\, \delta^{(3)}(\vec{\pi}_1 - \vec{\pi}'')\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, \psi^\dagger(\vec{\pi}_1, t)\, \psi^\dagger(\vec{\pi}_2, t)\, \psi(\vec{\pi}'', t)\, \psi(\vec{\pi}''', t)$$

$$= \int d^3\pi_1 d^3\pi_2\; \psi^\dagger(\vec{\pi}_1, t)\, \psi^\dagger(\vec{\pi}_2, t)\, \hat{v}(\hat{\vec{\pi}}_1, \hat{\vec{p}}_1, \hat{\vec{\pi}}_2, \hat{\vec{p}}_2)\, \psi(\vec{\pi}_1, t)\, \psi(\vec{\pi}_2, t)$$

[Hence proved].

So, now, even in the case of interactions, we can use this formalism.

- So, if the total N-particle Hamiltonian is, $\sum_{i=1}^{N} \hat{h}_i + \hat{v}_{(N)}$, where the $\hat{h}_i$ has some potential "V", and $\hat{v}_{(N)}$ is the interaction between the particles, for example, Coulomb interaction.

The above is the operator in particle mechanics language.

In the harmonic oscillator language on the other hand, the total Hamiltonian is:-

$$\hat{H}_{\text{total}} = \hat{H} + \hat{V}.$$

Now, in terms of $\psi, \psi^\dagger$'s, we have:-

$$\hat{H}_{\text{total}} = \int d^3r\ \psi^\dagger(\vec{r},t)\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right)\psi(\vec{r},t)$$

$$+ \int d^3r_1\, d^3r_2\, \psi^\dagger(\vec{r}_1,t)\psi^\dagger(\vec{r}_2,t)\cdot \hat{v}\left(\hat{\vec{r}}_1, \hat{\vec{p}}_1, \hat{\vec{r}}_2, \hat{\vec{p}}_2\right)\psi(\vec{r}_1,t)\psi(\vec{r}_2,t).$$

- N.B.:- If we can find the exact eigenstates and the exact eigenvalues (i.e. diagonalise), then we can solve the problem exactly. The final Hamiltonian might not look like a Harmonic oscillator form.

$$\hat{H} = \sum_n e_n a_n^\dagger a_n + \sum_{m,n,p,q} v_{mn,pq}\, a_m^\dagger a_n^\dagger a_p a_q.$$

If we can solve this exactly, we can solve in principle, $\sum_{i=1}^{N} \hat{h}_i + \hat{v}_{(ij)}$. If we can not solve exactly, we apply some kind of perturbation theory.

- Try for a time dependent Hamiltonian. Then, we can not expand in the basis of the Hamiltonian.
  We can actually choose any basis.
  We can expand the wavefunction now in the form, $\sum_{mn} f_{mn}(t)\, a_m^\dagger a_n$. Where now, $f_{mn}(t)$ is time

dependent unlike the e_n's.

These a_m's and a_n's are not the same as the old ones. Here, we get cross terms.
The formalism will still go through.

- Once we have developed the second quantised theory and the particle number in our system is not conserved, then we add some other Hermitian term to the existing Hamiltonian like,

$$\sum_{m,n,p} c_{mnp}\, a_m^\dagger a_n^\dagger a_p + \sum_{m,n,p} c^*_{mnp}\, a_p^\dagger a_n a_m .$$

This part clearly does not preserve the particle number.

- <u>One-body operator:-</u>

$$\hat{B} = \sum_{m,n} \int d^3r\, u_m^*(\vec{r})\, b(\hat{\vec{r}}, \hat{\vec{p}})\, u_n(\vec{r})\, a_m^\dagger a_n$$

$$= \int \psi^\dagger(\vec{r},t)\, b(\hat{\vec{r}}, \hat{\vec{p}})\, \psi(\vec{r},t)\, d^3r$$

Now, we try to prove the converse by writing,

$$\psi(\vec{r},t) = \sum_n a_n(t)\, u_n(\vec{r})$$

and $$\psi^\dagger(\vec{r},t) = \sum_m a_m^\dagger(t)\, u_m^*(\vec{r})$$

Plugging these in, we get:-

$$\hat{B} = \sum_{m,n} \int d^3r\, a_m^\dagger(t)\, u_m^*(\vec{r})\, b(\hat{\vec{r}}, \hat{\vec{p}})\, a_n(t)\, u_n(\vec{r})$$

$$= \sum_{m,n} a_m^\dagger(t)\, a_n(t) \int d^3r\, u_m^*(\vec{r})\, b(\hat{\vec{r}}, \hat{\vec{p}})\, u_n(\vec{r})$$

or $\hat{B} = \sum_{m,n} b_{mn}\, a_m^\dagger a_n \quad (\because b_{mn} = \int d^3x\, u_m^*(\vec{x})\, b(\hat{\vec{x}}, \hat{\vec{p}})\, u_n(\vec{x}))$.

- **Two-body operator** :-

$$\hat{V} = \sum_{m,n,p,q} V_{mn,pq}\, a_m^\dagger a_n^\dagger a_p a_q \text{ ; where}$$

$$V_{mn,pq} = \int d^3x_1 d^3x_2\; u_m^*(\vec{x}_1)\, u_n^*(\vec{x}_2)\, \hat{V}(\hat{\vec{x}}_1, \hat{\vec{p}}_1, \hat{\vec{x}}_2, \hat{\vec{p}}_2) \cdot u_p(\vec{x}_1) \cdot u_q(\vec{x}_2)$$

Plugging this in $\hat{V}$, we get :-

$$\hat{V} = \sum_{m,n,p,q} \int d^3x_1 d^3x_2\; u_m^*(\vec{x}_1) u_n^*(\vec{x}_2)\, \hat{V}(\hat{\vec{x}}_1, \hat{\vec{p}}_1, \hat{\vec{x}}_2, \hat{\vec{p}}_2) \cdot u_p(\vec{x}_1) \cdot u_q(\vec{x}_2)\, a_m^\dagger a_n^\dagger a_p a_q .$$

Now, $\sum_m a_m^\dagger u_m^*(\vec{x}_1) = \psi^\dagger(\vec{x}_1, t)$ etc.

$$\therefore \hat{V} = \int d^3x_1 d^3x_2\; \psi^\dagger(\vec{x}_1, t)\, \psi^\dagger(\vec{x}_2, t)\, \hat{V}(\hat{\vec{x}}_1, \hat{\vec{p}}_1, \hat{\vec{x}}_2, \hat{\vec{p}}_2) \cdot \psi(\vec{x}_1, t)\, \psi(\vec{x}_2, t)$$

Now, going in the other way, we write,
$\psi(\vec{x}, t) = \sum_n a_n(t)\, u_n(\vec{x})$ etc. to get :-

$$\hat{V} = \sum_{m,n,p,q} \int d^3x_1 d^3x_2\; a_m^\dagger(t)\, u_m^*(\vec{x}_1)\, a_n^\dagger(t)\, u_n^*(\vec{x}_2) \cdot \hat{V}(\hat{\vec{x}}_1, \hat{\vec{p}}_1, \hat{\vec{x}}_2, \hat{\vec{p}}_2)\, a_p(t)\, u_p(\vec{x}_1)\, a_q(t)\, u_q(\vec{x}_2)$$

$$= \sum_{m,n,p,q} a_m^\dagger(t)\, a_n^\dagger(t)\, a_p(t)\, a_q(t) \int d^3x_1 d^3x_2\; u_m^*(\vec{x}_1) u_n^*(\vec{x}_2) \cdot \hat{V}(\hat{\vec{x}}_1, \hat{\vec{p}}_1, \hat{\vec{x}}_2, \hat{\vec{p}}_2) \cdot u_p(\vec{x}_1)\, u_q(\vec{x}_2)$$

$$= \sum_{m,n,p,q} V_{mn,pq}\, a_m^\dagger(t)\, a_n^\dagger(t)\, a_p(t)\, a_q(t) .$$

20.1.2011

- How to manipulate with the fields without their mode expansions, i.e. how to work directly with the fields?

Now, we have to deal with this continuous index $\vec{n}$. To overcome this difficulty, we have to consider them as a discrete set of points, i.e. we have to take some kind of a cubic lattice.

In the $\psi(\vec{n},t)$, we let this $\vec{n} \to w(i_x, i_y, i_z)$; where the i_x, i_y, i_z are integers and "w" is the lattice spacing.

We think of $\psi(\vec{n},t) \to \psi_{\vec{i}}(t)$; where $\vec{i} \equiv (i_x, i_y, i_z)$.
We will work with them and at the end let $w \to 0$.

We now want to change from the continuum language to the discrete language.

So, now our integration,

$$\int d^3n \to w^3 \sum_{\{i_x, i_y, i_z\}}$$

Taking the limit $w \to 0$, gives us back the integration.

We now consider, $\psi_{\vec{i}}(t)$'s as the coordinate variables.

In this variable, we now calculate,

$$\frac{\partial \psi_{\vec{i}}}{\partial \psi_{\vec{j}}} = \delta_{i_x j_x} \delta_{i_y j_y} \delta_{i_z j_z}$$

If $\vec{i} = \vec{j}$, then this is 1, else it is 0.

We will see that this does not behave well as $w \to 0$.

Actually $\sum_{\{i_x, i_y, i_z\}} \xrightarrow[w \to 0]{} \frac{1}{w^3} \int d^3 r$, diverges.

Thus, to avoid these divergences, we define:-

$$\frac{\delta}{\delta \psi(\vec{r})} = \frac{1}{w^3} \frac{\partial}{\partial \psi_{\vec{i}}}$$

Then $\frac{\delta \psi(\vec{r}')}{\delta \psi(\vec{r})} = \frac{1}{w^3} \frac{\partial \psi_{\vec{i}'}}{\partial \psi_{\vec{i}}} = \frac{1}{w^3} \delta_{i_x i_x'} \delta_{i_y i_y'} \delta_{i_z i_z'}$.

We here took, $\vec{r} = w(i_x, i_y, i_z)$

$\vec{r}' = w(i_x', i_y', i_z')$

If $\vec{r}'$ and $\vec{r}$ are different points on the lattice, then the above quantity is zero.

- Properties:- (i) $\frac{\delta \psi(\vec{r}')}{\delta \psi(\vec{r})} = 0$ if $\vec{r}' \neq \vec{r}$

(ii) $\int d^3 r \frac{\delta \psi(\vec{r}')}{\delta \psi(\vec{r})} \overset{w \to 0}{=} w^3 \sum_{\{i_x, i_y, i_z\}} \frac{1}{w^3} \delta_{i_x i_x'} \delta_{i_y i_y'} \delta_{i_z i_z'}$

$= 1.$

Thus, we see that $\frac{\delta \psi(\vec{r}')}{\delta \psi(\vec{r})}$ has exactly the properties of the Dirac-delta function when we take a continuum limit (i.e. $w \to 0$), i.e.

$$\frac{\delta \psi(\vec{r}')}{\delta \psi(\vec{r})} \xrightarrow[w \to 0]{} \delta^{(3)}(\vec{r} - \vec{r}')$$

[We do this once and for all. We will not discretise everytime. Then we will work with the continuous variables].

If we have,

$\partial_x \psi(\vec{r},t)$, we write it in the discretised form as:-

$$\partial_x \psi(\vec{r},t) = \frac{1}{w}\left[\psi_{\hat{x}_{x+1},\hat{y},\hat{z}}(t) - \psi_{\hat{x},\hat{y},\hat{z}}(t)\right]$$

$$\therefore \partial_x \partial_x \psi(\vec{r},t) = \frac{1}{w}\partial_x \psi_{\hat{x}_{x+1},\hat{y},\hat{z}}(t) - \frac{1}{w}\partial_x \psi_{\hat{x},\hat{y},\hat{z}}(t)$$

$$= \frac{1}{w}\cdot\frac{1}{w}\left[\psi_{\hat{x}_{x+2},\hat{y},\hat{z}}(t) - \psi_{\hat{x}_{x+1},\hat{y},\hat{z}}(t)\right]$$

$$- \frac{1}{w}\cdot\frac{1}{w}\left[\psi_{\hat{x}_{x+1},\hat{y},\hat{z}}(t) - \psi_{\hat{x},\hat{y},\hat{z}}(t)\right]$$

$$= \frac{1}{w^2}\left[\psi_{\hat{x}_{x+2},\hat{y},\hat{z}}(t) - 2\psi_{\hat{x}_{x+1},\hat{y},\hat{z}}(t) + \psi_{\hat{x},\hat{y},\hat{z}}(t)\right]$$

Thus, we can (in the Lagrangian or the Action) represent the $\vec{\nabla}^2$ in terms of this.

[We should recover the rotational invariance].

In the $\hat{h}$, we have:-

$$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

- Let "F" be a function of $\{\psi_{\vec{i}}(t)$ and $\dot{\psi}_{\vec{i}}(t)\}$, i.e. a function of the collection of such variables.

- For example:- $L = \int \psi^*(\vec{r},t)\left(i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} - \hat{h}\psi(\vec{r},t)\right)d^3r$; where $\hat{h} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})$.

We can reinterpret "L" in terms of the discrete variables $\psi_{\vec{i}}$'s and $\dot{\psi}_{\vec{i}}$'s.

We can write $\psi^* = \psi^*_{\vec{i}}(t)$

$$\therefore \quad L = w^3 \sum_{\{i_x, i_y, i_z\}} \psi^*_{\vec{i}}(t) \left(i\hbar \dot{\psi}_{\vec{i}}(t) - \hat{h}\, \psi_{\vec{i}}(t) \right)$$

The variation of "F" can be written as:-

$$\delta F = \sum_{\{i_x, i_y, i_z\}} \left(\frac{\partial F}{\partial \psi_{\vec{i}}} \delta \psi_{\vec{i}} + \frac{\partial F}{\partial \dot{\psi}_{\vec{i}}} \delta \dot{\psi}_{\vec{i}} + \text{complex conjugate} \right)$$

Now, $\dfrac{\partial F}{\partial \psi_{\vec{i}}} = w^3 \dfrac{\delta F}{\delta \psi(\vec{r}, t)}$ and $\dfrac{\partial F}{\partial \dot{\psi}_{\vec{i}}} = w^3 \dfrac{\delta F}{\delta \dot{\psi}(\vec{r}, t)}$.

We can also write $w^3 \sum_{\{i_x, i_y, i_z\}}$ as $\int d^3 r$.

Thus, multiplying and dividing each term on the R.H.S. by w^3, we get:-

$$\delta F = \int d^3 r \left(\frac{\delta F}{\delta \psi(\vec{r}, t)} \delta \psi(\vec{r}, t) + \frac{\delta F}{\delta \dot{\psi}(\vec{r}, t)} \delta \dot{\psi}(\vec{r}, t) + \text{complex conjugate} \right).$$

For functional derivatives, we can use the chain rule for ordinary derivatives

The w^3 cancels (the normalisation has it in the denominator while the integration $\longrightarrow$ sum has it in the numerator)

$$L = \int d^3 r\, \psi^*(\vec{r}, t) \left(i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} - \hat{h} \psi(\vec{r}, t) \right)$$

$$\mathcal{H} = \sum_{\vec{i}} \left(\frac{1}{w^3} \cdot w^3 \right) \frac{\partial L}{\partial \dot{\psi}_{\vec{i}}} \cdot \dot{\psi}_{\vec{i}} - L$$

$$= \int d^3 r \frac{\delta L}{\delta \dot{\psi}(\vec{r}, t)} \dot{\psi}(\vec{r}, t) - L$$

Again, $L = \int d^3x' \, \psi^*(\vec{x}',t) \left\{ i\hbar \dot{\psi}(\vec{x}',t) - \hat{h}\psi(\vec{x}',t) \right\}$

We think of the Lagrangian as a function of coordinates and velocities (they being independent).

To find :- $\dfrac{\delta L}{\delta \dot{\psi}(\vec{x},t)} = \int d^3x' \, \psi^*(\vec{x}',t) \left\{ i\hbar \dfrac{\delta \dot{\psi}(\vec{x}',t)}{\delta \dot{\psi}(\vec{x},t)} \right\}$

Just as $\dfrac{\delta \psi(\vec{x}',t)}{\delta \psi(\vec{x},t)} = \delta^{(3)}(\vec{x}-\vec{x}')$, here also,

$$\frac{\delta \dot{\psi}(\vec{x}',t)}{\delta \dot{\psi}(\vec{x},t)} = \delta^{(3)}(\vec{x}-\vec{x}')$$

$$\therefore \frac{\delta L}{\delta \dot{\psi}(\vec{x},t)} = \int d^3x' \, \psi^*(\vec{x}',t) \, i\hbar \, \delta^{(3)}(\vec{x}-\vec{x}')$$

$$= i\hbar \, \psi^*(\vec{x},t).$$

So, the Hamiltonian is given by :-

$$\int d^3x \, i\hbar \, \psi^*(\vec{x},t) \dot{\psi}(\vec{x},t) - \int d^3x \, \psi^*(\vec{x},t) \left(i\hbar \dot{\psi}(\vec{x},t) - \hat{h}\psi(\vec{x},t) \right)$$

$$= \int d^3x \, \psi^*(\vec{x},t) \, \hat{h} \psi(\vec{x},t)$$

This is the same result we obtained by the mode expansion of the wave functions. [See page 46.].

[At this stage, we are using classical field theory, so here we have "*" and not "†".]

- Another useful notation is that of the conjugate momentum.

In the discrete form, the momentum conjugate to $\psi_{\vec{x}}$ is :-

$$p_{\vec{x}} = \frac{\partial L}{\partial \dot{\psi}_{\vec{x}}}$$

∴ the Poisson Brackets are :-

$$\{\psi_{\vec{i}}, p_{\vec{j}}\}_{P.B.} = \delta_{\vec{i},\vec{j}} = \delta_{i_x j_x} \delta_{i_y j_y} \delta_{i_z j_z}$$

It will be useful not to use $\vec{p}_{\vec{i}}$, but to use a normalised quantity.

So, we define, $\Pi(\vec{x}) = \frac{1}{w^3} p_{\vec{i}}$.

$$\{\psi(\vec{x}), \Pi(\vec{x}')\}_{P.B.} \text{ (at equal times)}.$$

$$= \frac{1}{w^3} \delta_{i_x i'_x} \delta_{i_y i'_y} \delta_{i_z i'_z} \xrightarrow{\text{Lt. } w \to 0} \delta^{(3)}(\vec{x} - \vec{x}')$$

$[\because \vec{x} = w\vec{i}]$.

Thus, if we take the $w \to 0$ limit, we get the Dirac-delta function.

$$\Pi(\vec{x}) = \frac{1}{w^3} \frac{\partial L}{\partial \dot{\psi}_{\vec{i}}} = \frac{\delta L}{\delta \dot{\psi}(\vec{x}, t)}$$

[In this notation, we do not have to worry about the w's].

- We will, in field theory, directly define $\Pi(\vec{x})$, and use this definition of the Poisson-bracket, i.e.

$$\{\psi(\vec{x}), \Pi(\vec{x}')\}_{P.B.} = \delta^{(3)}(\vec{x} - \vec{x}').$$

- In quantum theory, these ψ's and Π's are replaced by operators and we have to use the notation,

$$[\psi(\vec{x}, t), \Pi(\vec{x}', t)] = i\hbar\, \delta^{(3)}(\vec{x} - \vec{x}')$$

Now, let us go back to the Schrödinger problem.

$$L = \int d^3x'\, \psi^*(\vec{x}', t) \left(i\hbar \dot{\psi}(\vec{x}', t) - \hat{h} \psi(\vec{x}', t) \right)$$

$\Pi(\vec{x},t) = i\hbar\,\psi^*(\vec{x},t) \longrightarrow i\hbar\,\psi^\dagger(\vec{x},t)$ in the quantum theory.

[See page 59.].

We get then,

$[\psi(\vec{x},t),\ \psi^\dagger(\vec{x}',t)]\ i\hbar = i\hbar\,\delta^{(3)}(\vec{x}-\vec{x}')$

$\Rightarrow [\psi(\vec{x},t),\ \psi^\dagger(\vec{x}',t)] = \delta^{(3)}(\vec{x}-\vec{x}')$.

Thus, we recover the result that we obtained from the mode expansion of the ψ's and the $\psi^\dagger$'s. [See page 95.].

- **N.B.:-** The a_n's are discrete from the physical view point, whereas the $\psi_{\vec{x}}$'s are not discrete from the physical view point because eventually we let $w \to 0$.

The a_n's and the $\psi_{\vec{x}}$'s are still on the same footing. The "n" index represented the energy eigenstates. The "$\vec{x}$" index represents the position eigenstates. [See page 50.].

- **Identical Fermions:-** We again start with the single particle Schrödinger equation.

Let us (as in the case of bosons) consider "N" identical mutually non-interacting fermions, each moving under a potential $V(\vec{x})$.

The Hamiltonian is:-

$$\sum_{i=1}^{N} \hat{h}_i \ ; \text{ where } \hat{h}_i \equiv -\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{x}_i).$$

Let us (as in the case of bosons) suppose that the $u_n(\vec{x})$'s are eigenstates of $\hat{h}\left(= -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})\right)$

$$\therefore \hat{h}\,u_n(\vec{x}) = e_n\,u_n(\vec{x})$$

- **N.B.:-** As far as a single particle is concerned, there is no distinction between a boson and a fermion.

Now, to construct a basis in terms of the single particle wave functions.

We write,

$$u_{\{n_1,\ldots,n_N\}}(\vec{r}_1,\ldots,\vec{r}_N) = \frac{1}{\sqrt{N!}}\,[\,u_{n_1}(\vec{r}_1)\ldots u_{n_N}(\vec{r}_N) + \text{all permutations of } \vec{r}_1,\ldots,\vec{r}_N \times (-1)^{N_p}\,];$$

where "N_p" is the number of exchanges involved in the permutation.

Q:- How many permutations to go from $1,\ldots,N$ to a given permutation. There are many ways "N_p" is not fixed.
But whether "N_p" is odd or even is fixed.

Here, we do not consider the spin property of the fermions and the bosons.

But given $V(\vec{r})$ [the same], there is no way to distinguish between a fermion and a boson till there is one particle.

- Example:- If $N=3$,

$$u_{\{n_1,n_2,n_3\}}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \frac{1}{\sqrt{3!}}\,[\,u_{n_1}(\vec{r}_1)\,u_{n_2}(\vec{r}_2)\,u_{n_3}(\vec{r}_3) - u_{n_1}(\vec{r}_2)\,u_{n_2}(\vec{r}_1)\,u_{n_3}(\vec{r}_3) - u_{n_1}(\vec{r}_1)\,u_{n_2}(\vec{r}_3)\,u_{n_3}(\vec{r}_2) - u_{n_1}(\vec{r}_3)\,u_{n_2}(\vec{r}_2)\,u_{n_3}(\vec{r}_1) + u_{n_1}(\vec{r}_2)\,u_{n_2}(\vec{r}_3)\,u_{n_3}(\vec{r}_1) + u_{n_1}(\vec{r}_3)\,u_{n_2}(\vec{r}_1)\,u_{n_3}(\vec{r}_2)\,].$$

This is completely antisymmetric under the exchange of any two positions.

Additional feature :- If any of the two n_i's are equal, then $u_{\{n_1,\dots,n_N\}}(\vec{r}_1,\dots,\vec{r}_N)$ vanishes.

i.e. if $n_i = n_j$ for any pair of (i,j), then the state is zero.

Here also (like bosons), we can take an occupation number representation.

Here, u_1 appears m_1 times (say)
u_2 appears m_2 times (say)
⋮

Here another distinction with bosons is each $m_i = 0$ or 1.

Q:- Can an equivalent representation with a Harmonic oscillator be found?

Ans:- It can not be mapped to a Harmonic oscillator, but it can be mapped to an equivalent system which is abstract and can not be related to a harmonic oscillator.

- The equivalent system:- For every energy eigenstate u_n, introduce a pair of operators $a_n, a_n^\dagger$ satisfying the following relations:-

$\{a_m, a_n\} = 0$; $\{a_m^\dagger, a_n^\dagger\} = 0$; $\{a_m, a_n^\dagger\} = \delta_{mn}$, where for any two operators "A", "B", we define,

$\{A, B\} = AB + BA$ (anti-commutator).

We are thus constructing an equivalent quantum system by hand. Then, we would like to find the rules.

These a's and $a^\dagger$'s are not the creation and annihilation operators

of a harmonic oscillator as in the latter case, they do not anti-commute.

We now build a Hilbert space.

- The Hilbert space:- We define the vacuum (ground state), $|0\rangle$ such that,

$$a_n|0\rangle = 0 \quad \text{for every "n".}$$

Then the basis states are of the form:-

first representation :-

$$a_{n_1}^\dagger a_{n_2}^\dagger \ldots\ldots a_{m_N}^\dagger \leftrightarrow u_{\{n_1,\ldots,n_N\}}(\vec{\pi}_1,\ldots,\vec{\pi}_N)$$

second representation (occupation number representation) :-

$$(a_1^\dagger)^{m_1} (a_2^\dagger)^{m_2} \ldots\ldots |0\rangle$$

- claim:- We have an exact map between the quantum theory of both the states.

We have to apply the symmetry property exactly.

If any two n's are the same, then the state is zero.

Proof :- $\{a_n^\dagger, a_m^\dagger\} = 0$

or $a_n^\dagger a_m^\dagger + a_m^\dagger a_n^\dagger = 0$

If $m = n$, then

$$2(a_n^\dagger)^2 = 0$$

$$\Rightarrow (a_n^\dagger)^2 = 0$$

Thus, if two $a_{n_i}^\dagger$'s are the same, then the wave function vanishes.

Thus, it passes the first property, i.e. if the m_i's are more than 1, then the state is zero.

We have to check the matrix elements of the operators in the two states must be the same.

The Hamiltonian in this description is :-

$$\hat{H} = \sum_n e_n a_n^\dagger a_n .$$

More generally, if we have a one-body operator,

$$\hat{b}_{(N)} = \sum_{i=1}^{N} b(\hat{\vec{r}}_i, \hat{\vec{p}}_i)$$ [Each term depends on the coordinate and momentum of the i^{th} particle].

The equivalent representation is :-

$$\hat{B} = \sum_{m,n} b_{mn} a_m^\dagger a_n \; ; \text{ where } b_{mn} = \int d^3r \, u_m^*(\vec{r}) \, b(\vec{r}, \vec{p}) \, u_n(\vec{r}).$$

Now, to prove that :-

$$\langle u_n | \hat{b}_{(N)} | u_{n'} \rangle = \langle n | \hat{B} | n' \rangle .$$

Proof :- R.H.S. $= \sum_{K=1}^{\infty} \sum_{L=1}^{\infty} b_{KL} \langle 0 | a_{n_1} \cdots a_{n_N} a_K^\dagger a_L \, a_{n_1'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$

$$= \sum_{K=1}^{\infty} \sum_{L=1}^{\infty} b_{KL} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} [\delta_{n_N,K} - a_K^\dagger a_{n_N}] \cdot [\delta_{n_1',L} - a_{n_1'}^\dagger a_L] a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$= \sum_{K,L=1}^{\infty} b_{KL} \delta_{K,n_N} \delta_{L,n_1'} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$- \sum_{K,L=1}^{\infty} b_{KL} \delta_{K,n_N} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_{n_1'}^\dagger a_L \, a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$- \sum_{L,L=1}^{\infty} b_{KL} \delta_{L,n_1'} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_K^\dagger a_{n_N} a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$+ \sum_{K,L=1}^{\infty} b_{KL} \langle 0 | a_{n_1} \cdots a_{n_{N-1}} a_K^\dagger a_{n_N} a_{n_1'}^\dagger a_L \, a_{n_2'}^\dagger \cdots a_{n_N'}^\dagger | 0 \rangle$$

$$\text{R.H.S.} = \sum_{\kappa,\lambda=1}^{\infty} b_{\kappa\lambda}\,\delta_{\kappa,n_N}\,\delta_{\lambda,n_1'}\,\langle 0|a_{n_1}\cdots a_{n_{N-1}}\,a_{n_2'}^{\dagger}\cdots a_{n_N'}^{\dagger}|0\rangle$$

$$-\sum_{\kappa,\lambda=1}^{\infty} b_{\kappa\lambda}\,\delta_{\kappa,n_N}\,\langle 0|a_{n_1}\cdots a_{n_{N-1}}\,a_{n_1'}^{\dagger}[\delta_{\lambda,n_2'}-a_{n_2'}^{\dagger}a_{\lambda}]\cdots a_{n_N'}^{\dagger}|0\rangle$$

$$-\sum_{\kappa,\lambda=1}^{\infty} b_{\kappa\lambda}\,\delta_{\lambda,n_1'}\,\langle 0|a_{n_1}\cdots a_{n_{N-2}}[\delta_{n_{N-1},\kappa}-a_{\kappa}^{\dagger}a_{n_{N-1}}].\,a_{n_2'}^{\dagger}\cdots a_{n_N'}^{\dagger}|0\rangle$$

$$+\sum_{\kappa,\lambda=1}^{\infty} b_{\kappa\lambda}\,\langle 0|a_{n_1}\cdots a_{n_{N-2}}[\delta_{\kappa,n_{N-1}}-a_{\kappa}^{\dagger}a_{n_{N-1}}].\,a_{n_N}a_{n_1'}^{\dagger}.[\delta_{n_2',\lambda}-a_{n_2'}^{\dagger}a_{\lambda}]\cdots a_{n_N'}^{\dagger}|0\rangle$$

$$=\sum_{\kappa,\lambda=1}^{\infty}\sum_{i=1}^{N}\sum_{j=1}^{N}(-1)^{i+j}\,b_{\kappa\lambda}\,\delta_{\kappa,n_i}\,\delta_{\lambda,n_j'}\,\langle 0|a_{n_1}\cdots \not{a}_{n_i}\cdots a_{n_N}\,a_{n_1'}^{\dagger}\cdots a_{n_j'}^{\dagger}\cdots a_{n_N'}^{\dagger}|0\rangle$$

Where $\not{a}_{n_i}$ and $\not{a}_{n_j'}^{\dagger}$ are explained in page 19.

Here, we have used the fact that,

$$\{a_{n_i}, a_{\kappa}^{\dagger}\} = \delta_{n_i,\kappa}$$

From page 20. and 21., we write :-

$$\text{R.H.S.} = \sum_{i=1}^{N}\sum_{j=1}^{N}(-1)^{i+j}\,b_{n_i,n_j'}\,\delta(n_1,\cdots,\not{n}_i,\cdots,n_N;\,n_1',\cdots,\not{n}_j',\cdots n_N')$$

$$\text{L.H.S.} = \int d^3r_1\cdots d^3r_N\,u^{*}_{\{n_1',\cdots,n_N'\}}(\vec{r}_1,\cdots,\vec{r}_N)\,\hat{b}_{(N)}\,u_{\{n_1',\cdots,n_N'\}}(\vec{r}_1,\cdots,\vec{r}_N)$$

Now, $u_{\{n_1',\cdots,n_N'\}}(\vec{r}_1,\cdots,\vec{r}_N)$ is by construction a function which is completely antisymmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

Again $\hat{b}_{(N)}$ is completely symmetric under the exchange of any two particles.

Thus, $\hat{b}_{(N)}\,u_{\{n_1',\cdots,n_N'\}}(\vec{r}_1,\cdots,\vec{r}_N)$ is completely antisymmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

Again, $u_{s m_1, \ldots, m_N}(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}} [u_{m_1}(\vec{r}_1) \cdots u_{m_N}(\vec{r}_N)$
+ all permutations of $\vec{r}_1, \ldots, \vec{r}_N \times (-1)^{N_p}$]

This term is also antisymmetric under $\vec{r}_i \leftrightarrow \vec{r}_j$ (for any pair of "i", "j").

So instead of calculating the (N!) integrals separately, we perform only the first and multiply by $(N!) \times (-1)^{N_p}$.

$\left(u_1(\vec{r}_1) u_2(\vec{r}_2) - u_2(\vec{r}_1) u_1(\vec{r}_2) \right] ($ . . .

For fermions, there is no field theory, whose quantisation will give us these rules.

The best we can do is that we take a classical field theory, then instead of replacing the poisson bracket by $\frac{1}{i\hbar}[\,,\,]$, we do it by $\frac{1}{i\hbar}\{\,,\,\}$, i.e. anti-commutator bracket. We will then be arriving at the results.

Though, we must remember that, this is not a standard rule and that there is not any known classical limit of the results we obtained for the fermions.

[As, it has a Hilbert space, the linearity of the wave functions, ensures that they form a quantum state.

Any quantum operator $\hat{O}$ satisfies,

$$i\hbar\frac{\partial\hat{O}}{\partial t} = [\hat{O}, \hat{H}].$$

Thus, here also the standard rules of quantum mechanics hold.]

- Let us consider a harmonic oscillator. Let, both fermions and bosons have any energy levels.

If we now replace the identity,

$$[\hat{x}, \hat{p}] = i\hbar \text{ by,}$$

$\{\hat{x}, \hat{p}\} = i\hbar$, then we will not get something sensible. The system will be different.

Thus, for both bosons and fermions, we will have to use, $[\hat{x}, \hat{p}] = i\hbar$.

Thus is a reason, we are getting different results for a bosonic and a fermionic systems.

Suppose a fermion moves in a coulomb potential. We quantise

using commutation and not anti-commutation. The anti-commutation comes during the second quantisation.

Thus, any result of quantising a classical limit, we have to replace $\{,\}_{P.B.}$ by $\frac{1}{i\hbar}[,]$. Fermions are not a result of first-quantising a classical system.

- $\{\psi, \psi^*\} = -\{\psi^*, \psi\}$ is not natural.
  A poisson-bracket is anti-symmetric in ψ, ψ^*.

- If we take grassmann variables, it is not a classical theory anymore.

- classical limit of Harmonic oscillators are coherent states, $\exp(\lambda a_m^\dagger)|0\rangle$.

This is not possible for fermions. A given $(a_m^\dagger)$ can be applied atmost once.

21.1.2011

In (1+1)-D, we can have particles like para fermions. Here, we can pump in some of the particles.

We generalise statistics by not generalising the symmetry conditions, but by specifying the number of particles.

We have,

$$i\hbar \frac{d\hat{O}}{dt} = [\hat{O}, \hat{H}].$$

If $[\hat{O}, \hat{H}] = 0$, then $\hat{O} \neq \hat{O}(t)$. We then formulate the whole problem in the Heisenberg picture.

• To find the relativistic generalisation of what we have been doing.

One particle Schrödinger equation gives:-

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \psi.$$

Having a potential breaks even the translational invariance.
So, let us first consider free particles, i.e. $V(\vec{r}) = 0$.

Thus, now, the energy eigenstates become continuous.
[We can always put the particle in a box and discretise its momentum and hence its energy.

So, the energy eigenstates are of the form,

$$\frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}, \text{ where } (k_x, k_y, k_z) = \hbar(\kappa_x, \kappa_y, \kappa_z)$$

Therefore, we get:-

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi = \frac{\hbar^2}{2m} (\kappa_x^2 + \kappa_y^2 + \kappa_z^2) \psi$$

Thus, the energy eigenvalues are:-

$$E = \frac{1}{2m} (k_x^2 + k_y^2 + k_z^2).$$

This does not have Lorentz invariance but only Galilean invariance.

We want to generalise Schrödinger equation, so that "E" and "$\vec{p}$" follow Lorentz formula. Then, we second quantise.

• We generalise to the relativistic system :-

We will use the following units (just to simplify); $\hbar = 1$, $c = 1$.

We want, $E = \sqrt{\vec{p}^2 + m^2}$ [actually $E = \sqrt{\vec{p}^2 c^2 + m^2 c^4}$].

We still have the identification,

$\frac{i\hbar\partial}{\partial t} \longrightarrow$ Energy,

$-i\hbar \frac{\partial}{\partial x} \longrightarrow$ momentum.

We are looking for an operator (matter equation), such that $e^{-i(Et - \vec{k}\cdot\vec{x})}$ is a solution when $E = \sqrt{\vec{k}^2 + m^2}$.

We have,

$$i\hbar \frac{\partial}{\partial t} e^{-i(Et - \vec{k}\cdot\vec{x})} = E e^{-i(Et - \vec{k}\cdot\vec{x})}$$

$$\text{and } -i\hbar \frac{\partial}{\partial x} e^{-i(Et - \vec{k}\cdot\vec{x})} = k_x e^{-i(Et - \vec{k}\cdot\vec{x})}$$

} $\hbar = c = 1$.

What changes is the relation between "E" and "$\vec{p}$", the operators will not change.

To get rid of the square root, we write,

$$E^2 = \vec{k}^2 + m^2 \qquad (\because \hbar = 1,\ c = 1).$$

∴ We write,

$$-\frac{\partial^2}{\partial t^2}\psi = -\vec{\nabla}^2\psi + m^2\psi \quad [\text{using the previous two relations}].$$

or $$\left[-\frac{\partial^2}{\partial t^2} + \vec{\nabla}^2 - m^2\right]\psi = 0$$

or $[\Box - m^2]\psi = 0$; where $\Box = -\frac{\partial^2}{\partial t^2} + \vec{\nabla}^2$ is the D'Alembertian operator.

Here, we use the metric $(-1, 1, 1, 1)$.

The above is the Klein-Gordon equation.

Check:- If we have, $\psi = e^{-iEt + i\vec{k}\cdot\vec{x}}$, then

$(\Box - m^2)\psi = 0$

$\Rightarrow -(-iE)^2 + (i\vec{k})^2 - m^2 = 0$

or $E^2 = \vec{k}^2 + m^2$

or $E = \pm\sqrt{\vec{k}^2 + m^2}$

Thus, irrespective of what sign, we choose for "E", the Klein-Gordon equation is satisfied.

We have got more than what we had wanted !!!!!!!

The spectrum, as we see, contains both positive and negative energy levels. i.e. particles with negative energies are allowed here, which we do not want.

Now, "$|\vec{k}|$" can be as large as we can think of, then, there will not be any bound on the negative energy levels.

If, it were bounded, we could have just shifted the zero of the energy. Here, we can not do that, because there is an infinity bound for the negative energy levels.

Thus, this first quantised equation is not manifestly positive.

But, we will see that, if we second quantise this equation (as we did for the Schrödinger equation), then the equation will be manifestly positive.

• N.B. :- In Schrödinger equation, the time evolution [$i\hbar\,\partial/\partial t$] would even make a real wave-function evolve as a complex one.

On the contrary, the Klein-Gordon equation is real [because of $\partial^2/\partial t^2$ and $\vec{\nabla}^2$], and a real wave-function always evolves as a real wave-function.

Schrödinger equation is:-

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2m}\vec{\nabla}^2\psi \quad \text{(for a free particle)}.$$

We just give $\psi(t=0)$ and this fixes the time evolution. If $\psi(t=0)$ is real, it will become complex because of the "i".

In contrast, the Klein-Gordon equation is:-

$$\frac{\partial^2\psi}{\partial t^2} = (\vec{\nabla}^2 - m^2)\psi.$$

So, here, we will have to specify both $\psi(t=0)$ and $\dot{\psi}(t=0)$ and let it evolve. As, it is a second order equation in both "t" and "$\vec{x}$", and has no "i" hanging in the equation, so if $\psi(t=0)$ and $\dot{\psi}(t=0)$ are real, so will ~~they~~ be at all times. It will never become complex.

By restricting to real, we are putting a condition on the Fourier modes; there is no "i".

We can solve the Klein-Gordon equation numerically.

We can add the complex conjugate of the "ψ" to this one (as "ψ^*" is the solution to the same Klein-Gordon equation).

But "ψ^*" did not satisfy the same Schrödinger

equation, the equation will be :-

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^*.$$

Thus, in the Schrödinger case, the energy eigenstates obviously can not be real as the energy operator is $i\frac{\partial}{\partial t}$.

Here, in the Klein-Gordon case, we restrict "ψ" to be real. If "ψ" were a complex field, we could have taken its real and complex parts separately.

$\psi = \psi_R + i\psi_I$. Each of these will separately satisfy the Klein-Gordon equation.

A complex field is equivalent to two real fields.

• Notation :- $x^0 = t$, $x^1 = x$, $x^2 = y$, $x^3 = z$,

and we will also write,

$$\Box = -\frac{\partial^2}{\partial t^2} + \vec{\nabla}^2$$
$$= \eta^{\mu\nu}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu};$$

where $\eta^{00} = -1$; $\eta^{ij} = \delta_{ij}$; $\eta^{0i} = \eta^{i0} = 0$ $(i, j = 1, 2, 3)$.

• N.B.:- We must note that the Klein-Gordon equation is not a proper first quantised theory.

In the second quantised (relativistic) theory with appropriate non-relativistic limit, we will get the second quantised non-relativistic theory.

• N.B. :- In Schrödinger equation, even if we take $V(\vec{r})$ as complex, the relative difference between $\vec{\nabla}^2$ and $V(\vec{r})$ can never make this a

completely real equation.

- Now, we take the Klein-Gordon equation, treat it as a classical equation and then quantise it.

We try to write an action for this.

We write, the action :-

$$S = \frac{1}{2}\int dt\, d^3x\ \phi\,[\Box - m^2]\,\phi$$; here $\left(\frac{1}{2}\right)$ is the normalisation factor.

We replaced $\psi \longrightarrow \phi$ to distinguish Klein-Gordon field from schroödinger field.

The normalisation factor does not affect the classical equation.

Now, $\delta S = \frac{1}{2}\int dt\, d^3x \left[\delta\phi\,[\Box - m^2]\,\phi + \phi\,[\Box - m^2]\,\delta\phi\right]$.

We integrate the second term by parts.

$$\int dt\, d^3x\ \phi\,\Box\,\delta\phi$$

$$= -\int dt\, d^3x\, \phi \frac{\partial^2(\delta\phi)}{\partial t^2} + \int dt\, d^3x\ \phi\,\vec{\nabla}^2(\delta\phi)$$

$$= -\int d^3x \left[\phi \cancel{\frac{\partial(\delta\phi)}{\partial t}}^{\,0}\right] + \int d^3x\, dt\, \frac{\partial\phi}{\partial t}\cdot\frac{\partial(\delta\phi)}{\partial t}$$

$$= \int d^3x \left[\frac{\partial\phi}{\partial t}\cancel{\delta\phi}^{\,0}\right] - \int d^3x\, dt\, \frac{\partial^2\phi}{\partial t^2}\,\delta\phi + \int dt\, d^3x\, \vec{\nabla}^2\phi\,\delta\phi$$

$$+ \int dt\, d^3x\, \vec{\nabla}^2\phi\,\delta\phi$$

$$= \int dt\, d^3x\,(\Box\phi)\,\delta\phi$$

Thus, we write,

$$\delta S = \frac{1}{2}\int dt\, d^3x \{\delta\phi(\Box - m^2)\phi + \delta\phi\,\Box\phi - m^2\phi\,\delta\phi\}$$

$\delta S = 0$ for arbitrary $\delta\phi$.

Thus, the integrand must vanish,

$\therefore$ We get :-

$$\frac{1}{2}.2\,[(\Box - m^2)\phi] = 0$$

or $(\Box - m^2)\phi = 0$

$(E^2 - p^2)$ is an invariant here.

Here, the Lagrangian is :-

$$L = \frac{1}{2}\int d^3x\, \phi\,[\Box - m^2]\,\phi$$

$$= \frac{1}{2}\int d^3x\, \phi\left[-\frac{\partial^2}{\partial t^2} + \vec{\nabla}^2 - m^2\right]\phi$$

$\phi(\vec{x},t) \rightarrow$ "$\vec{x}$" is like a label and we think of "ϕ" as a dynamical variable.

The Lagrangian, here, depends on the second time derivative of the coordinate.

Normally in classical physics, Lagrangian is a function of coordinates, time and the first derivative (in time) of the coordinates.

We could obviously add a first time derivative of any arbitrary function to the Lagrangian without affecting the equations of motion.

- But, if $L = L(\dot{q})$, we always do not have a Hamiltonian formulation.

The usual Lagrangian formalism usually has,

$$L = L(q, \dot{q}).$$

But now, we write the Action in a different way.

$$S = \frac{1}{2}\int dt\, d^3x\, \phi[\Box - m^2]\phi$$

$$= \frac{1}{2}\int dt\, d^3x\, \phi\left[-\frac{\partial^2}{\partial t^2} + \vec{\nabla}^2 - m^2\right]\phi$$

We integrate the time-part, by parts.

We get :-

$$S = \frac{1}{2}\int dt\, d^3x \left(\frac{\partial\phi}{\partial t}\right)^2 + \frac{1}{2}\int dt\, d^3x\, \phi[\vec{\nabla}^2 - m^2]\phi$$

To get a covariant looking form, we can also integrate the $\vec{\nabla}^2$-part by parts. It is not necessary though.

- Then, we get :-

$$S = \frac{1}{2}\int dt\, d^3x \left[\left(\frac{\partial\phi}{\partial t}\right)^2 - (\vec{\nabla}\phi)^2 - m^2\phi^2\right]$$

$$\text{or } S = \frac{1}{2}\int dt\, d^3x \left[-\eta^{\mu\nu}\frac{\partial\phi}{\partial x^\mu}\cdot\frac{\partial\phi}{\partial x^\nu} - m^2\phi^2\right]$$

The conjugate momentum is defined as :-

$$\pi(\vec{x}, t) = \frac{\delta L}{\delta\dot{\phi}(\vec{x}, t)} = \dot{\phi}(\vec{x}, t)$$

$$L = \frac{1}{2}\int d^3x' \left[\left(\frac{\partial\phi(\vec{x}', t)}{\partial t}\right)^2 - (\vec{\nabla}\phi(\vec{x}', t))^2 - m^2(\phi(\vec{x}', t))^2\right]$$

$$\therefore \frac{\delta L}{\delta \dot{q}(\vec{x},t)} = \frac{1}{\varkappa}\int d^3x'\, \varkappa\, \dot{\phi}(\vec{x}',t)\, \delta^{(3)}(\vec{x}'-\vec{x}) = \dot{\phi}(\vec{x},t)$$

$$\left[\because \frac{\delta \dot{\phi}^2(\vec{x}',t)}{\delta \dot{\phi}(\vec{x},t)} = \frac{\delta \dot{\phi}^2(\vec{x}',t)}{\delta \dot{\phi}(\vec{x}',t)} \cdot \frac{\delta \dot{\phi}(\vec{x}',t)}{\delta \dot{\phi}(\vec{x},t)} = 2\dot{\phi}(\vec{x}',t)\, \delta^{(3)}(\vec{x}'-\vec{x})\right].$$

[similarly, $(\vec{\nabla}\phi)^2$ can be written as :-

$$\left\{\frac{1}{\omega}\left(\phi_{\tilde{x}+1,\tilde{y},\tilde{z}} - \phi_{\tilde{x},\tilde{y},\tilde{z}}\right)\right\}^2 + \cdots\cdots\Big].$$

We will have to write a commutation relation between $\Pi(\vec{x},t)$, $\phi(\vec{x},t)$.

~~N.B~~ If we choose a different definition of $\Pi(\vec{x},t)$, we might not get a manifestly Lorentz invariance.

So, the Hamiltonian is :-

$$H = \sum \frac{\partial L}{\partial \dot{\phi}} \cdot \dot{\phi} - L$$

$$= \int d^3x \frac{\delta L}{\delta \dot{\phi}(\vec{x},t)} \cdot \dot{\phi}(\vec{x},t) - L$$

$$= \int d^3x \left\{\Pi(\vec{x},t)\, \dot{\phi}(\vec{x},t)\right\} - \frac{1}{2}\int d^3x \left[\dot{\phi}^2(\vec{x},t) - (\vec{\nabla}\phi)^2 - m^2\phi^2\right]$$

$$= \frac{1}{2}\int d^3x \left\{\Pi^2(\vec{x},t) + (\vec{\nabla}\phi)^2 + m^2\phi^2\right\}$$

- Here, we note that each term is positive definite.
- The momentum operator has to be a function of space
  → translational symmetry.

In Π, ϕ, the indices do not match up, so, we can not identify them directly as Lorentz four vectors.

N.B. This Hamiltonian is an analogue of what we got for the Schrödinger problem.

$$H_{S.E.} = \int d^3x \, \psi^* \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \psi$$

The $\vec{\nabla}^2$ term can be integrated by parts and the $V(\vec{r})\psi$ can be considered as an analogue of $m^2\phi^2$.

The Klein-Gordon equation gave negative energy when we considered the wave equation. But here, we are considering something different.

- If we take "ϕ" to be real, it can not be an eigenstate of $i\frac{\partial}{\partial t}$, i.e., it can not be an energy eigenstate if it is real.

But, here, we are considering the Hamiltonian of the field theory.

- Previously (in the Schrödinger case, we expanded the ψ's in terms of the a_n's and we simplified the Hamiltonian.

- Here, we do a similar thing. We go to a different basis, the plane wave basis.

- We introduce new variables,

$$\tilde{\phi}(\vec{k},t) = \int e^{-i\vec{k}\cdot\vec{x}} \, \phi(\vec{x},t) \, \frac{d^3x}{(2\pi)^{3/2}}$$

and $\tilde{\Pi}(\vec{k},t) = \int e^{-i\vec{k}\cdot\vec{x}}\, \Pi(\vec{x},t)\, \frac{d^3x}{(2\pi)^{3/2}}$.

These are the Fourier transforms of $\phi(\vec{x},t)$ and $\Pi(\vec{x},t)$.
We must note that, we have not touched time at all.
Thus, if we know $\tilde{\phi}(\vec{k},t)$ and $\tilde{\Pi}(\vec{k},t)$, we can reconstruct $\phi(\vec{x},t)$ and $\Pi(\vec{x},t)$ and vice versa.

These are just an identical (alternate) set of variables.
[It is just like instead of using $v_1, v_2, \ldots$, we use a linear combination of them].

The Hamiltonian will look simpler in these variables.

We have (from definition),

$$\{\phi(\vec{x},t),\ \phi(\vec{x}',t)\}_{P.B.} = 0$$

$$\{\Pi(\vec{x},t),\ \Pi(\vec{x}',t)\}_{P.B.} = 0$$

and $\{\phi(\vec{x},t),\ \Pi(\vec{x}',t)\}_{P.B.} = \delta^{(3)}(\vec{x}-\vec{x}')$

Using these relations, we can, very well, calculate the Poisson Brackets of $\tilde{\phi}(\vec{k},t)$, $\tilde{\Pi}(\vec{k},t)$.

Now, $\{\tilde{\phi}(\vec{k},t),\ \tilde{\phi}(\vec{k}',t)\}_{P.B.} = \int \frac{d^3x\, d^3x'}{(2\pi)^3}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'}\, \{\phi(\vec{x},t), \phi(\vec{x}',t)\}$ (the Poisson bracket $\to 0$)

$$= 0$$

Similarly, $\{\tilde{\Pi}(\vec{k},t), \tilde{\Pi}(\vec{k}',t)\}_{P.B.} = 0$

and $\{\tilde{\phi}(\vec{k},t),\ \tilde{\Pi}(\vec{k}',t)\}_{P.B.} = \int \frac{d^3x\, d^3x'}{(2\pi)^3}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'}\, \{\phi(\vec{x},t), \Pi(\vec{x}',t)\}$

$$= \int \frac{d^3x\, d^3x'}{(2\pi)^3}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'}\, \delta^{(3)}(\vec{x}-\vec{x}')$$

or $\{\tilde{\phi}(\vec{k},t),\ \tilde{\Pi}(\vec{k}',t)\} = \int \frac{d^3x}{(2\pi)^3} e^{-i(\vec{k}+\vec{k}')\cdot\vec{x}}$

$= \delta^{(3)}(\vec{k}+\vec{k}')$

It is in the momentum space.

This is actually, the statement of momentum conservation.

Here we have a $\delta^{(3)}(\vec{k}+\vec{k}')$, we will see later how we get a $\delta^{(3)}(\vec{k}-\vec{k}')$.

To show that,

$$H = \frac{1}{2}\int d^3k \left[\tilde{\Pi}(\vec{k},t)\tilde{\Pi}(-\vec{k},t) + (\vec{k}^2+m^2)\tilde{\phi}(\vec{k},t)\tilde{\phi}(-\vec{k},t)\right]$$

We start with,

$$H = \frac{1}{2}\int d^3x \left[\dot{\phi}^2(\vec{x},t) + (\vec{\nabla}\phi(\vec{x},t))^2 + m^2\phi^2(\vec{x},t)\right],$$

and we use,

$$\dot{\phi}(\vec{x},t) = \pi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}}\ \tilde{\Pi}(\vec{k},t)$$

$$\text{and } \phi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}}\ \tilde{\phi}(\vec{k},t)$$

$\therefore$ We write,

$$H = \frac{1}{2}\int \frac{d^3x}{(2\pi)^3}\int d^3k\, d^3k' \left[\tilde{\Pi}(\vec{k},t)\tilde{\Pi}(\vec{k}',t) + (i\vec{k})\cdot(i\vec{k}')\tilde{\phi}(\vec{k},t)\tilde{\phi}(\vec{k}',t) + m^2\tilde{\phi}(\vec{k},t)\tilde{\phi}(\vec{k}',t)\right] e^{i(\vec{k}+\vec{k}')\cdot\vec{x}}$$

Writing $\vec{x} = -\vec{y}$, we get $d^3x = -d^3y$.

$$\therefore H = -\frac{1}{2}\int d^3k\, d^3k' \left[\tilde{\Pi}(\vec{k},t)\tilde{\Pi}(\vec{k}',t) - \vec{k}\cdot\vec{k}'\tilde{\phi}(\vec{k},t)\tilde{\phi}(\vec{k}',t) + m^2\tilde{\phi}(\vec{k},t)\tilde{\phi}(\vec{k}',t)\right]\delta^{(3)}(\vec{k}+\vec{k}')$$

Writing $\vec{k}' = -\vec{k}''$, we get $-d^3k' = d^3k''$.

∴ We get :-

$$H = \frac{1}{2}\int d^3k\, d^3k'' \left[\tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k}'',t) + (\vec{k}\cdot\vec{k}'' + m^2)\tilde{\phi}(\vec{k},t)\tilde{\phi}(-\vec{k}'',t)\right] \delta^{(3)}(\vec{k}-\vec{k}'')$$

$$\text{or } H = \frac{1}{2}\int d^3k \left[\tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) + (k^2+m^2)\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)\right]$$

Now, we had required ϕ, Π to be real but not $\tilde{\phi}, \tilde{\Pi}$ to be real, because they have an 'i' in the exponential.

But, we must note that, they can not be arbitrary complex variables.

We have :-

$$\phi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}}\, e^{i\vec{k}\cdot\vec{x}}\, \tilde{\phi}(\vec{k},t)$$

$$\text{and } \Pi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}}\, e^{i\vec{k}\cdot\vec{x}}\, \tilde{\Pi}(\vec{k},t).$$

Now, if $\tilde{\phi}$ is an arbitrary complex function of $(\vec{k},t)$, then $\phi(\vec{x},t)$ is not necessarily real.

We need to put some conditions such that (ϕ, Π) are real.

Our condition is:-

$$\left(\tilde{\phi}(\vec{k},t)\right)^* = \tilde{\phi}(-\vec{k},t)$$

Proof :- $\tilde{\phi}^*(\vec{k},t) = \int e^{-i\vec{k}\cdot\vec{x}}\, \phi(\vec{x},t)\, \frac{d^3x}{(2\pi)^{3/2}} = \tilde{\phi}(-\vec{k},t)$

Similarly, $\left(\tilde{\Pi}(\vec{k},t)\right)^* = \tilde{\Pi}(-\vec{k},t)$.

Now, if we calculate,

$$\{\tilde{\phi}(\vec{x},t),\ \tilde{\Pi}^*(\vec{x}',t)\}_{P.B.}$$

$$= \int \frac{d^3x\, d^3x'}{(2\pi)^3} e^{-i\vec{k}\cdot\vec{x}} e^{i\vec{k}'\cdot\vec{x}'} \{\phi(\vec{x},t), \Pi(\vec{x}',t)\}_{P.B.}$$

$$= \int \frac{d^3x\, d^3x'}{(2\pi)^3} e^{-i\vec{k}\cdot\vec{x}} e^{i\vec{k}'\cdot\vec{x}'} \delta^{(3)}(\vec{x}-\vec{x}')$$

$$= \int \frac{d^3x}{(2\pi)^3} e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}}$$

$$= \delta^{(3)}(\vec{k}-\vec{k}')$$

We will next take a classical system, and the variables $\tilde{\phi}(\vec{k},t)$ and $\tilde{\Pi}(\vec{k},t)$ and the conditions, $(\tilde{\phi}(\vec{k},t))^* = \tilde{\phi}(-\vec{k},t)$ and $(\tilde{\Pi}(\vec{k},t))^* = \tilde{\Pi}(-\vec{k},t)$, and replace the $*$'s by the $\dagger$'s and replace $\{,\}_{P.B.}$ by $\frac{1}{i\hbar}[,]$, and we consider these $\tilde{\phi}$'s and $\tilde{\Pi}$'s as operators and try to find the spectrum.

If there was no $(-\vec{k})$, then, we could have had it like

$$\vec{p}^2 + (\vec{k}+m^2)\vec{x}^2.$$

[N.B. :- In the expression, $\frac{\vec{p}^2}{2} + \frac{1}{2}k\vec{x}^2$, where "$k$" is the stiffness factor, so the expression is not exactly symmetric under $\vec{p} \leftrightarrow \vec{x}$.]

We can write the terms as $\sum_{\vec{k}}$ (instead of $\int d^3k$) by discretising. Then each term can be thought of as a harmonic oscillator.

But, this is not necessary.

Let us have two terms,

$$H = \frac{1}{2}\left(p_1^2 + K_1 q_1^2\right) + \frac{1}{2}\left(p_2^2 + K_2 q_2^2\right).$$

Now, we take $\tilde{q}_1 = q_1 + q_2$, $\tilde{q}_2 = q_1 - q_2$, $\tilde{p}_1 = p_1 + p_2$ and $\tilde{p}_2 = p_1 - p_2$.

We then get,

$$q_1 = \frac{1}{2}(\tilde{q}_1 + \tilde{q}_2)$$

$$q_2 = \frac{1}{2}(\tilde{q}_1 - \tilde{q}_2)$$

$$p_1 = \frac{1}{2}(\tilde{p}_1 + \tilde{p}_2)$$

$$p_2 = \frac{1}{2}(\tilde{p}_1 - \tilde{p}_2)$$

We then can write the Hamiltonian in terms of these new variables.

$$H = \frac{1}{2}\left[\frac{1}{4}\left[\tilde{p}_1^2 + \tilde{p}_2^2 + 2\tilde{p}_1\tilde{p}_2\right] + \frac{K_1}{4}\left[\tilde{q}_1^2 + \tilde{q}_2^2 + 2\tilde{q}_1\tilde{q}_2\right]\right]$$

$$+ \frac{1}{2}\left[\frac{1}{4}\left[\tilde{p}_1^2 + \tilde{p}_2^2 - 2\tilde{p}_1\tilde{p}_2\right] + \frac{K_2}{4}\left[\tilde{q}_1^2 + \tilde{q}_2^2 - 2\tilde{q}_1\tilde{q}_2\right]\right]$$

Now if $K_1 = K_2$, then,

$$H = \frac{1}{2}\left[\frac{1}{2}\left[\tilde{p}_1^2 + \tilde{p}_2^2\right] + \frac{K}{2}\left[\tilde{q}_1^2 + \tilde{q}_2^2\right]\right]$$

So, now also, we can interpret $\tilde{q}_1, \tilde{q}_2, \tilde{p}_1, \tilde{p}_2$ as the coordinates and the momenta.

- To find the conjugate to $\phi(\vec{x},t)$.

We have, $L = \int d^3x \left[\pi^2(\vec{x},t) - (\vec{\nabla}\phi)^2 - m^2\phi^2\right]$

$$\text{or } L = \frac{d^3x}{(2\pi)^3}\int d^3k\, d^3k' \left\{ \tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(\vec{k}',t) - \left[(i\vec{k})\cdot(i\vec{k}') + m^2\right] \tilde{\phi}(\vec{k},t)\,\tilde{\phi}(\vec{k}',t) \right\} \cdot \underbrace{e^{i(\vec{k}+\vec{k}')\cdot\vec{x}}}_{\delta^{(3)}(\vec{k}-\vec{k}'')}$$

$$= -\int d^3k\, d^3k' \left\{ \tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k}'',t) + \left[\vec{k}\cdot(-\vec{k}'') - m^2\right] \tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k}'',t) \right]$$

[In the last step, we replaced $\vec{k}'$ by $-\vec{k}''$, thus $-d^3k' = d^3k''$].

$$\text{or } L = \int d^3k \left\{ \tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) - (k^2+m^2)\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t) \right\}$$

$\therefore \quad \dot{\tilde{\phi}}(\vec{k}',t) = \tilde{\Pi}(\vec{k}',t)$

$\therefore$ Conjugate momentum to $\tilde{\phi}(\vec{k}',t)$ is :-

$$\frac{\delta L}{\delta \dot{\tilde{\phi}}(\vec{k}',t)} = \frac{\delta L}{\delta \tilde{\Pi}(\vec{k}',t)}$$

$$= \int d^3k\, \tilde{\Pi}(-\vec{k},t)\,\delta^{(3)}(\vec{k}-\vec{k}')$$

$$= \tilde{\Pi}(-\vec{k}',t) = \tilde{\Pi}^*(\vec{k}',t)$$

[$\because \quad \frac{\delta L}{\delta \tilde{\Pi}(\vec{k}',t)} = \int d^3k \frac{\delta\{\tilde{\Pi}(\vec{k},t)\}}{\delta \tilde{\Pi}(\vec{k},t)} \cdot \frac{\delta \tilde{\Pi}(\vec{k},t)}{\delta \tilde{\Pi}(\vec{k}',t)}\, \tilde{\Pi}(-\vec{k},t)$

$$= \int d^3k\, \delta^{(3)}(\vec{k}'-\vec{k})\,\tilde{\Pi}(-\vec{k},t)$$

$$= \tilde{\Pi}(-\vec{k}',t) \ ].$$

- Can we write,

$$i\frac{\partial \psi}{\partial t} = E\psi = \sqrt{-\vec{\nabla}^2+m^2}\ \psi \ ?$$

Now, if we transform, $\psi(\vec{x},t) \longrightarrow \tilde{\psi}(\vec{k},t)$,

then $\sqrt{-\vec{\nabla}^2+m^2} \longrightarrow \sqrt{\vec{k}^2+m^2}$.

Then, $\sqrt{-\vec{\nabla}^2+m^2}\ \psi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} \sqrt{\vec{k}^2+m^2}\ \tilde{\psi}(\vec{k},t)$

or $\boxed{-\vec{\nabla}^2 + m^2}\ \psi(\vec{x},t) = \int \frac{d^3\vec{k}}{(2\pi)^{3/2}} \boxed{\vec{k}^2 + m^2} \int \frac{d^3\vec{x}'}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}'} \psi(\vec{x}',t)$

This is clearly, a non-local theory.

Like, if we add terms like,

$(\psi(\vec{x},t))^2$, mimicking interactions, then we get a non-local theory.

- But, $[\Box - m^2]\phi + \lambda\phi^2 = 0$ still gives us a local theory.

In the non-linear case, it will not superpose, but, in the linear case, if there is a potential,

$$[\Box - m^2 + V(\vec{x})]\,\phi = 0$$

$$\left[\frac{-\partial^2}{\partial t^2} + \vec{\nabla}^2 - m^2 + V(\vec{x})\right]\phi = 0.$$

Then, we will have to choose the eigenfunctions of $\{\vec{\nabla}^2 - m^2 + V(\vec{x})\}$ operator.

27.1.2011

For the Klein-Gordon field, the action is,

$$S = \int dt\, d^3x\, \frac{1}{2}\left[(\partial_t\phi)^2 - (\vec{\nabla}\phi)^2 - m^2\phi^2\right]$$

We then traded in "ϕ" with its Fourier transform.

We thus introduced,

$$\tilde{\phi}(\vec{k},t) = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}}\,\phi(\vec{x},t).$$

We defined, $\pi(\vec{x},t) = \frac{\delta L}{\delta \dot{\phi}(\vec{x},t)}$; $\tilde{\pi}(\vec{k},t) = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} \pi(\vec{x},t)$,

i.e. $\tilde{\pi}(\vec{k},t) = \frac{\delta L}{\delta \dot{\tilde{\phi}}(\vec{k},t)}$.

Given this, the Hamiltonian,

$$H = \frac{1}{2}\int d^3k \left[\tilde{\pi}(\vec{k},t)\,\tilde{\pi}(-\vec{k},t) + (\vec{k}^2+m^2)\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)\right]$$

and we also had the Poisson-Bracket relations,

$$\{\tilde{\phi}(\vec{k},t),\ \tilde{\phi}(\vec{k}',t)\}_{P.B.} = 0,\quad \{\tilde{\pi}(\vec{k},t),\ \tilde{\pi}(\vec{k}',t)\}_{P.B.} = 0,$$
$$\{\tilde{\phi}(\vec{k},t),\ \tilde{\pi}(\vec{k}',t)\}_{P.B.} = \delta^{(3)}(\vec{k}+\vec{k}').$$

We also had the relations,

$$(\tilde{\phi}(\vec{k},t))^* = \tilde{\phi}(-\vec{k},t)$$
$$\text{and } (\tilde{\pi}(\vec{k},t))^* = \tilde{\pi}(-\vec{k},t)$$

We now try to quantise this theory.

We now consider $\tilde{\phi}, \tilde{\pi}$ as operators and their complex conjugate as the $\dagger$'s.

$\therefore$ We get :-

$$(\tilde{\phi}(\vec{k},t))^\dagger = \tilde{\phi}(-\vec{k},t)$$
$$\text{and } (\tilde{\pi}(\vec{k},t))^\dagger = \tilde{\pi}(-\vec{k},t)$$

and $[\tilde{\phi}(\vec{k},t), \tilde{\pi}(\vec{k}',t)] \equiv i\,\delta^{(3)}(\vec{k}+\vec{k}')$ [taking $\hbar = 1$].

The Hamiltonian now becomes an operator.

We define new operators which will have the same properties as the creation, annihilation operators.

We define :-

$$a(\vec{k},t) = \frac{1}{\sqrt{2}} \left(\omega_{\vec{k}}^{1/2} \tilde{\phi}(\vec{k},t) + i\, \omega_{\vec{k}}^{-1/2} \tilde{\Pi}(\vec{k},t) \right);$$

where $\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$,

$$a^\dagger(\vec{k}',t) = \frac{1}{\sqrt{2}} \left(\omega_{\vec{k}'}^{1/2} \tilde{\phi}^\dagger(\vec{k}',t) - i\, \omega_{\vec{k}'}^{-1/2} \tilde{\Pi}^\dagger(\vec{k}',t) \right)$$

$$= \frac{1}{\sqrt{2}} \left(\omega_{\vec{k}'}^{1/2} \tilde{\phi}(-\vec{k}',t) - i\, \omega_{\vec{k}'}^{-1/2} \tilde{\Pi}(-\vec{k}',t) \right).$$

$$\therefore \left[a(\vec{k},t), a^\dagger(\vec{k}',t) \right]$$

$$= -\frac{i}{2} \omega_{\vec{k}}^{1/2} \omega_{\vec{k}'}^{-1/2} \left[\tilde{\phi}(\vec{k},t), \tilde{\Pi}(-\vec{k}',t) \right]$$

$$+ \frac{i}{2} \omega_{\vec{k}}^{-1/2} \omega_{\vec{k}'}^{1/2} \left[\tilde{\Pi}(\vec{k},t), \tilde{\phi}(-\vec{k}',t) \right]$$

$$= -\frac{i}{2} \omega_{\vec{k}}^{1/2} \omega_{\vec{k}'}^{-1/2} \cdot i\, \delta^{(3)}(\vec{k} - \vec{k}')$$

$$+ \frac{i}{2}(-i)\, \delta^{(3)}(-\vec{k}' + \vec{k})$$

$$= \left(\frac{1}{2} + \frac{1}{2} \right) \delta^{(3)}(\vec{k} - \vec{k}') = \delta^{(3)}(\vec{k} - \vec{k}')$$

Similarly, $\left[a(\vec{k},t), a(\vec{k}',t) \right]$

$$= \frac{i}{2} \omega_{\vec{k}}^{1/2} \omega_{\vec{k}'}^{-1/2} \left[\tilde{\phi}(\vec{k},t), \tilde{\Pi}(\vec{k}',t) \right]$$

$$+ \frac{i}{2} \omega_{\vec{k}}^{-1/2} \omega_{\vec{k}'}^{1/2} \left[\tilde{\Pi}(\vec{k},t), \tilde{\phi}(\vec{k}',t) \right]$$

$$= \frac{i}{2} \omega_{\vec{k}}^{1/2} \omega_{\vec{k}'}^{-1/2} \cdot i\, \delta^{(3)}(\vec{k} + \vec{k}') + \frac{i}{2} \omega_{\vec{k}}^{-1/2} \omega_{\vec{k}'}^{1/2} (-i)\, \delta^{(3)}(\vec{k} + \vec{k}')$$

$$= 0.$$

Similarly, $[a^\dagger(\vec{k},t),\ a^\dagger(\vec{k}',t)] = 0$.

Now, $\hat{H} = \frac{1}{2}\int d^3k\ [\tilde{\Pi}(\vec{k},t)\tilde{\Pi}(-\vec{k},t) + \omega_{\vec{k}}^2\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)]$

Now, we want to get $\tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t)$
and $\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)$, so, we multiply,

$a(\vec{k},t)$ by $a^\dagger(\vec{k},t)$.

$$\therefore a(\vec{k},t)\,a^\dagger(\vec{k},t) = \frac{1}{2}[\omega_{\vec{k}}\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t) + \omega_{\vec{k}}^{-1}\tilde{\Pi}(\vec{k},t)\tilde{\Pi}(-\vec{k},t) - i\,\tilde{\phi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) + i\,\tilde{\Pi}(\vec{k},t)\tilde{\phi}(-\vec{k},t)]$$

Now, we want to remove the last two terms.

$$\text{Now, } a^\dagger(\vec{k},t)\,a(\vec{k},t) = \frac{1}{2}[\omega_{\vec{k}}\tilde{\phi}(-\vec{k},t)\,\tilde{\phi}(\vec{k},t) + \omega_{\vec{k}}^{-1}\tilde{\Pi}(-\vec{k},t)\tilde{\Pi}(\vec{k},t) + i\,\tilde{\phi}(-\vec{k},t)\,\tilde{\Pi}(\vec{k},t) - i\,\tilde{\Pi}(-\vec{k},t)\,\tilde{\phi}(\vec{k},t)]$$

Now, $[\tilde{\phi}(-\vec{k},t),\ \tilde{\Pi}(\vec{k},t)]$

$$= i\delta^{(3)}(\vec{k}-\vec{k}) = i\delta^{(3)}(0)$$

$$\therefore \tilde{\phi}(-\vec{k},t)\,\tilde{\Pi}(\vec{k},t) = \tilde{\Pi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t) + i\,\delta^{(3)}(\vec{k}=0)$$

$$\therefore a(\vec{k},t)\,a^\dagger(\vec{k},t) + a^\dagger(\vec{k},t)\,a(-\vec{k},t)$$

$$= \frac{1}{2}[2\omega_{\vec{k}}\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t) + 2\,\omega_{\vec{k}}^{-1}\tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) - i\,\tilde{\phi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) + i\,\tilde{\Pi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t) + i\,\tilde{\phi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) - i\,\tilde{\Pi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)]$$

$$= \omega_{\vec{k}}^{-1}\tilde{\Pi}(\vec{k},t)\,\tilde{\Pi}(-\vec{k},t) + \omega_{\vec{k}}\,\tilde{\phi}(\vec{k},t)\,\tilde{\phi}(-\vec{k},t)$$

$$\therefore \hat{H} = \frac{1}{2}\int d^3k\ \omega_{\vec{k}}\left[a(\vec{k},t)\, a^\dagger(\vec{k},t) + a^\dagger(-\vec{k},t)\, a(-\vec{k},t)\right]$$

Now, in the second term, we do $\vec{k} \longrightarrow -\vec{k}$, then we get:-

$$\int_{-\infty}^{+\infty} d^3k\ a^\dagger(-\vec{k},t)\, a(-\vec{k},t) \longrightarrow -\int_{+\infty}^{-\infty} d^3k\ a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

$$= \int_{-\infty}^{+\infty} d^3k\ a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

Thus, the second term is invariant under $\vec{k} \to -\vec{k}$.

Thus, $\hat{H} = \frac{1}{2}\int d^3k\ \omega_{\vec{k}}\left[a(\vec{k},t)\, a^\dagger(\vec{k},t) + a^\dagger(\vec{k},t)\, a(\vec{k},t)\right]$

Now, we have,

$$\left[a(\vec{k},t),\ a^\dagger(\vec{k},t)\right] = \delta^{(3)}(\vec{k}-\vec{k}) = \delta^{(3)}(0)$$

$$\therefore a(\vec{k},t)\, a^\dagger(\vec{k},t) = \delta^{(3)}(0) + a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

Thus, $$\hat{H} = \int d^3k\ \omega_{\vec{k}}\, a^\dagger(\vec{k},t)\, a(\vec{k},t) + \frac{1}{2}\left(\int d^3k\ \omega_{\vec{k}}\right)\delta^{(3)}(\vec{k}=0).$$

Now, the second term is an infinite constant. This overall constant is irrelevant, when we are interested in calculating the difference in energy between two states. The overall energy is completely arbitrary. It is only the difference in the energy of two levels that counts. Thus, we ignore the second term and simply write the Hamiltonian operator as:-

$$\hat{H} = \int d^3k\ \omega_{\vec{k}}\, a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

- **N.B:** Now, in the infinite term, we note that there are two very different kinds of infinities involved.

The term, $\int d^3k\, \omega_{\vec{k}} = \int d^3k \sqrt{\vec{k}^2+m^2}$ increases without bound with increasing $|\vec{k}|$.

Again, $\delta^{(3)}(\vec{k}=0)$ is another infinity because the spacetime has infinite volume.

If we take a box of finite volume, then, this divergence could be gotten rid of.

These kinds of divergences are known as ultraviolet (or short-distance) divergence. This occurs for very high energy / momentum (i.e. at very small distances).

We do not know whether this formula is valid for very high energies.

But, we can always put a cut-off.

We must note that, even in classical mechanics, the zero of the potential energy does not have any meaning. A zero level is always fixed and differences in energies are considered with respect to that level.

- N.B. energy is a source of gravity. So, when we encounter gravity, we can not leave out this second term. Thus, we face problems quantising gravity.

But, for our case at hand, we can choose a certain zero level.

In every problem, we should decide on what we should subtract. We should measure the difference in energies of the two levels.

we will never be able to measure this infinite term.

But, if we have independent oscillators with interactions, then what we subtract does not only depend on the oscillators but also on their interactions with each other.

Like, if we add a λx^4 to the existing $\frac{1}{2}kx^2$ term to the simple harmonic oscillator, then the zero level changes.

• N.B. If we take a system with no particles and say that it has zero energy and now if we add a particle with negative energy and take it to $-\infty$, then this is not allowed.

The individual energies should not be unbounded from below.

Thus, the Klein-Gordon equation, in the first quantised form, does not make much sense.

There, we had negative infinity (in the first quantised form).

But here (i.e., in the second quantised form), we have a positive infinity only. Thus, if we fix a zero level, everything is specified.

This way, we are fixing the zero-energy level. We can fix an "E_0". That energy will be for no particles. Then, adding particles is unambiguous.

• N.B. In the classical system "N" (the number of particles) is large.

Now, in the quantum system, if we did not have the $\frac{1}{2}\hbar\omega$, then there would have been no difference in the classical limit.

Thus, it is a purely quantum mechanical term that we are removing.

Here, this extra term is an analogous term, which is a quantum effect.

Here also, we can not measure simultaneously, $\phi, \tilde{\Pi}$ or q, Π, as they do not commute.

There are infinite numbers of Π's and ϕ's at infinite number of spacetime points.

The difference between the two points can be as small as possible but still, there can be an infinite number of points in between these two points. This is the ultraviolet divergence at small volumes.

If we consider a lattice, and if its volume is $1\,cm^3$, then there are finite number of points. But if we take this volume to infinity, then the number of points also tend to Infinity.

- Summary :- (i) one infinity is due to the infinite volume in space,
  (ii) another infinity is due to an infinite number of points between two points in space.

Thus, we drop the constant (infinite) term and take the Hamiltonian,

$$\hat{H} = \int d^3\vec{k}\, \omega_{\vec{k}}\, a^{\dagger}(\vec{k},t)\, a(\vec{k},t).$$

Then, we would like to build the eigenstates (at time $t=0$).

For every $\vec{k}$, it is like a harmonic oscillator.

So, the ground state is denoted by $|0\rangle$ such that for all $\vec{k}$, $a(\vec{k},t=0) \equiv a(\vec{k})$

and $a(\vec{k})|0\rangle = 0$.

But at any time 't', we will get the same spectrum, thus, $a(\vec{k},t)|0\rangle = 0$.

Thus, by construction, we have measured the ground state energy to be zero because,

$$\hat{H}|0\rangle = \int d^3k\, \omega_{\vec{k}}\, a^\dagger(\vec{k},t)\, a(\vec{k},t)|0\rangle = 0.$$

The first excited state will be $a^\dagger(\vec{k},t)|0\rangle$.

We will have, $\hat{H}\, a^\dagger(\vec{k},t)|0\rangle = \omega_{\vec{k}}\, a^\dagger(\vec{k},t)|0\rangle$.

Proof:- $\hat{H}\, a^\dagger(\vec{k},t)|0\rangle = \int d^3k'\, \omega_{\vec{k}'}\, a^\dagger(\vec{k}',t)\, a(\vec{k}',t)\, a^\dagger(\vec{k},t)|0\rangle$

$$= \int d^3k'\, \omega_{\vec{k}'}\, a^\dagger(\vec{k}',t)\left[\delta^{(3)}(\vec{k}-\vec{k}') + a^\dagger(\vec{k},t)\,\cancel{a(\vec{k}',t)}^{\,0}\right]|0\rangle$$

$$= \omega_{\vec{k}}\, a^\dagger(\vec{k},t)|0\rangle \quad [\text{Hence proved}].$$

$\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$.

Thus, single particle momentum states can be there with energy values, $\omega_{\vec{k}} = \sqrt{\vec{k}^2+m^2}$.

• N.B. Now, if we can measure the momentum eigenvalues, $\vec{k}$, i.e. if we can get the momentum eigenstates (by constructing the momentum operator), then we can say that the states are (the above ones) single particle momentum states.

Now, a second excited state may be,

$$a^\dagger(\vec{k}_1,t)\; a^\dagger(\vec{k}_2,t)|0\rangle.$$

Then $\hat{H}\, a^\dagger(\vec{k}_1,t)\, a^\dagger(\vec{k}_2,t)|0\rangle$

$$= \int d^3k\; \omega_{\vec{k}}\; a^\dagger(\vec{k},t)\, a(\vec{k},t)\, a^\dagger(\vec{k}_1,t)\, a^\dagger(\vec{k}_2,t)|0\rangle$$

$$= \int d^3k\; \omega_{\vec{k}}\; a^\dagger(\vec{k},t)\left[\delta^{(3)}(\vec{k}-\vec{k}_1) + a^\dagger(\vec{k}_1,t)\, a(\vec{k},t)\right]. \; a^\dagger(\vec{k}_2,t)|0\rangle$$

$$= \omega_{\vec{k}_1}\, a^\dagger(\vec{k}_1,t)\, a^\dagger(\vec{k}_2,t)|0\rangle + \int d^3k\; \omega_{\vec{k}}\; a^\dagger(\vec{k},t)\, a^\dagger(\vec{k}_1,t)\left[\delta^{(3)}(\vec{k}-\vec{k}_2) + a^\dagger(\vec{k}_2,t)\, a(\vec{k},t)\right]|0\rangle$$

$$= (\omega_{\vec{k}_1} + \omega_{\vec{k}_2})\, a^\dagger(\vec{k}_1,t)\, a^\dagger(\vec{k}_2,t)|0\rangle \qquad \left[\because [a^\dagger(\vec{k}_1,t), a^\dagger(\vec{k}_2,t)] = 0\right].$$

Thus, this denotes a two particle state given by two vectors with the total energy, $\sqrt{\vec{k}_1^2+m^2} + \sqrt{\vec{k}_2^2+m^2}$, where $\vec{k}_1$ is the momentum of one particle and $\vec{k}_2$ is that of the other particle.

- One particle level can be considered by the continuous parameter

The momentum eigenvalue (to be found later) in this case is $\vec{k}_1 + \vec{k}_2$.

Now, even if $\vec{k}_1 + \vec{k}_2 = 0$, the total energy is not zero as there is a $\sqrt{\vec{k}_1^2+m^2}$ and a $\sqrt{\vec{k}_2^2+m^2}$ which is a characteristic of two particles.

We can compare our second quantised Klein-Gordon Hamiltonian with the second quantised Schrödinger Hamiltonian.

In the Klein-Gordon case,

$$\hat{H}_{K.G.} = \int d^3k \sqrt{\vec{k}^2 + m^2}\; a^\dagger(\vec{k},t)\, a(\vec{k},t).$$

In the Schrödinger case,

$\hat{H}_S = \sum_n \epsilon_n a_n^\dagger a_n$; where the ϵ_n's are the single particle energy eigenvalues.

Here, the above Hamiltonian is for free particles.

Now, if we have a Schrödinger equation without a potential "V", then the ϵ_n's for free particles would have become continuous and then,

$$\hat{H}_S = \int d^3k \left(\frac{\vec{k}^2}{2m}\right) a^\dagger(\vec{k},t)\, a(\vec{k},t).$$

The equal-time commutation relations would be

$[a(\vec{k}), a(\vec{k}')] = 0,$

$[a^\dagger(\vec{k}), a^\dagger(\vec{k}')] = 0,$

and $[a(\vec{k}), a^\dagger(\vec{k}')] = \delta^{(3)}(\vec{k}-\vec{k}')$ [in both cases].

In $\hat{H}_{K.G.}$, $\sqrt{\vec{k}^2 + m^2}$ is actually, $\sqrt{\vec{k}^2 c^2 + m^2 c^4}$.

Now, for large "m" or small $|\vec{k}|$, we have,

$$\sqrt{\vec{k}^2 + m^2} \simeq m + \frac{\vec{k}^2}{2m} + \ldots\ldots$$

("m" is a constant term).

Thus, we see that in the non-relativistic limit, the structures of the two Hamiltonians, $\hat{H}_{Klein}$ and $\hat{H}_S$ are similar.

• N.B. But, we must note that at the first quantised level, the Klein-Gordon equation did not have a perfectly physical interpretation (because of infinite lower bound in energy) but the Schrödinger equation did have a perfectly physical interpretation.

Thus, though at the starting point, the Schrödinger equation was a single derivative in time and the Klein-Gordon equation involved a double derivative in time, yet, both yielded almost similar results. The latter is the relativistic version of the former.

Now, for $V=0$, the Schröding equation reads:-

$$i\frac{\partial\psi}{\partial t} = \hat{h}\psi = -\frac{1}{2m}\vec{\nabla}^2\psi \quad (\hbar=1).$$

Now, if we take, $\psi = e^{i\vec{u}\cdot\vec{x}}$ to be a solution, then,

$$-\frac{1}{2m}\vec{\nabla}^2\psi = -\frac{(i\vec{u})^2}{2m}e^{i\vec{u}\cdot\vec{x}} = \frac{\vec{u}^2}{2m}e^{i\vec{u}\cdot\vec{x}}.$$

Now, we want to find some operator which acting on $e^{i\vec{u}\cdot\vec{x}}$ would give $\sqrt{\vec{u}^2+m^2}$. Is it altogether possible?

We use the Fourier transform of $\psi(\vec{x},t)$ as:-

$$\tilde{\psi}(\vec{u},t) = \frac{1}{(2\pi)^{3/2}}\int e^{-i\vec{u}\cdot\vec{x}}\,\psi(\vec{x},t)\,d^3x.$$

We have,

$$\hat{H} = \int d^3x\, \psi^*(\vec{x},t)\ \hat{h}\ \psi(\vec{x},t)$$

$$= -\frac{1}{2m}\int d^3x \int \frac{d^3u}{(2\pi)^{3/2}} \int \frac{d^3u'}{(2\pi)^{3/2}}\, e^{i\vec{u}'\cdot\vec{x}}\, \tilde{\psi}^*(\vec{u}',t)\, \vec{\nabla}^2\, e^{-i\vec{u}\cdot\vec{x}}\, \tilde{\psi}(\vec{u},t)$$

$$= +\int \frac{d^3x}{(2\pi)^3} \int d^3u \int d^3u'\, e^{i(\vec{u}'-\vec{u})\cdot\vec{x}}\, \tilde{\psi}^*(\vec{u}',t)\, \frac{\vec{u}^2}{2m}\, \tilde{\psi}(\vec{u},t)$$

$$= \int d^3u \int d^3u'\, \delta^{(3)}(\vec{u}'-\vec{u})\, \tilde{\psi}^*(\vec{u}',t)\, \frac{\vec{u}^2}{2m}\, \tilde{\psi}(\vec{u},t)$$

$$\text{or } \hat{H} = \int d^3u\, \tilde{\psi}^*(\vec{u},t)\, \frac{\vec{u}^2}{2m}\, \tilde{\psi}(\vec{u},t).$$

We would like to find a $\hat{h}_{rel}$, such that :-

$$\hat{h}_{rel}\, e^{i\vec{u}\cdot\vec{x}} = \sqrt{\vec{u}^2+m^2}\ e^{i\vec{u}\cdot\vec{x}}.$$

Then we could have used the same Schrödinger equation. But, alas, we can not find a simple $\hat{h}_{rel}$.

There is linearity in "ψ", not in momentum.
We have to find a local differential operator.

Definition of $\hat{h}_{rel}$:- Given a function $\psi(\vec{x},t)$, $\hat{h}_{rel}$ should give another function.

Way about :- If we take the function $\psi(\vec{x},t)$, take its Fourier transform, multiply it by $\sqrt{\vec{u}^2+m^2}$ and take its inverse Fourier transform.

We define, $\hat{h}_{rel}\,\psi(\vec{x},t) = \frac{1}{(2\pi)^{3/2}} \int d^3u\, e^{i\vec{u}\cdot\vec{x}} \left(\sqrt{\vec{u}^2+m^2} \int \frac{d^3y}{(2\pi)^{3/2}}\, e^{-i\vec{u}\cdot\vec{y}}\, \psi(\vec{y},t) \right)$

Then, we will get:-

$S = \int d^3x\ \psi^*(\vec{x},t)\left(i\frac{\partial}{\partial t} - \hat{h}_{rel}\right)\psi(\vec{x},t)$ and quantise it and get the same $\hat{H}$, i.e.

$$\hat{H} = \int d^3x\ \sqrt{\vec{\nabla}^2+m^2}\ \hat{a}^{\dagger}(\vec{x},t)\hat{a}(\vec{x},t).$$

Local operator :- Depends on "ψ" and its derivative at all "x". But, clearly $\hat{h}_{rel}$ is not a local operator.

Only, if the operator is a polynomial in momentum, it is local, else, it is not so.

We now want to know about the interactions. In the Klein-Gordon case, the action,

$$S = \frac{1}{2}\int[(\partial_\mu\phi)^2 - (\vec{\nabla}\phi)^2 - m^2\phi^2]\,d^4x.$$

We have to know 'ϕ' and its derivatives at the same point.

We may think of each "ϕ" as a coordinate variable. If we couple two oscillators widely separated by two points in space, then it is a non-local scenario.

We may add $\hat{h}_{rel}[\psi^*(\vec{x},t)\ \psi^*(\vec{x},t)\ \psi(\vec{x},t)\ \psi(\vec{x},t)]$ which looks local, i.e. at the same space point. But actually, this is not local.

Because this formalism is not manifestly local (it has an action at a distance), we can not add such terms like, $\hat{h}_{rel}[\psi^*(\vec{x},t)\ \psi^*(\vec{x},t)\ \psi(\vec{x},t)\psi(\vec{x},t)]$.

It has a product of one $\psi^*(\vec{x},t)$ at one point and a 'ψ' at a completely different space-point. We do not know what kind of interactions will have an action at a distance.

Thus, in our theory, we should add every term to the Lagrangian which are at the same space points.
Here, we need the information at all points.
Any such Hamiltonian has a conserved particle number.

The number operator is,
$\hat{N} = \int d^3x\ a^\dagger(\vec{x})\, a(\vec{x})$ and in the Schrödinger problem, it is:-
$\hat{N} = \int d^3x\ \psi^\dagger(\vec{x},t)\ \psi(\vec{x},t)$.
We could have maintained the conservation by demanding that every term has the same number of ψ's and $\psi^\dagger$'s.
We can write the $a, a^\dagger$ in terms of the ϕ, Π's in the Klein-Gordon case, then the expression for the number operator (local) for ϕ, Π is complicated.

- **N.B.** So, typically, local interactions in the Klein-Gordon theory, do not conserve $\hat{N}$.

- Example:- If we add to the action,
$\Delta S = \int dt \int d^3x\ (\phi(\vec{x},t))^4$, then the extra term in the Lagrangian would be:-

$\Delta L = \int d^3x\ (\phi(\vec{x},t))^4$ and the extra term in the Hamiltonian would be:-
$\Delta H = -\int d^3x\ (\phi(\vec{x},t))^4$.

We can write $\phi(\vec{x},t)$ as a linear combination of a's and $a^\dagger$'s. Thus, we will have terms with equal number of a's and $a^\dagger$'s as well as unequal number of ~~them~~. For example, we will have terms like,

$$aaaa,\ aaaa^\dagger,\ aaaa^\dagger a^\dagger, \text{ and so on.}$$

So, local interactions written in terms of $\phi(\vec{x},t)$ do not conserve the number of particles.

So, in this theory, with high energy, we can get more particles.

But if someone does not bother about locality but only wants particle conservation, then he/she can work with $\psi, \psi^\dagger$. One could then add to the original action, some terms with equal number of ψ's and $\psi^\dagger$'s. Then we must use the Schrödinger representation.

But, in the relativistic case, we want locality. We do not want the transmission of signal > the speed of light.

So, we can not conserve particle number.

The number operator commutes with the Lorentz transformation operator, which can be checked by giving the system, a Lorentz boost.

We can not assign a charge to a given event. For local operators, we have ~~to~~ integrate over.

In relativity, if we have sufficient energy, we can create more particles.

We can always carry a particle and its antiparticle. relativity does not forbid it.

Two particle states have a different kind of dispersion relation.

On doing second quantisation, we get the correct spectrum.

For quadratic Lagrangians, we will get particle representation.

When there are cubic and / or higher order terms in the Lagrangian, we use perturbation theory. We can see scattering among particles.

In the first case, we solve a first quantised case and in the second quantisation case, we always start with the action for a single particle.

In Schrödinger picture, the time derivative is of order 1. There, we get the same spectrum for both the first and the second quantised cases. But, there is no guarantee that it will happen for all.

But, on the other hand, in the Klein-Gordon picture, in the first quantised theory, we get the energy spectrum as,

$\omega = \pm \sqrt{\vec{k}^2 + m^2}$, but in the second quantised theory, we only get the positive energy spectrum.

For fermions, we will assume that all the negative energy states have been filled up by the fermions.

[negative energy states are completely filled up].

We can always put a fermion in the positive energy level. (These are single particle states).

On the other hand, if we remove a negative energy electron (excite it so that it goes and occupies a positive energy level), then a "hole" is created. Then the total energy > the ground state energy.

But, for bosons, we can never fill the negative energy states completely, as we can always put more bosons to any energy level.

- We have, $[\phi(\vec{x},t), \Pi(\vec{y},t)] = i\delta^{(3)}(\vec{x}-\vec{y})$.
  We can think of $\Pi(\vec{y},t) = -i\dfrac{\delta}{\delta\phi(\vec{y},t)}$ just like in quantum mechanics, we take, $\hat{p} = -i\dfrac{\delta}{\delta x}$.

  Now, we imagine that there is a functional $F[\phi]$, then,

$$[\phi(\vec{x},t), \Pi(\vec{y},t)]F[\phi]$$
$$= -i\left[\phi(\vec{x},t), \frac{\delta}{\delta\phi(\vec{y},t)}\right]F[\phi]$$
$$= -i\left[\phi(\vec{x},t)\frac{\delta F[\phi]}{\delta\phi} - \frac{\delta}{\delta\phi}\{\phi F[\phi]\}\right]$$
$$= -i\left[\phi(\vec{x},t)\frac{\delta F[\phi]}{\delta\phi(\vec{y},t)} - \phi(\vec{x},t)\frac{\delta F[\phi]}{\delta\phi(\vec{y},t)} - F[\phi]\,\delta^{(3)}(\vec{x}-\vec{y})\right]$$
$$\left(\because \frac{\delta\phi(\vec{x},t)}{\delta\phi(\vec{y},t)} = \delta^{(3)}(\vec{x}-\vec{y})\right).$$

  or $[\phi(\vec{x},t), \Pi(\vec{y},t)]F[\phi] = iF[\phi]\delta^{(3)}(\vec{x}-\vec{y})$.

• Symmetries and conservation laws (Noether's theorem):-

Let us begin with some general system.

Suppose, we have a classical field theory with fields $\phi_1(x), \phi_2(x)$, ... (i.e. multiple fields).

These fields can either be scalar fields, or components of vector fields. In our study, we will not make any assumptions.

The action will be denoted as a functional,

$S = S[\{\phi_n(x)\}]$, where $x = (\vec{x}, t)$.

• Definitions:- A function gives a number, if we specify the arguments.

A functional gives a number, if we specify the functions, i.e. $\phi_1(x), \phi_2(x), \ldots$.

Example:- The Klein-Gordon action functional is:-

$$S = \frac{1}{2}\int dt \int d^3x \left[(\partial_t \phi)^2 - (\vec{\nabla}\phi)^2 - m^2\phi^2\right].$$

We now talk about a transformation of the fields.

The notion of a transformation is that, given a set of functions $\phi_1(x), \phi_2(x), \ldots, \phi_n(x)$, there is a rule which transforms these functions to $\tilde{\phi}_1(x), \tilde{\phi}_2(x), \ldots, \tilde{\phi}_n(x)$.

Thus, a transformation is a rule to generate new functions from a given set of functions.

The rule should be such that if we have any set of functions, then we can find the new set of functions.

Just like in quantum mechanics one can have $3N$ coordinates for N-particles. A classical field theory can have multiple number of fields.

The transformation is generally written as :-

$$\tilde{\phi}_s(y) = F_s\,[\{\phi_r(x)\}, y].$$

Here F_s denotes a functional of all these functions.
This is the most general form of the transformation.

"$\tilde{\phi}$" is a function of "y" for every point "y" and is a functional of all the fields, "ϕ".

Thus, we have to know all the ϕ_r's at all the space-time points.

We define a symmetry as when the transformation keeps the action unchanged. Thus, then the transformation generates a symmetry when,

$$S[\{\tilde{\phi}_r(x)\}] = S[\{\phi_r(x)\}] \text{ for all possible choices of } \{\phi_r(x)\}.$$

We have to put certain boundary conditions on the $\phi_r(x)$'s.

For a symmetry, the value of the action for these two sets of fields have to be the same.

• Example :- Space - time translation.

It is defined as :-

$\tilde{\phi}_r(x) \equiv \phi_r(x+a)$; where '$a$' is a constant 4-vector.

This is a transformation.

Now, we ask the question whether it is a symmetry or not. The answer obviously depends on what action we choose.

Let us for example choose the free scalar field,

i.e. $S[\phi] = \frac{1}{2}\int d^4x \left[-\eta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - m^2\phi^2 \right]$; where $\partial_\mu \equiv \frac{\partial}{\partial x^\mu}$.

Now, to check whether this is a symmetry under the above transformation, we calculate,

$$S[\tilde{\phi}] = \frac{1}{2}\int d^4x \left[-\eta^{\mu\nu}\partial_\mu\tilde{\phi}(x)\,\partial_\nu\tilde{\phi}(x) - m^2[\tilde{\phi}(x)]^2 \right]$$

$$= \frac{1}{2}\int d^4x \left[-\eta^{\mu\nu}\frac{\partial}{\partial x^\mu}\phi(x+a)\frac{\partial}{\partial x^\nu}\phi(x+a) - m^2\{\phi(x+a)\}^2 \right]$$

Now, we define $y^\mu = x^\mu + a^\mu$.

Then, $\frac{\partial}{\partial x^\mu} = \frac{\partial}{\partial y^\nu}\cdot\frac{\partial y^\nu}{\partial x^\mu} = \frac{\partial}{\partial y^\nu}\,\delta^\nu_\mu = \frac{\partial}{\partial y^\mu}$

and $d^4x = dx^0\,dx^1\,dx^2\,dx^3 = dy^0\,dy^1\,dy^2\,dy^3 = d^4y$.

[$\because$ a^μ is a constant four vector].

The range of integration ($-\infty$ to $+\infty$) remains the same (assume).

Then, by the above assumption, we get:-

$$S[\tilde{\phi}] = \frac{1}{2}\int d^4y \left[-\eta^{\mu\nu}\frac{\partial\phi(y)}{\partial y^\mu}\cdot\frac{\partial\phi(y)}{\partial y^\nu} - m^2\{\phi(y)\}^2\right]$$

Now, "y" is a dummy integration variable which we can very well write as "x".

Thus, we get:-

$$S[\tilde{\phi}] = \frac{1}{2}\int d^4x \left[-\eta^{\mu\nu}\frac{\partial\phi(x)}{\partial x^\mu}\cdot\frac{\partial\phi(x)}{\partial x^\nu} - m^2\{\phi(x)\}^2\right]$$

$$= S[\phi].$$

Thus, the above transformation is a symmetry in this case.

- N.B. We must note that adding a total time derivative to the action, does not change it. This is already allowed in this formalism. When a total derivative is added, it always integrates to zero at the boundary.

  We will assume that the fields fall off sufficiently fast at the boundary.

But, for the above action, a constant transformation, i.e. $\phi \to \tilde{\phi} = \phi + c$ ($c \equiv$ constant), will not be a symmetry because by no way, the term, $m^2\{\phi + c\}^2$ will give us $S[\tilde{\phi}] = S[\phi]$.

The condition that the symmetry holds is irrespective of the initial field configuration.

- N.B. If the initial fields $\phi_\pi(\vec{x},t)$ satisfy the equations of motion, then so do the $\tilde{\phi}_\pi(\vec{x},t)$'s.

That is, whatever variation we take in "$\phi_r(\vec{x},t)$", if we take in "$\tilde{\phi}_r(\vec{x},t)$", we will get the same equations of motion.

But, we should never use the equations of motion to prove symmetry.

We will check symmetry for "$\tilde{\psi}$" very close to "ψ", where we will have only first order correction terms.

- Example:- Let us consider the Schrödinger field theory.

The action is:- $S = \int dt \int d^3x \; \psi^*(\vec{x},t) \left[i \frac{\partial \psi(\vec{x},t)}{\partial t} - \hat{h} \psi(\vec{x},t) \right]$,
where we have taken $\hbar = 1$ and
$\hat{h} = -\frac{1}{2m} \vec{\nabla}^2 + V(\vec{x})$ as a differential operator.

Now, we ask if the transformation,

(i) $\tilde{\psi}(\vec{x},t) = \psi(\vec{x}+\vec{a}, t+a^0)$ a symmetry or not.

This is clearly not a symmetry because if we write,
$y^\mu = x^\mu + a^\mu$, then the form of the potential,
$V(x^\mu) = V(y^\mu - a^\mu)$ will change.

But for time independent potentials, the transformation,

$\tilde{\psi}(\vec{x},t) = \psi(\vec{x}, t+a^0)$ is a symmetry.

(ii) We can multiply "ψ" by some phase "α".

Then $\tilde{\psi}(\vec{x},t) = e^{i\alpha} \psi(\vec{x},t)$ [$\alpha \equiv$ constant].

Then $S[\tilde{\psi}(\vec{x},t)] = \int dt \int d^3x \; \psi^*(\vec{x},t) \, e^{-i\alpha} \left[i \frac{\partial}{\partial t} - \hat{h} \right] e^{i\alpha} \psi(\vec{x},t)$

$= S[\psi(\vec{x},t)]$.

The exponential terms cancel out.

Thus, $\tilde{\psi}(\vec{x},t) = e^{ia}\,\psi(\vec{x},t)$ is a symmetry in this case.

All of the above are examples of continuous symmetry. There are always some parameters (a^0, a) which would be continuous.

Analogous to the phase shift, in the scalar case, $\tilde{\phi} = -\phi$ is a symmetry. This is termed a discrete symmetry.

As the scalar field action has all quadratic terms, just by looking into it, we can say that $\tilde{\phi}(\vec{x},t) = -\phi(\vec{x},t)$ is a symmetry.

- Infinitesimal symmetries:- We can choose "$\tilde{\phi}$" close to "ϕ". So, from continuous symmetry, we can go to an infinitesimal symmetry by taking the parameters to be infinitesimal.

- Example :- We have, $\tilde{\phi}(x) = \phi(x+a)$. An infinitesimal symmetry means that, we want to choose "a^μ" such that,

$$\tilde{\phi}(x) = \phi(x+a) \approx \phi(x).$$

Property :- We imagine "a^μ" to be small (infinitesimal), such that,

$$\tilde{\phi}(x) = \phi(x) + a^\mu \frac{\partial \phi}{\partial x^\mu} + \mathcal{O}(a^2).$$

Here, we consider bounded functions and as long as $\frac{\partial \phi}{\partial x^\mu}$ is continuous in the limit $a \to 0$, we get :-

$$\tilde{\phi}(x) \to \phi(x)$$

• Example:- In the case,

$\tilde{\psi}(\vec{x},t) = e^{-i\alpha}\psi(\vec{x},t)$, in the limit $\alpha \to 0$, we get $\tilde{\psi}(\vec{x},t) = (1 - i\alpha)\psi(\vec{x},t) + \mathcal{O}(\alpha^2)$ + higher order terms.

$= \psi(\vec{x},t) - i\alpha\psi(\vec{x},t) + \mathcal{O}(\alpha^2) + \cdots$

• Now, we suppose that we have an infinitesimal transformation with some set of parameters $\epsilon^1, \epsilon^2, \cdots, \epsilon^K$ which are infinitesimal under which $\phi \approx \tilde{\phi}$.

Suppose, at this stage, we do not know whether it is a symmetry (i.e. the transformation) or not.

We calculate, $S[\tilde{\phi}] - S[\phi]$, irrespective of whether it is a symmetry or not. The difference is very small.

We get, $S[\tilde{\phi}] - S[\phi] = \sum_K \epsilon_K G_K + \mathcal{O}(\epsilon^2)$, where the G_K's are some functionals of $\{\phi_x(x)\}$ and we ignore the $\mathcal{O}(\epsilon^2)$ terms.

We define this (i.e. the infinitesimal transformation) to be a symmetry if all the G_K's are individually zeroes.

• Example:- Again, if we consider,

$S = \int dt \int d^3x\, \psi^*(\vec{x},t)\left[-i\frac{\partial}{\partial t} - \hat{h}\right]\psi(\vec{x},t)$ and the transformation,

$\tilde{\psi}(\vec{x},t) = \psi(\vec{x},t) + i\epsilon\psi(\vec{x},t)$ [we take "α" as "ϵ" here],

then, $S[\tilde{\psi}] - S[\psi] = \mathcal{O}(\epsilon^2)$.

Proof:- $S[\tilde{\psi}] = \int dt \int d^3x \{\psi^*(\vec{x},t) - i\epsilon \psi^*(\vec{x},t)\}[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V] \cdot \{\psi(\vec{x},t) + i\epsilon\psi(\vec{x},t)\}$.

$$= \int dt \int d^3x\, \psi^*(\vec{x},t)[i\frac{\partial}{\partial t} - \hat{h}]\psi(\vec{x},t)$$
$$- i\epsilon \int dt \int d^3x\, \psi^*(\vec{x},t)[i\frac{\partial}{\partial t} - \hat{h}]\psi(\vec{x},t)$$
$$+ i\epsilon \int dt \int d^3x\, \psi^*(\vec{x},t)[i\frac{\partial}{\partial t} - \hat{h}]\psi(\vec{x},t)$$
$$+ \epsilon^2 \int dt \int d^3x\, \psi^*(\vec{x},t)[i\frac{\partial}{\partial t} - \hat{h}]\psi(\vec{x},t)$$

$\therefore S[\tilde{\psi}] - S[\psi] = \epsilon^2 S[\psi] = O(\epsilon^2)$.

[Hence proved].

This means that the corresponding G_{rs}'s are zeroes and thus, this transformation is a symmetry.

∴ often we may not know off-hand what the transformations are like. So, we deal with the infinitesimal transformations and check whether the first order variation is zero or not.

- N.B. If we use the equations of motion [assuming that "ψ" satisfies the equations of motion] and get $\delta S = 0$ for all $\psi, \tilde{\psi}$, then this is an empty statement as we have already assumed that $\psi, \tilde{\psi}$ satisfy the equations of motion.

- We now take some infinitesimal symmetry transformation,

$\delta\tilde{\phi}_s(y) = \tilde{\phi}_s(y) - \phi_s(y) = \epsilon H_s[\{\phi_r(x)\}, y]$; where these H_s's are functionals.

Suppose we have checked that the above infinitesimal transformation is a symmetry,

i.e. $S[\tilde{\phi}] - S[\phi] = O(\epsilon^2)$.

Now, we define a new transformation, $\hat{\phi}_s(y)$ such that,

$\hat{\phi}_s(y) - \phi_s(y) = \epsilon(y)\, H_s[\{\phi_r(x)\}, y]$. That is, we have replaced the infinitesimal parameter by an infinitesimal function.

This is not going to be a symmetry in general.

We will calculate this,

$$S[\{\hat{\phi}_s(y)\}] - S[\{\phi_s(y)\}] = \int d^4x\, \partial_\mu \epsilon(x)\, J^\mu[\{\phi_r(y)\}, x]$$

for some functional J^μ.

The only reason that it may fail to be zero is because when the derivatives are acting on $\epsilon(y)$, they do not give zeroes as the $\epsilon(y)$'s are not constants as the ϵ's we previously had. Then, we knew that the variation is zero.

In this case, we will have terms where there will be atleast one derivative acting on "ϵ". If we have more derivatives acting on "ϵ", we integrate by parts, till we get only one derivative on "ϵ".

We will assume that the boundary terms, i.e. $\phi \xrightarrow{\infty} 0$ and $\partial_\mu \phi \xrightarrow{\infty} 0$.

If $\phi_s(y)$ satisfies the equations of motion, then,

$\int d^4x\, \partial_\mu \epsilon(x) J^\mu = 0$ for any $\epsilon(x)$.

Integrating by parts and demanding that J^μ vanishes at the boundary, we will get :-

$\int d^4x\, \epsilon(x)\, \partial_\mu J^\mu = 0$ for any $\epsilon(x)$,
which will in turn imply that,
$\partial_\mu J^\mu(x) = 0$.

- Exercise :- For the schrödinger field theory, the action is :-

$$S = \int d^3x\, dt\, \psi^*(\vec{x},t) \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V \right] \psi(\vec{x},t).$$

Previously, we had the following transformation,
$\hat{\psi}(\vec{x},t) = \psi(\vec{x},t) + i\epsilon\,\psi(\vec{x},t)$, which generated a symmetry (see pages 112-113).

Now, we consider the transformation,
$\hat{\psi}(\vec{x},t) = \psi(\vec{x},t) + i\,\epsilon(\vec{x},t)\,\psi(\vec{x},t)$.

We should first check that the terms without the derivatives of "$\epsilon(x)$" must cancel.

Check :-

$$S[\hat{\psi}] = \int dt \int d^3x \left[\psi^*(\vec{x},t) - i\epsilon(\vec{x},t)\,\psi^*(\vec{x},t) \right] \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V \right] \cdot \left[\psi(\vec{x},t) + i\epsilon(\vec{x},t)\psi(\vec{x},t) \right]$$

$$= S[\psi] - i\int dt \int d^3x\, \epsilon(\vec{x},t)\,\psi^*(\vec{x},t) \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V \right] \psi(\vec{x},t)$$
$$+ i\int dt \int d^3x\, \psi^*(\vec{x},t) \left[i\left(\frac{\partial \epsilon}{\partial t}\right)\psi(\vec{x},t) + i\epsilon(\vec{x},t)\frac{\partial \psi(\vec{x},t)}{\partial t} \right.$$
$$\left. + \frac{1}{2m}\vec{\nabla}\cdot(\psi\vec{\nabla}\epsilon + \epsilon\vec{\nabla}\psi) - V\epsilon(\vec{x},t)\psi(\vec{x},t) \right]$$
$$+ O(\epsilon^2) \text{ (neglect)}$$

or $S[\hat{\psi}] - S[\psi] = -i\int dt \int d^3x\, \epsilon(\vec{x},t)\psi^*(\vec{x},t) \left[\frac{1}{2m}\vec{\nabla}^2 - V \right] \psi(\vec{x},t)$
$$+ i\int dt \int d^3x\, \psi^*(\vec{x},t) \left[i\left(\frac{\partial \epsilon}{\partial t}\right)\psi(\vec{x},t) + \frac{1}{2m}\cdot 2\,\vec{\nabla}\psi\cdot\vec{\nabla}\epsilon \right.$$
$$+ \frac{1}{2m}\epsilon(\vec{x},t)\vec{\nabla}^2\psi(\vec{x},t)$$
$$+ \frac{1}{2m}\{\vec{\nabla}^2\epsilon(\vec{x},t)\}\psi(\vec{x},t)$$
$$\left. - V\epsilon(\vec{x},t)\psi(\vec{x},t) \right]$$

$$\text{or } S[\hat{\psi}] - S[\psi] = -\int dt \int d^3x \left\{ \frac{\partial \epsilon(\vec{x},t)}{\partial t} \right\} \psi^*(\vec{x},t)\psi(\vec{x},t)$$

$$+ \frac{\hbar}{m} \int dt \int d^3x \, \vec{\nabla}\epsilon \cdot (\vec{\nabla}\psi)\psi^*$$

$$+ \frac{\hbar}{2m} \int dt \int_S [\vec{\nabla}\epsilon(\vec{x},t)\, \psi^*\psi] \cdot d\vec{S}$$

$$- \frac{\hbar}{2m} \int dt \int d^3x \, \vec{\nabla}\epsilon(\vec{x},t) \cdot \vec{\nabla}(\psi^*\psi)$$

The surface integral vanishes and we get :-

$$S[\hat{\psi}] - S[\psi] = -\int dt \int d^3x \left\{ \frac{\partial \epsilon(\vec{x},t)}{\partial t} \right\} \psi^*(\vec{x},t)\psi(\vec{x},t)$$

$$- \frac{\hbar}{2m} \int dt \int d^3x \, \vec{\nabla}\epsilon(\vec{x},t) \cdot \{ \psi^*\vec{\nabla}\psi + \psi\vec{\nabla}\psi^* - 2\psi^*\vec{\nabla}\psi \}$$

$$= \int d^4x \, \partial_\mu \epsilon(\vec{x},t)\, J^\mu$$

where $J^\mu = \left(-\psi^*(\vec{x},t)\psi(\vec{x},t), \frac{\hbar}{2m}[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*] \right)$

$$J^0 = -\psi^*(\vec{x},t)\psi(\vec{x},t) = -|\psi(\vec{x},t)|^2$$

and $J^i = \frac{\hbar}{2m}[\psi^*(\vec{x},t)\partial_i\psi(\vec{x},t) - \psi(\vec{x},t)\partial_i\psi^*(\vec{x},t)]$

Now, $\partial_\mu J^\mu = \partial_0 J^0 + \partial_i J^i$

$$= -\frac{\partial}{\partial t}\{\psi^*(\vec{x},t)\psi(\vec{x},t)\} + \frac{\hbar}{2m}\vec{\nabla}\cdot[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*]$$

$$= -\psi^*\frac{\partial\psi}{\partial t} + \left(-\psi\frac{\partial\psi^*}{\partial t}\right) + \frac{\hbar}{2m}\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi + \frac{\hbar}{2m}\psi^*\vec{\nabla}^2\psi$$

$$- \frac{\hbar}{2m}\vec{\nabla}\psi\cdot\vec{\nabla}\psi^* - \frac{\hbar}{2m}\psi\vec{\nabla}^2\psi^*$$

$$= \hbar\psi^*\left(-\frac{1}{2m}\vec{\nabla}^2\psi + (-\hbar)\frac{\partial\psi}{\partial t}\right) + \hbar\psi\left(-\frac{1}{2m}\vec{\nabla}^2\psi^* + \hbar\frac{\partial\psi^*}{\partial t}\right)$$

Now, the Schrödinger equation is:-

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2m}\vec{\nabla}^2\psi + V\psi$$

and its conjugate equation is:-

$$-i\frac{\partial\psi^*}{\partial t} = -\frac{1}{2m}\vec{\nabla}^2\psi^* + V\psi^*.$$

Thus, $\partial_\mu J^\mu = -i\psi^*(-V\psi) + i\psi(-V\psi^*)$

$= i\psi^* V\psi - i\psi V\psi^*$

$= 0.$

Thus, the charges are conserved. This gives us the conserved charges for this theory.

Thus, the time derivative $J^0 = -\psi^*\psi$ and the space derivatives, $J^i = \frac{i}{2m}(\psi^*\partial_i\psi - \psi\partial_i\psi^*)$ are conserved.

16.2.2011

We assumed that our theory has certain symmetries.

We assumed that there are many fields $\phi_1, \phi_2, \ldots$ and the corresponding action is:- $S[\{\phi_r(x)\}]$.

We then defined a transformation of the field,

$\tilde{\phi}_r(x) = F_r[\{\phi_s(y)\}; x]$; the "x" is there as we need to define $\tilde{\phi}_r(x)$ at every spacetime point "x".

We declared the above transformation to be a symmetry, if:-

$$S[\{\tilde{\phi}_r(x)\}] = S[\{\phi_r(x)\}].$$

i.e., the action evaluated in the new field configuration = the action evaluated at the old field configuration.

We then introduced the continuous symmetry, where the transformation was labelled by some continuous parameters $a_1, a_2, \ldots$.

Often, it is a useful convention that if we set the a_i's $= 0$, then $\tilde{\phi}_r = \phi_r$.

This is chosen as the origin of the parameter space.

• example :- (i) Translations :- Here, the transformation rule was :-

$\tilde{\phi}(x) = \phi(x+a)$; where 'a' is a constant 4-vector, (a^0, a^1, a^2, a^3).

If $a^\mu = 0$, then, $\tilde{\phi}(x) = \phi(x)$.

(ii) In the Schrödinger field theory, we defined, the transformation (found to be a symmetry) as :-

$$\psi(\vec{x}, t) = e^{i\alpha}\, \psi(\vec{x}, t)$$

Now, setting $\alpha = 0$, we get :-

$$\tilde{\psi}(\vec{x}, t) = \psi(\vec{x}, t)$$

Of course, we could have written,

$\tilde{\psi}(\vec{x}, t) = e^{i(\alpha+2)}\psi(\vec{x}, t)$ for example which again would have been a symmetry. In that case, $\alpha = -2 \Rightarrow \tilde{\psi}(\vec{x}, t) = \psi(\vec{x}, t)$.

Then, we introduced the notion of infinitesimal transformation where the transformation parameter is not zero but is infinitesimally small (i.e. small a^μ's, so that :-

$\tilde{\phi}_r(x) \approx \phi_r(x)$ (very close to but not exactly equal).

In this case, we could write the transformation as:-

$$\tilde{\phi}_r(x) = \phi_r(x) + \epsilon f_r[\{\phi_s(y)\}, x] + \mathcal{O}(\epsilon^2) + \cdots ;$$

where "f_r" is a functional and "ϵ" is an infinitesimal parameter.

Based on infinitesimal transformations, we derived a relation between symmetries and conservation laws.

Let us imagine that the above transformation is a symmetry. We then make "ϵ" as a function of "x" (space-time), $\epsilon(x)$. "S" then is no longer a symmetry in general.

Then, $S[\tilde{\phi}] - S[\phi] \neq 0$

$= \int d^4x \, \partial_\mu \epsilon(x) J^\mu(x)$, where $J^\mu(x)$ is a functional of the fields and a function of "x".

The reason for this generic form is that, it is linear in "ϵ". If "ϵ" is a constant, this difference obviously vanishes. The non-zero result is due to the derivative of "ϵ".

Now, the above relation implies (if throughout we assume that the fields fall off at ∞), that,

$$\int d^4x \, \epsilon(x) \partial_\mu J^\mu(x) = 0,$$

iff the equations of motion hold, then, thus for any "ϕ", to first order,

$$S[\tilde{\phi}] - S[\phi] \simeq 0,$$

i.e. $S[\tilde{\phi}] - S[\phi] = O(\epsilon^2)$

$\Rightarrow \partial_\mu J^\mu = 0$, i.e. when the equations of motion hold.

There are 4-components of J^μ, we do not assume Lorentz invariance.

- Let us now consider the Schroidinger problem :-

The action, $S = \int dt\, d^3x\, \psi^*(x) \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V(x) \right] \psi(x)$.

The symmetry condition is :-

$$\tilde{\psi} = e^{i\alpha}\psi .$$

For infinitesimal symmetry transformation, $\alpha = \epsilon$.

Then, $\tilde{\psi} = \psi + i\epsilon\psi$.

Now, we consider the transformation,

$\tilde{\psi}(x) = \psi(x) + i\epsilon(x)\psi(x)$ and calculate $S[\tilde{\psi}]$.

Then $S[\tilde{\psi}] = \int dt\, d^3x \left[\psi^*(x) - i\epsilon(x)\psi^*(x) \right] \cdot \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V(x) \right] \cdot \left[\psi(x) + i\epsilon(x)\psi(x) \right]$.

$$= S[\psi] + \int dt\, d^3x \left[-i\epsilon(x)\psi^*(x) \right] \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V(x) \right] \psi(x)$$

$$+ \int dt\, d^3x\, \psi^* x \left[i\frac{\partial}{\partial t} + \frac{1}{2m}\vec{\nabla}^2 - V(x) \right] \left[i\epsilon(x)\psi(x) \right] .$$

Now, we get :-

$$S[\tilde{\psi}] - S[\psi] = \int dt\, d^3x \left[-i\epsilon(x)\psi^*(x) \right] \left[i\frac{\partial \psi(x)}{\partial t} + \frac{1}{2m}\nabla^2\psi(x) - V(x)\psi(x) \right]$$

$$+ \int dt\, d^3x\, \psi^*(x) \Big[i\frac{\partial (i\epsilon(x))}{\partial t}\psi(x) - \epsilon(x)\frac{\partial \psi(x)}{\partial t}$$

$$+ \frac{i}{2m}\epsilon(x)\nabla^2\psi(x) + \frac{i}{2m}\psi(x)\nabla^2\epsilon(x)$$

$$+ \frac{i}{m}\vec{\nabla}\epsilon(x)\cdot\vec{\nabla}\psi(x) - iV(x)\epsilon(x)\psi(x) \Big]$$

Thus, we get :-

$$S[\tilde{\psi}] - S[\psi] = \int dt\, d^3x \left[-\psi^*(x) \frac{\partial \epsilon(x)}{\partial t} \psi(x) \right.$$

$$\left. + \frac{i\hbar}{2m} \psi^*(x) \psi(x) \vec{\nabla}^2 \epsilon(x) \right.$$

$$\left. + \frac{i\hbar}{m} \psi^*(x) \vec{\nabla} \epsilon(x) \cdot \vec{\nabla} \psi(x) \right].$$

Now, the second term is :-

$$\frac{i\hbar}{2m} \int dt\, d^3x\, \psi^* \vec{\nabla}^2 \epsilon(x)\, \psi(x)$$

$$= \frac{i\hbar}{2m} \int dt\, d^3x\, \vec{\nabla} \cdot \left(\vec{\nabla} \epsilon(x)\, \psi^*(x) \psi(x) \right)$$

$$- \frac{i\hbar}{2m} \int dt\, d^3x\, \vec{\nabla} \epsilon(x) \cdot \vec{\nabla} (\psi^*(x) \psi(x))$$

Now, the first term can be converted to a surface integral which vanishes at the boundary.

Thus, we get :-

$$S[\tilde{\psi}] - S[\psi] = \int dt\, d^3x \left[\frac{\partial \epsilon(x)}{\partial t} (-\psi^*(x) \psi(x)) \right.$$

$$\left. + \frac{i\hbar}{2m} \vec{\nabla} \epsilon(x) \cdot \left[-\psi^*(x) \vec{\nabla} \psi(x) - \psi(x) \vec{\nabla} \psi^*(x) \right.\right.$$

$$\left.\left. + 2\psi^*(x) \vec{\nabla} \psi(x) \right] \right]$$

$$= \int dt\, d^3x \left[\frac{\partial \epsilon(x)}{\partial t} (-\psi^*(x) \psi(x)) \right.$$

$$\left. + \frac{i\hbar}{2m} \vec{\nabla} \epsilon(x) \cdot \left[\psi^*(x) \vec{\nabla} \psi(x) - \psi(x) \vec{\nabla} \psi^*(x) \right] \right]$$

$$= \int dt\, d^3x\, \partial_\mu \epsilon(x)\, J^\mu(x) ;$$

where $J^0(x) = -\psi^*(x) \psi(x)$

and $J^i(x) = \frac{i\hbar}{2m} \left[\psi^*(x) \partial_i \psi(x) - (\partial_i \psi^*(x)) \psi(x) \right].$

This is a conserved current in the Schrödinger picture.

[See proof in pages 116–117.]

$\partial_\mu J^\mu = 0$

$\therefore \int dt \int d^3x \, \partial_\mu J^\mu = 0.$

$\Rightarrow \int dt \int d^3x \, \partial_0 J^0 + \int dt \int d^3x \, \partial_i J^i = 0$

Now, the second term vanishes if the fields $\to 0$ at infinity.

$\Rightarrow Q = \int d^3x \, J^0$ is conserved.

conserved charge calculated at a fixed time slice.

The conserved charge remains the same provided the fields evolve with the equation of motion.

[The conservation laws hold when the equations of motion are satisfied.

It can be different in different frames though.].

- Symmetry of Maxwell's source free equations:-

$$S = \int d^4x \, (\vec{E}^2 - \vec{B}^2).$$

But this action is not symmetric under $\vec{E} \leftrightarrow \vec{B}$.

$\vec{\nabla} \cdot \vec{B} = 0$

and $\vec{\nabla} \cdot \vec{E} = 0$ (if no charge density).

These equations are symmetric under the rotation of $\vec{E}$ and $\vec{B}$.

[There are cases where even the action principle is not known.

If we can find such an action, we can then use Noether's procedure else not].

- For simplicity we now take the Klein-Gordon field "ϕ^4" :-

$$S = \int d^4x \left[-\frac{1}{2} \eta^{\rho\sigma} \partial_\rho \phi \, \partial_\sigma \phi - \frac{1}{2} m^2 \phi^2 \right].$$

We now consider a symmetry,

$$\tilde{\phi}(x) = \phi(x+a) \quad (\text{i.e. translation}).$$

To show that this is a symmetry, we just shift the integration variable from x to $y = (x+a)$.

We now take $a^\mu = \epsilon^\mu$ (infinitesimal),

then, $\tilde{\phi}(x) = \phi(x) + \epsilon^\mu \partial_\mu \phi(x)$.

This calls for a four-conserved charge.

For the Schrödinger equation, we had one parameter "α" and hence one conserved charge.

Now, we assume $\epsilon^\mu(x)$.

Then, $S[\tilde{\phi}] = \int d^4x \Big[-\frac{1}{2}\eta^{\rho\sigma} \partial_\rho (\phi(x) + \epsilon^\mu(x)\partial_\mu\phi(x)) \partial_\sigma (\phi(x) + \epsilon^\nu(x)\partial_\nu\phi(x))$
$- \frac{1}{2} m^2 (\phi(x) + \epsilon^\mu(x)\partial_\mu\phi(x))(\phi(x) + \epsilon^\nu(x)\partial_\nu\phi(x)) \Big]$

$= S[\phi] + \int d^4x \Big[-\frac{1}{2}\eta^{\rho\sigma} \partial_\rho\phi(x) \partial_\sigma(\epsilon^\mu(x)\partial_\mu\phi(x))$
$+ -\frac{1}{2}\eta^{\rho\sigma} \partial_\rho(\epsilon^\mu(x)\partial_\mu\phi(x)) \partial_\sigma\phi(x) \Big]$

$+ \int d^4x \Big[-\frac{1}{2} m^2 \big[\phi(x)\epsilon^\nu(x)\partial_\nu\phi(x) + \phi(x)\epsilon^\mu(x)\partial_\mu\phi(x) \big]$
$+ O(\epsilon^2)$

Now, $\eta^{\rho\sigma}\partial_\rho\phi(x)\partial_\sigma(\epsilon^\mu(x)\partial_\mu\phi(x)) = \eta^{\rho\sigma}\partial_\sigma\phi(x)\partial_\rho(\epsilon^\mu(x)\partial_\mu\phi(x))$

$\therefore S[\tilde{\phi}] - S[\phi] = -\int d^4x \big[\eta^{\rho\sigma}\partial_\rho\phi(x)\partial_\sigma(\epsilon^\mu(x)\partial_\mu\phi(x))\big]$
$- \int d^4x\, \phi(x)\epsilon^\mu(x)\partial_\mu\phi(x) m^2 + O(\epsilon^2)$

$= -\int d^4x \Big[\eta^{\rho\sigma}\partial_\rho\phi(x)\big(\partial_\sigma\epsilon^\mu(x)\big)\partial_\mu\phi(x)$
$+ \eta^{\rho\sigma}\partial_\rho\phi(x)\partial_\sigma\big(\partial_\mu\phi(x)\big)\epsilon^\mu(x)$
$+ m^2\phi(x)\epsilon^\mu(x)\partial_\mu\phi(x) \Big]$

Now, we can write,

$$\phi(x)\partial_\mu\phi(x) = \frac{1}{2}\partial_\mu[\phi(x)]^2$$

And $\eta^{\beta\sigma}\partial_\beta\phi(x)\{\partial_\sigma\partial_\mu\phi(x)\}$ as $\eta^{\beta\sigma}\partial_\sigma\phi(x)\{\partial_\beta\partial_\mu\phi(x)\}$

Thus, this term can be written as:-

$$\frac{1}{2}\eta^{\beta\sigma}\partial_\mu[\partial_\beta\phi(x)\partial_\sigma\phi(x)] \quad [\because \partial_\beta\partial_\mu \equiv \partial_\mu\partial_\beta \text{ etc.}].$$

$$\therefore S[\tilde{\phi}] - S[\phi] = -\int d^4x\,[\eta^{\beta\sigma}\partial_\beta\phi(x)(\partial_\sigma\epsilon^\mu(x))\partial_\mu\phi(x) + \frac{1}{2}\partial_\mu[\eta^{\beta\sigma}\partial_\beta\phi(x)\partial_\sigma\phi(x)]\epsilon^\mu(x) + \frac{m^2}{2}\partial_\mu[\phi(x)]^2\epsilon^\mu(x)].$$

Now, we integrate by parts the last two terms and let the boundary terms $\to 0$ at the boundary. Then, we get:-

$$S[\tilde{\phi}] - S[\phi] = \int d^4x\,[-\eta^{\beta\sigma}\partial_\beta\phi(x)(\partial_\sigma\epsilon^\mu(x))\partial_\mu\phi(x) + \frac{1}{2}\partial_\mu\epsilon^\mu(x)\eta^{\beta\sigma}\partial_\beta\phi(x)\partial_\sigma\phi(x) + \frac{1}{2}\partial_\mu\epsilon^\mu(x)m^2[\phi(x)]^2].$$

$$= \int d^4x\,\partial_\nu\epsilon^\mu(x)[-\eta^{\beta\nu}\partial_\beta\phi(x)\partial_\mu\phi(x) + \frac{1}{2}\delta_\mu{}^\nu\eta^{\beta\sigma}\partial_\beta\phi(x)\partial_\sigma\phi(x) + \frac{1}{2}\delta_\mu{}^\nu m^2[\phi(x)]^2].$$

or $S[\tilde{\phi}] - S[\phi] = \int d^4x\,\partial_\nu\epsilon^\mu(x)\,T_{(\mu)}^{\nu}$; The "μ" index shows that there are four different conserved currents, for each component there is one conserved current. Each conserved current again has four components.

$$\therefore T_{(\mu)}^{\nu} = \frac{1}{2}\delta_\mu{}^\nu\eta^{\beta\sigma}\partial_\beta\phi(x)\partial_\sigma\phi(x) + \frac{1}{2}\delta_\mu{}^\nu m^2[\phi(x)]^2 - \eta^{\beta\nu}\partial_\beta\phi(x)\partial_\mu\phi(x).$$

The continuity equation then is:-

$$\partial_\tau J^\tau_{(\mu)} = 0.$$

There will be four such equations, one for each "μ".

[When we write $\frac{dQ}{dt} = 0$, then J^τ should be zero at the boundary.].

[$\mu \equiv$ depends on what symmetry we are considering.

$J^\tau_{(0)} \equiv$ time translation

$J^\tau_{(1)} = x^1$ translation, and so on.].

To prove that,

$$\partial_\tau J^\tau_{(\mu)} = 0.$$

Proof :- $\partial_\tau \left[\frac{1}{2} \delta_\mu{}^\tau \eta^{\beta\sigma} \partial_\beta \phi(x) \partial_\sigma \phi(x) + \frac{1}{2} \delta_\mu{}^\tau m^2 [\phi(x)]^2 - \eta^{\beta\tau} \partial_\beta \phi(x) \partial_\mu \phi(x) \right].$

$$= \frac{1}{2} \partial_\mu \left[\eta^{\beta\sigma} \partial_\beta \phi(x) \partial_\sigma \phi(x) \right] + \frac{m^2}{2} \partial_\mu [\phi(x)]^2 - \partial^\beta (\partial_\beta \phi(x) \partial_\mu \phi(x)).$$

$$= \frac{1}{2} \partial_\mu [\partial_\beta \phi(x) \partial^\beta \phi(x)] + \frac{m^2}{2} 2 \phi(x) \partial_\mu \phi(x) - (\partial^\beta \partial_\beta \phi(x)) \partial_\mu \phi(x) - \partial_\beta \phi(x) \partial^\beta \partial_\mu \phi(x)$$

[The Klein - Gordon equation is :-

$$\partial^\beta \partial_\beta \phi(x) + m^2 \phi(x) = 0.]$$

$\therefore$ we get :-

$$\partial_\tau J^\tau_{(\mu)} = \frac{1}{2} (\partial_\mu \partial_\beta \phi(x)) \partial^\beta \phi(x) + \frac{1}{2} \partial_\beta \phi(x) \partial_\mu \partial^\beta \phi(x) + m^2 \phi(x) \partial_\mu \phi(x) - m^2 \phi(x) \partial_\mu \phi(x) - \partial_\beta \phi(x) \partial^\beta \partial_\mu \phi(x)$$

Now, the first term is :-

$$\frac{1}{2}\partial^{\beta}\phi(x)\,(\partial_{\mu}\partial_{\beta}\phi(x))$$
$$-\frac{1}{2}\partial_{\beta}\phi(x)\,(\partial_{\mu}\partial^{\beta}\phi(x))$$

Thus, the first and the second terms are equal.

$\therefore$, we get :-

$$\partial_{\tau}J_{(\mu)}^{\tau} = \partial_{\beta}\phi(x)\,(\partial_{\mu}\partial^{\beta}\phi(x)) - \partial_{\beta}\phi(x)\,(\partial^{\beta}\partial_{\mu}\phi(x))$$

Now, the second term is :-

$$\partial_{\beta}\phi(x)\,(\partial^{\beta}\partial_{\mu}\phi(x)) - \partial_{\beta}\phi(x)\,(\partial_{\mu}\partial^{\beta}\phi(x))$$

$\therefore \partial_{\tau}J_{(\mu)}^{\tau} = 0$. [Hence proved].

- The energy momentum tensor is defined as :-

$$T^{\nu\tau} = -\eta^{\mu\nu}J_{(\mu)}^{\tau} \quad [\text{'}-\text{'} \text{ sign is a convention}].$$

Thus, we get from

$$\partial_{\tau}J_{(\mu)}^{\tau} = 0$$
$$\Rightarrow \partial_{\tau}(-\eta^{\mu\nu}J_{\mu}^{(\tau)}) = 0$$

or $\partial_{\tau}T^{\nu\tau} = 0$;

and $T^{\nu\tau} = -\frac{1}{2}\eta^{\nu\tau}\eta^{\beta\sigma}\partial_{\beta}\phi(x)\,\partial_{\sigma}\phi(x) - \frac{1}{2}\eta^{\nu\tau}m^{2}[\phi(x)]^{2} + \eta^{\beta\tau}\eta^{\nu\mu}\partial_{\beta}\phi(x)\,\partial_{\mu}\phi(x)$.

The conserved charges are defined as :-

$P^{\nu} = \int T^{\nu 0}\,d^{3}x$ and $P^{0} = \int T^{00}\,d^{3}x$; where 0 is the index of 'J'.

$$\therefore P^i = \int T^{i0}\, d^3x$$

$$= \int \Big[-\tfrac{1}{2}\eta^{i0}\,\eta^{\rho\sigma}\,\partial_\rho\phi(x)\,\partial_\sigma\phi(x) - \tfrac{1}{2}\eta^{i0}\,m^2\,[\phi(x)]^2 + \eta^{\rho 0}\,\eta^{i\mu}\,\partial_\rho\phi(x)\,\partial_\mu\phi(x)\Big]\, d^3x$$

Now, as $i \neq 0$, the first two terms vanish.

In the second term, the non-zero contribution comes from $\rho = 0$ and $\mu = i$. Thus,

$$P^i = -\int \partial_i\phi(x)\,\partial_0\phi(x)\, d^3x$$

$$\text{and } P^0 = \int T^{00}\, d^3x = \int \Big[-\tfrac{1}{2}\eta^{00}\,\eta^{\rho\sigma}\,\partial_\rho\phi(x)\partial_\sigma\phi(x) - \tfrac{1}{2}\eta^{00}\,m^2[\phi(x)]^2 + \eta^{\rho 0}\,\eta^{0\mu}\,\partial_\rho\phi(x)\,\partial_\mu\phi(x)\Big] d^3x$$

Now, the last two terms gives:-

$$\tfrac{1}{2}m^2[\phi(x)]^2 + \partial_0\phi(x)\,\partial_0\phi(x)$$

and the first term is:- $\tfrac{1}{2}\eta^{\rho\sigma}\,\partial_\rho\phi(x)\partial_\sigma\phi(x)$.

Again, we get:-

$$P^0 = \tfrac{1}{2}\int d^3x\, \big[-(\partial_0\phi(x))^2 + (\vec{\nabla}\phi)^2 + m^2[\phi(x)]^2\big] + \int d^3x\,(\partial_0\phi(x))^2$$

$$= \tfrac{1}{2}\int d^3x\, \big[(\partial_0\phi(x))^2 + (\vec{\nabla}\phi)^2 + m^2[\phi(x)]^2\big] = H$$

Now, coming back to $P^i = -\int \partial_i\phi(x)\,\partial_0\phi(x)\, d^3x$

$$\text{or } P^i = -\int d^3x \int \frac{d^3k}{(2\pi)^3}\int d^3k'\, \partial_i e^{i\vec{k}\cdot\vec{x}}\, \tilde{\phi}(\vec{k},t)\, e^{-i\vec{k}'\cdot\vec{x}}\, \tilde{\pi}(\vec{k}',t)$$

$$\text{or} \quad P^i = -\int d^3k \int d^3k' \,(-ik_i)\, \delta(\vec{k}+\vec{k}')\, \tilde{\phi}(\vec{k},t)\, \tilde{\Pi}(\vec{k}',t)$$

$$= -\int d^3k\,(-ik_i)\, \tilde{\phi}(\vec{k},t)\, \tilde{\Pi}(-\vec{k},t)$$

Now, in terms of a's and $a^\dagger$'s, we have :-

$$\frac{1}{\sqrt{2}}\omega_{\vec{k}}^{1/2}\tilde{\phi}(\vec{k},t) + \frac{i}{\sqrt{2}}\omega_{\vec{k}}^{-1/2}\tilde{\Pi}(\vec{k},t) = a(\vec{k},t)$$

$$\text{and} \quad \frac{1}{\sqrt{2}}\omega_{\vec{k}}^{1/2}\tilde{\phi}(-\vec{k},t) - \frac{i}{\sqrt{2}}\omega_{\vec{k}}^{-1/2}\tilde{\Pi}(-\vec{k},t) = a^\dagger(\vec{k},t)$$

$$\therefore \quad \frac{2}{\sqrt{2}}\omega_{\vec{k}}^{1/2}\tilde{\phi}(\vec{k},t) = a(\vec{k},t) + a^\dagger(-\vec{k},t)$$

$$\text{or} \quad \tilde{\phi}(\vec{k},t) = \frac{1}{\sqrt{2}}\omega_{\vec{k}}^{-1/2}\left[a(\vec{k},t) + a^\dagger(-\vec{k},t)\right]$$

$$\text{and} \quad \frac{2i}{\sqrt{2}}\omega_{\vec{k}}^{-1/2}\tilde{\Pi}(-\vec{k},t) = a(-\vec{k},t) - a^\dagger(\vec{k},t)$$

$$\text{or} \quad \tilde{\Pi}(-\vec{k},t) = \frac{1}{\sqrt{2}i}\omega_{\vec{k}}^{1/2}\left[a(-\vec{k},t) - a^\dagger(\vec{k},t)\right]$$

Thus, putting these in the expression of P^i, we get :-

$$P^i = -\frac{1}{2}\int d^3k\, k_i \left[a(\vec{k},t) + a^\dagger(-\vec{k},t)\right]\left[a(-\vec{k},t) - a^\dagger(\vec{k},t)\right]$$

$$= -\frac{1}{2}\int d^3k\, k_i \left[a(\vec{k},t)\,a(-\vec{k},t) - a(\vec{k},t)\,a^\dagger(\vec{k},t) + a^\dagger(-\vec{k},t)\,a(-\vec{k},t) - a^\dagger(-\vec{k},t)\,a^\dagger(\vec{k},t)\right]$$

We may apply these on the single particle states. This will produce an eigenvalue, which is 'k_i'. //

17.2.2011

We consider the term :-

$$I = -\frac{1}{2}\int_{-\infty}^{\infty} d^3k\, k_i \left[a(\vec{k},t)\, a(-\vec{k},t)\right]$$

If we now transform $\vec{k} \leftrightarrow -\vec{k}$, then, we get :-

$$I = -\frac{1}{2}\int_{\infty}^{-\infty}(-d^3k)(-k_i)\,[a(-\vec{k},t)\,a(\vec{k},t)]$$

$$= \frac{1}{2}\int_{-\infty}^{\infty} d^3k\, k_i [a(\vec{k},t)\,a(-\vec{k},t)] \qquad (\because [a(\vec{k},t),\, a(\vec{k}',t)] = 0).$$

$$= -I$$

Thus, this term is antisymmetric under $\vec{k} \to -\vec{k}$ and hence this integral is zero.

Similarly $\frac{1}{2}k_i\, a^\dagger(-\vec{k},t)\, a^\dagger(\vec{k},t)$

$$\xrightarrow[\vec{k}\to-\vec{k}]{} -\frac{1}{2}k_i\, a^\dagger(\vec{k},t)\, a^\dagger(-\vec{k},t)$$

$$= -\frac{1}{2}k_i\, a^\dagger(-\vec{k},t)\, a^\dagger(\vec{k},t)$$

$$(\because [a^\dagger(\vec{k},t), a^\dagger(\vec{k}',t)] = 0).$$

Hence this integral also vanishes.

$$\therefore P_i = -\frac{1}{2}\int d^3k\, k_i [-a(\vec{k},t)\, a^\dagger(\vec{k},t) + a^\dagger(-\vec{k},t)\, a(-\vec{k},t)]$$

Again, in the last term, we change $\vec{k} \to -\vec{k}$.

$$\therefore -\frac{1}{2}\int_{-\infty}^{\infty} d^3k\, k_i\, a^\dagger(-\vec{k},t)\, a(-\vec{k},t)$$

$$\xrightarrow[\vec{k}\to-\vec{k}]{} \frac{1}{2}\int_{\infty}^{-\infty}(-d^3k)\, k_i\, a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

$$= \frac{1}{2}\int_{-\infty}^{\infty} d^3k\, k_i\, a^\dagger(\vec{k},t)\, a(\vec{k},t)$$

$$\therefore P_i = \frac{1}{2}\int_{-\infty}^{\infty} d^3k\, k_i [a(\vec{k},t)\, a^\dagger(\vec{k},t) + a^\dagger(\vec{k},t)\, a(\vec{k},t)]$$

Now, $[a(\vec{k},t), a^\dagger(\vec{k}',t)] = \delta^{(3)}(\vec{k}-\vec{k}')$

$$\therefore a(\vec{k},t)\, a^\dagger(\vec{k},t) = a^\dagger(\vec{k},t)\, a(\vec{k},t) + \delta^{(3)}(0)$$

$$\text{or } P_i = \int d^3k\, k_i\, a^\dagger(\vec{k},t)\, a(\vec{k},t) + \frac{1}{2}\int d^3k\, k_i\, \delta^{(3)}(0).$$

Now, $\delta^{(3)}(\vec{x}) = \frac{1}{(2\pi)^3}\int d^3x\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}$

If we now set $\vec{x}=0$, we get :-

$$\delta^{(3)}(0) = \frac{1}{(2\pi)^3}\int d^3x = \frac{V}{(2\pi)^3}\,;$$ where "V" is the volume of space.

The constant infinity is due to this infinite volume.

We can regularise this by considering the field theory to lie in a finite box, the momentum will then be a discrete sum.

In this integral,

$$\int d^3k\, k_i \xrightarrow[\vec{k}\to-\vec{k}]{} -\int d^3k\, k_i$$

Now, instead of $-\infty$ to $+\infty$, we let dk_x, dk_y, dk_z run from $-\Lambda$ to Λ and we get :-

$$\int_{-\Lambda}^{\Lambda} dk_x \int_{-\Lambda}^{\Lambda} dk_y \int_{-\Lambda}^{\Lambda} dk_z\, k_i = 0 \qquad [i \equiv x,y,z]$$

The vacuum itself carries some momentum which we can not measure.

The vacuum can also carry some energy (the ground state energy), but, we can only measure the differences in the two energy levels.

We can always measure some quantity with respect to that carried by the vacuum.

We can not fix any actual origin of momentum or energy.

When we consider gravity, it matters whether the vacuum carries momentum or energy.

$E = \sqrt{\vec{k}^2 + m^2}$ is actually a difference of the single particle energy state to that of the vacuum.

∴ So, we eventually drop the $\frac{1}{2}\int d^3k\, k_i\, \delta^{(3)}(0)$ integral which gives us an infinite constant.

†

- N.B. :- We take the Quantum Field Theory in a finite box and put some periodic boundary conditions on it. Then, we will get a Kronecker delta with a factor of $(L/2\pi)$ for every direction, which will give us $V/(2\pi)^3$ with the delta functions.

- N.B. :- In the presence of gravity, by somehow regularising for momentum, we can never regularise for energy because of the k^2 term. We can not regularise that.

We, thus, can not couple this Quantum Field Theory to gravity, it produces infinite divergences.

Thus, we arrive at :-

$$\hat{P}_i = \int d^3k\, k_i \left[a^\dagger(\vec{k},t)\, a(\vec{k},t) \right]$$

Thus, by design, we get :-

$$\hat{P}_i |0\rangle = 0 \quad (\because a(\vec{k},t)|0\rangle = 0 \text{ for all } \vec{k}).$$

Now, we apply it on a single particle state, to get :-

$$\hat{P}_i\, a^\dagger(\vec{k},t)|0\rangle = \int d^3k'\, k_i'\, a^\dagger(\vec{k}',t)\, a(\vec{k}',t)\, a^\dagger(\vec{k},t)|0\rangle$$

$$= \int d^3k'\, k_i'\, a^\dagger(\vec{k}',t)\left[a^\dagger(\vec{k},t)\, a(\vec{k}',t) + \delta^{(3)}(\vec{k}-\vec{k}') \right]|0\rangle$$

The first term vanishes (i.e. $a(\vec{k}',t)|0\rangle = 0$), we thus get:-

$$\hat{P}_i\, a^\dagger(\vec{k},t)|0\rangle = \int d^3k'\, K_i'\, a^\dagger(\vec{k}',t)\,\delta^{(3)}(\vec{k}-\vec{k}')|0\rangle$$
$$= K_i\, a^\dagger(\vec{k},t)|0\rangle$$

Thus, "K_i" is the momentum carried by the state $a^\dagger(\vec{k})|0\rangle$ in the i^{th} direction.

Previously, we had seen that this single particle state carries an energy, $\omega_{\vec{k}} = \sqrt{\vec{k}^2+m^2}$ [see page 96.].

For any other relation, we will not have any particle interpretation. The particles emerge once we quantise.

The states obey the relations between the energy and the momentum as that by a single particle.

- So far we have seen that in the Noether's theorem, a continuous symmetry $\Rightarrow$ a conservation law. This tells us precisely how to find the conserved current J^μ.

- We would now like to prove the converse, i.e., given a conservation law, there is a symmetry.

We will prove it in a somewhat limited context. We will assume the Lagrangian to be a function of the fields and their first order time derivatives. [Just like the Hamiltonian depends on q, v].

We assume that "L" depends on $\{\phi_n\}$ and $\{\partial_t \phi_n\}$.

[N.B.:- Previously, in proving the original statement, the action was not assumed to be limited.]

[N.B.:- We will not involve any first order space derivatives,

we can always discretise them.]

For convenient notation, it is best to have both.

Let us consider a finite number of coordinate variables and their time derivatives.

To simplify notation, we consider a classical mechanics with coordinates $q_1, q_2, \ldots, q_N$ and velocities $v_1, v_2, \ldots, v_N$.

The Lagrangian then is:-

$$L(\{q_n\}, \{v_n\}).$$

We think this index "n" as a continuous variable or we can take their Fourier momentum modes.

Let us assume that $L \neq f(t)$.

[• N.B:- We can obviously include it and then our calculations will change a bit.].

In the Lagrangian formulation we take these $\{q_n\}$'s and $\{v_n\}$'s as independent variables.

To go to the Hamiltonian formulation, we define the conjugate momentum as:-

$$p_n = \frac{\partial L}{\partial v_n}; \quad \text{where } H(\{q_n\}, \{p_n\}) = \sum_n v_n p_n - L(\{q_n\}, \{v_n\}).$$

The total number of variables is $2N$.

We can also define the action. The action is a functional of the trajectory ("L" and "H" are functions of the $2N$ coordinates). The action "S" provides a number. We have to specify the trajectory and hence all the $\{q(t)\}$.

$\therefore S[\{q_r(t)\}] = \int dt\, L(\{q_r(t)\}, \{\frac{dq_r(t)}{dt}\})$; where

$\{\frac{dq_r(t)}{dt}\}$ is the slope(s) of the trajectory at every point.

Given a trajectory, the velocity at each point is fixed.
But, when the Lagrangian is concerned, we think $\{q_r\}$'s and $\{v_r\}$'s as independent variables.

Let us suppose that $Q(\{q_r\}, \{p_r\}, t)$ be a conserved charge. This means that $\frac{dQ}{dt} = 0$ when the equations of motion hold.

$\frac{\partial Q}{\partial t}$ might not be zero.

Writing explicitly, we get :-

$$\frac{dQ}{dt} = \sum_r \left[\frac{\partial Q}{\partial q_r} \cdot \frac{dq_r}{dt} + \frac{\partial Q}{\partial p_r} \cdot \frac{dp_r}{dt} \right] + \frac{\partial Q}{\partial t} = 0.$$

The Hamilton's equations tell us that :-

$$\frac{dq_r}{dt} = \frac{\partial H}{\partial p_r} \; ; \; \frac{dp_r}{dt} = -\frac{\partial H}{\partial q_r}.$$

$$\therefore \frac{dQ}{dt} = \sum_r \left[\frac{\partial Q}{\partial q_r} \cdot \frac{\partial H}{\partial p_r} - \frac{\partial Q}{\partial p_r} \cdot \frac{\partial H}{\partial q_r} \right] + \frac{\partial Q}{\partial t}$$

$$= \{Q, H\}_{P.B.} + \frac{\partial Q}{\partial t}.$$

The equations of motion tells us $\frac{dq_r}{dt}$ and $\frac{dp_r}{dt}$ in terms of functions of (p, q).

$\therefore \frac{dQ}{dt} = f(p, q, t) = 0$; $(\because H = H(p, q))$.

Thus, $f(p,q,t)$ has to vanish identically.

It does not depend on the equations of motion.
This must be zero, without the equations of motion.

Thus, if $\frac{dQ}{dt} \neq 0$, then, we can not make it zero by using the equations of motion.

Conservation law of course requires the equation of motion, but the expression we arrive at must be zero without the equations of motion's aid.

So, we conclude that :-

$$\sum_r \left[\frac{\partial Q}{\partial q_r} \cdot \frac{\partial H}{\partial p_r} - \frac{\partial Q}{\partial p_r} \cdot \frac{\partial H}{\partial q_r} \right] + \frac{\partial Q}{\partial t} = 0 .$$

A non-trivial function "Q" may not make this vanish.
In that case "Q" is not conserved at that point.

- N.B.:- We may complicate "Q" by taking in dependence of $\dot{q}_r$, $\dot{p}_r$ etc.

- We will now show that $q_r \to q_r + \epsilon \{ Q, q_r \}_{P.B.}$,

  i.e. $\tilde{q}_r = q_r + \epsilon \sum_s \left[\frac{\partial Q}{\partial q_s} \cdot \frac{\partial q_r}{\partial p_s} - \frac{\partial Q}{\partial p_s} \cdot \frac{\partial q_r}{\partial q_s} \right]$

  $= q_r - \epsilon \frac{\partial Q}{\partial p_r}$ is a symmetry of "S" (i.e. "S" does not change to the first order in "ϵ"). Here, we can not use the equations of motion.

$$S[\{\tilde{q}_n(t)\}] = \int dt\, L\left(\{\tilde{q}_n(t)\}, \{\frac{d\tilde{q}_n(t)}{dt}\}\right).$$

$$L = \sum_n v_n p_n - H.$$

$$\therefore \delta L = L(\{\tilde{q}_n(t)\}, \{\tilde{v}_n(t)\}) - L(\{q_n(t)\}, \{v_n(t)\})$$

$$= \delta\left(\sum_n v_n p_n - H\right)$$

$$= \sum_n (\delta v_n p_n + v_n \delta p_n) - \sum_n \left(\frac{\partial H}{\partial q_n}\delta q_n + \frac{\partial H}{\partial p_n}\delta p_n\right).$$

Now, $\frac{\partial H}{\partial p_n} = v_n$. Here "$v_n$" is not taken as $\frac{dq_n}{dt}$.

We are not using the equations of motion here, but just the Legendre transformation between "L" and "H".

[N.B.:- We want this "H" because we wrote $\frac{dQ}{dt}$ in terms of "H".].

$$\therefore \delta L = \sum_n (\delta v_n p_n + v_n \delta p_n) - \sum_n \left(\frac{\partial H}{\partial q_n}\delta q_n + v_n \delta p_n\right)$$

$$= \sum_n \left(\delta v_n p_n - \frac{\partial H}{\partial q_n}\delta q_n\right).$$

$$\therefore S[\{\tilde{q}_n(t)\}] - S[\{q_n(t)\}]$$

$$= \int dt \sum_n \left(\delta v_n p_n - \frac{\partial H}{\partial q_n}\delta q_n\right)$$

The action is to be evaluated at $\{q_n(t)\}$ and $\{\frac{dq_n(t)}{dt}\}$.

on the trajectory, we get :-

$\delta v_n = \frac{d}{dt}(\delta q_n)$, because on the trajectory, $v_n = \frac{dq_n}{dt}$ (by definition).

Thus, $S[\{\tilde{q}_n(t)\}] - S[\{q_n(t)\}]$

$$= \int dt \sum_n \left(\frac{d}{dt}(\delta q_n) p_n - \frac{\partial H}{\partial q_n}\delta q_n\right).$$

[• $L(\{q_r\}, \{v_r\})$ is an abstract function. It is better not to think it as the Lagrangian as of now.

• $H = \sum_r p_r v_r - L$; with $p_r = \frac{\partial L}{\partial v_r}$ = definition of Legendre transformation.

Given "L", we can calculate "H" and vice versa.
Given $\{v_r\}$ we can calculate $\{p_r\}$. We can invert this relation to give, $v_r = \frac{\partial H}{\partial p_r}$. Here, nowhere have we used the equations of motion, neither have we said $v_r = \dot{q}_r$.].

[• We can not use the Euler-Lagrange equations. Unless we put "v", we can not define the action].

At every given point on the trajectory, we have to calculate each of these quantities p_r, δq_r, H etc.

$$\therefore S[\{\tilde{q}_r(t)\}] - S[\{q_r(t)\}]$$

$$= \int dt \sum_r \left\{ -\frac{dp_r}{dt} \delta q_r - \frac{\partial H}{\partial q_r} \delta q_r \right\}$$

$$+ \int dt \sum_r \delta\left(\frac{dq_r}{dt} p_r\right)$$

We drop the second term at the boundary.

i.e. we drop, $\sum_r \int d\delta(q_r p_r)$ at the boundary.

Now, we use $\delta q_r = -\epsilon \frac{\partial Q}{\partial p_r}$.

∴ We get:-

$$S[\{\tilde{q}_r(t)\}] - S[\{q_r(t)\}]$$

$$= \int dt \sum_r \left(\epsilon \frac{\partial Q}{\partial p_r} \cdot \frac{dp_r}{dt} + \epsilon \frac{\partial Q}{\partial p_r} \frac{\partial H}{\partial q_r} \right)$$

Till now, we have not used anywhere that "Q" is conserved. Now, we use the fact that "Q" is conserved.

We then have,

$$\sum_r \left\{ \frac{\partial Q}{\partial q_r} \cdot \frac{\partial H}{\partial p_r} - \frac{\partial Q}{\partial p_r} \cdot \frac{\partial H}{\partial q_r} \right\} + \frac{\partial Q}{\partial t} = 0$$

$\therefore$ We get,

$$S[\{\tilde{q}_r(t)\}] - S[\{q_r(t)\}] = \int dt \left[\sum_r \left(\epsilon \left\{ \frac{\partial Q}{\partial p_r} \cdot \frac{dp_r}{dt} + \frac{\partial Q}{\partial q_r} \cdot \frac{\partial H}{\partial p_r} \right\} \right) + \epsilon \frac{\partial Q}{\partial t} \right]$$

Now, $\frac{\partial H}{\partial p_r} = v_r$.

We have to evaluate the term inside the braces along the trajectory. So, on the trajectory,

$$v_r = \frac{dq_r}{dt}.$$

$$\therefore S[\{\tilde{q}_r(t)\}] - S[\{q_r(t)\}] = \epsilon \int dt \left[\sum_r \left\{ \frac{\partial Q}{\partial p_r} \cdot \frac{dp_r}{dt} + \frac{\partial Q}{\partial q_r} \cdot \frac{dq_r}{dt} \right\} + \frac{\partial Q}{\partial t} \right]$$

Here also, we have not used the Euler-Lagrange's equations.

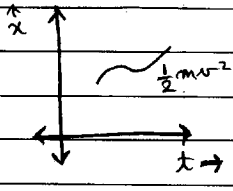
$$\therefore S[\{\tilde{q}_r(t)\}] - S[\{q_r(t)\}] = \epsilon \int dt \, \frac{dQ}{dt}$$

$$= \epsilon Q \Big|_{t_1}^{t_2}.$$

Thus, $\frac{dQ}{dt} = 0 \Rightarrow \delta q_r = -\epsilon \frac{\partial Q}{\partial p_r}$ is a symmetry of 'S'.

* **N.B.:-** $\frac{dQ}{dt}$ is not zero along the trajectory.

Let $L = \frac{1}{2} m v^2$



$\frac{1}{2}mv^2$ is different at different points.

$Q = mv$ is the conserved charge.

$$\frac{dQ}{dt} = m\frac{dv}{dt} = m\frac{d^2x}{dt^2}.$$

$\frac{d^2x}{dt^2} \neq 0$ for an arbitrary trajectory. The trajectory vanishes only for fixed points at t_1, t_2.
The boundary terms are zeroes.

For an arbitrary trajectory, we can choose it to fall off at two points.

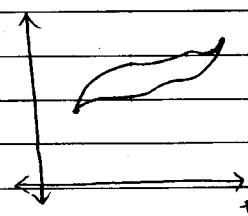
By invariance of the action, we mean it to be invariant upto boundary terms. It will then not affect the equations of motion.

Actually, we do not care about the boundary terms.

For derivation of the field equations, the boundary terms are irrelevant.

We might as well take trajectories where the boundary terms are zeroes.

If these are not zero, then also our equations of motion will hold.



$\delta S = 0$ between these two trajectories.