

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 14
Second Quantization Creation, Destruction and Number operators

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C.S.C.O. → complete set 'α' of compatible observables

Our system: N number of identical elementary particles

....even in the presence of "correlations"
indistinguishable 'elementary particles'

eg. a particular state of our N-particles system:

n_1	n_1 particles are in state α_1	N_1 Complete set of commuting Hermitian operators
n_2	n_2 particles are in state α_2	
n_3	n_3 particles are in state $\alpha_3 \dots$ etc.	

Eigenvalues respectively of occupation number operators

Description of : Bose-Einstein & Fermi-Dirac particles

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Greetings, so we will continue our discussion on Second Quantization and today we will introduce the creation, destruction and the number operators, the destruction operator also often referred to as the annihilation operator. And basically there are our many particle system will be described in terms of single particle quantum numbers. These are elementary identical particles, so they are indistinguishable they are elementary.

But we will continue to treat them as elementary particles even in the presence of correlations and even reconciling with indistinguishability because you may not be able to number them or identify them by some names or numbers or colours. But they do have their intrinsic properties which are fundamental to an elementary particle.

So, if you have an N particle system then even in the presence of correlations we can talk about a certain number like n_1 number of particles in state α_1 . Now what is α_1 ? α_1 is a set of quantum numbers we describe a particular single particle quantum state okay. So, there is a single particle quantum state it is not just one quantum number it can be a set of quantum numbers.

And these quantum numbers come from Eigen values of those operators which commute with each other corresponding to whatever measurements are compatible with each other. So, you will have n_1 number of particles in the state α_1 , n_2 particles in the state α_2 and so on.

So, this will be our description of the N particle system and this is way you would describe the system of indistinguishable elementary particles whether they are fermions or bosons.

But then of course this statistics is different. So, these are obtained as Eigen values of a complete set of commuting Hermitian operators. These are number operators so this number n1 is an Eigen value of a number operator which is capital N1 okay, n2 is an Eigen value of upper case N2 which is a Hermitian operator.

This is the number operator; these are called as occupation number operators. And this description is common to both the fermions and the bosons.

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Reference: Fetter & Walecka - 'Quantum Theory of Many Particle Systems' Chapter 1

In almost all cases of interest, the many-particle Hamiltonian has the following form: (for both Fermions/Bosons)

$$H = \sum_{k=1}^N T(x_k) + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N V(x_k, x_l)$$

eg. $x_k \rightarrow$ space-spin coordinate of fermions

$i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) = H\Psi(x_1, x_2, \dots, x_N, t)$ Schrodinger equation
-with appropriate boundary conditions on the wave function

Ψ : expressed in basis of single particle base functions $\psi_{R_k}(x_k)$
eg.: $\psi_{R_k}(x_k) \leftrightarrow \psi_{n_k l_k m_l m_s}(x_k)$ or $\psi_{R_k}(x_k) \leftrightarrow \psi_{n_k l_k j_k m_j}(x_k)$

$E_k \leftrightarrow \{n_k l_k m_l m_s\}$ or $E_k \leftrightarrow \{n_k l_k j_k m_j\}$
eigenvalues of 'one-electron' C.S.C.O.

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Now let us develop the Schrodinger equation and up to a certain point we will carry the formalism forward yes Suman (Question time: 03:23-not audible) the number of particles okay they are Eigen values give the number of particles in a particular single particle quantum state okay.

So, you have for both fermions as well as bosons let us say you have got a space in space spin space represented by x_k and a typical Hamiltonian for the many particle system is the sum of all the kinetic energy operators and certain two particle interactions. This is a typical you know Hamiltonian okay. The details will differ sometimes we will have more complex terms but notwithstanding the details.

By and large a many particle system will have will be described by a Hamiltonian of this kind in which the kinetic energy operators will sum over all the number of particles going from one to the total number of particles. And the two particle interactions represented by this V in

the case of fermions it could be the $1/r_{ij}$ but in general it could be some two particle interactions.

Now the Schrodinger equation for this system would be a function of these n coordinates each of these x_1, x_2 upto x_n is actually a set of 4 coordinates. So, there are $4n$ coordinates right, three space coordinates and once spin coordinate for each particle. They are collectively written as x_1 . So, there are these n coordinates and there is also a time dependence.

So, this is the Schrodinger equation and you need to solve them, solve this subject to whatever boundary conditions are appropriate for the physical situation under consideration. Now this wave function will be represented in a basis of single particle states, so these Ψ_i , so there are two kinds of Ψ which I have used one is this Ψ which if we may call this as an upper case Ψ .

And this is another Ψ which I may call as a lowercase ψ okay. Both are Ψ 's but this is the end particle wave function this is uppercase Ψ , this is a function of all of these end coordinates as well as time. And then you have these lowercase ψ functions which are the function of single particle coordinates x_k .

So, this probability amplitude is a measure of the probability amplitude that a particle at coordinate x_k will be in the quantum state E_k where E_k is a set of appropriate number of single particle quantum numbers. It is not just the energy it will have all other measurements which are compatible with the measurement of energy okay.

So, it could include the angular momentum, it could include spin and any other measurement which is compatible with the measurement of energy. So, E_k is a collective label and this in for one particle, one electron atoms for example this is the set of 4 quantum numbers n_l, j and m_j or it can also be n_l, m_l and m_s . But in the case of spin orbit interaction j and m_j are better quantum numbers and not m_l and m_s .

But you can always carry out transformations from one to the other using the Clebsch-Gordan coefficients. So, essentially E_k stands for a set of appropriate number of quantum numbers we describe the single particle states. And these come from Eigen values of a complete set of commuting operators corresponding to compatible observations.

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$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) = H \Psi(x_1, x_2, \dots, x_N, t) \quad (\text{for both Fermions/Bosons})$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N)$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1', E_2', \dots, E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N)$$

$\psi_{E_k}(x_k)$: time-independent one-particle functions
 eg.: $\psi_{E_k}(x_k) \leftrightarrow \psi_{n_k l_k m_k}(x_k)$ or $\psi_{E_k}(x_k) \leftrightarrow \psi_{n_k l_k m_k}(x_k)$

entire time-dependence of $\Psi(x_1, x_2, \dots, x_N, t)$
 is in the time-dependence of $C(E_1', E_2', \dots, E_N', t)$


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So, this is your Schrodinger equation and you can write it as a product of single particle functions. Look at the coefficient, the coefficient will of course depend on these quantum numbers as well as the time. But then a general and particle state which is been written on the left-hand side will be a linear superposition of all of these possibilities inclusive of a summation over E_1 prime, E_2 prime up to E_N prime.

So, there may be infinite possibilities in this set okay and all of these collectively represent the N particle system. Now this is the most general description of an N particle state, be it a system of fermions or bosons this part is common to both. So, you can write all of these multiple sigma notations as a single sigma notation. But the summation is over E_1 prime, E_2 prime all the way up to E_N prime, so you must sum over all of them.

These are time independent; the single particle states are independent of time okay. All the time dependence is in this coefficient C , this is where the time dependence is okay. So, there is of course a time dependence, the Schrodinger equation, the Schrodinger wave function is of course a time dependent function as you can see from here.

But the time dependence is not in these single particle states it is in this coefficient C . This is where the entire time dependence is in this t okay. So, the coefficients C are time dependent the single particle states are not. You can always develop a formalism in which you can make the single particle states also time dependent.

But that is a matter of detail and those are special techniques which are devised to deal with the many body problem, I will mention some of them as of the course develops further. But at this point we consider time independent one particle functions, one particle states and the time dependence completely absorbed in the coefficient C .

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(for both Fermions/Bosons)

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) = H \Psi(x_1, x_2, \dots, x_N, t)$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1} \sum_{E_2} \dots \sum_{E_N} C(E_1, E_2, \dots, E_N, t) \psi_{E_1}(x_1) \psi_{E_2}(x_2) \dots \psi_{E_N}(x_N)$$

$$\Psi(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N, t) = \pm \Psi(x_1, x_2, \dots, x_j, \dots, x_i, \dots, x_N, t)$$

$\begin{matrix} + \text{Bosons} & \rightleftarrows & - \text{Fermions} \\ \updownarrow & & \updownarrow \\ + B & \rightleftarrows & F \end{matrix}$

Necessary and sufficient condition is that the expansion coefficients themselves are symmetric or antisymmetric with respect to interchange corresponding quantum numbers.

$$C(E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N, t) = \pm C(E_1, E_2, \dots, E_j, \dots, E_i, \dots, E_N, t)$$

HW: prove it! $i \rightleftarrows j$

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So, now we know that if you interchange the *i*th and the *j*th particle, if there is an interchange between *i* and *j* particle then the wave function would either remain invariant, it will remain the same as before or one interchange will lead to a change of sign of the wave function. And that depends on whether you are dealing with fermions or bosons right. So, this is where the statistics comes in.

So, all the statistics is contained in the properties of the wave function. Now this is just a product of single particle states. And you are summing over all of them okay. So the statistics is not contained here the statistics is contained in the coefficient *C* okay. So, there is a one to one correspondence between the property that the wave function remains either invariant on interchange of particles for bosons or changes sign for fermions.

And the properties of the coefficient *C*, if you interchange two of these labels okay. So this is the necessary and sufficient condition that the expansion coefficients see themselves must be either symmetric or anti-symmetric. They are symmetric in the case of bosons and they are anti symmetric in the case of fermions.

The expansion coefficient *C* is where the symmetry is now sitting okay. And this is a necessary and sufficient condition you can prove this as a very simple exercise I have already given hints about you know where is the proof comes from. But essentially you notice that the statistics is now contained in the symmetry properties of the coefficient that under the interchange of the, these quantum states *E_j* and *E_i*.

If you interchange these quantum states okay. The coefficient C will either remain invariant or remain the same amplitude, same modulus but change its sign okay. Depending on your working with either Bose type of particles or Fermi particles.

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$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) = H \Psi(x_1, x_2, \dots, x_N, t) \quad (\text{for both Fermions/Bosons})$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1', E_2', \dots, E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N)$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N)$$

multiply the Schrodinger equation by $\psi_{E_1}(x_1)^\dagger \psi_{E_2}(x_2)^\dagger \dots \psi_{E_N}(x_N)^\dagger$
for a fixed set $\{E_1, E_2, \dots, E_N\}$

$$\psi_{E_1}(x_1)^\dagger \psi_{E_2}(x_2)^\dagger \dots \psi_{E_N}(x_N)^\dagger \times i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) =$$

$$= \psi_{E_1}(x_1)^\dagger \psi_{E_2}(x_2)^\dagger \dots \psi_{E_N}(x_N)^\dagger \times H \Psi(x_1, x_2, \dots, x_N, t)$$

Now, integrate over all coordinates

$$i\hbar \int dx_1 \int dx_2 \dots \int dx_N \psi_{E_1}(x_1)^\dagger \psi_{E_2}(x_2)^\dagger \dots \psi_{E_N}(x_N)^\dagger \times \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) =$$

$$= \int dx_1 \int dx_2 \dots \int dx_N \psi_{E_1}(x_1)^\dagger \psi_{E_2}(x_2)^\dagger \dots \psi_{E_N}(x_N)^\dagger \times H \Psi(x_1, x_2, \dots, x_N, t)$$

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So, this is what we have got and now the summation is over dummy indices, dummy variables the dummy variables are our primed variables E1 prime, E2 prime up to En prime. So, they are going to be summed over. So, what we are going to do is to multiply the Schrodinger equation by this product of single particle states but you take the adjoint okay. So, you multiplied by the adjoint of these single particle states.

By the product of these single particle states and for a particular set E1, E2 these are without primes okay. The prime variables appear in this summation so they are dummy labels we do not want to use them since we are multiplying it by a particular set E1, E2 up to En. So, you multiply the Schrodinger equation by this set.

Now this is the result of the left hand side you take the product of these single particle states with their adjoints and multiply the left hand side iħ cross del Psi by del t by this. And on the right hand side you have got the same factor pre multiplying h Psi okay. Now the next thing you do is integrate over all the coordinates. So, now your integration over x1 is actually not a single integration.

But it is integration over three space coordinates and the summation over the discrete spin coordinator okay. So, each integration corresponds to 4, one discrete sum and three integrations over the space variables. So, you integrate over all the coordinates, so this is iħ cross is coming from here, it is also over here and you integrate over dx1, dx2 up to xn this is the integrand which is on the left hand side.

Which is this product of single particle states take with their adjoints and multiplying del Psi by del t ih cross having written on the extreme left as a constant multiplier. So, that is your left hand side. On the right hand side you have got again an integration over all the coordinates x1 to xn. And what are you integrating is this product of single particle states with their adjoints pre multiplying xi okay.

Yes of course (Question time: 15:07 – not Audible) of course x1 is the particular coordinate okay certain interactions might couple a particle at x1 with a particle at x2 right. So, there can be an interaction V which depends on x1 and x2 and that is gone that goes into the Hamiltonian okay. So, that is sitting in this Hamiltonian here okay. (Refer Slide Time: 15:43)

$$i\hbar \int dx_1 \int dx_2 \dots \int dx_N \psi_{E_1}^*(x_1) \psi_{E_2}^*(x_2) \dots \psi_{E_N}^*(x_N) \times \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) =$$

$$= \int dx_1 \int dx_2 \dots \int dx_N \psi_{E_1}^*(x_1) \psi_{E_2}^*(x_2) \dots \psi_{E_N}^*(x_N) \times H \Psi(x_1, x_2, \dots, x_N, t)$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{k_1} \sum_{k_2} \dots \sum_{k_N} C(E_1, E_2, \dots, E_N, t) \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N)$$

$$i\hbar \int dx_1 \int dx_2 \dots \int dx_N \left[\frac{\partial}{\partial t} \sum_{k_1} \sum_{k_2} \dots \sum_{k_N} C(E_1, E_2, \dots, E_N, t) \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N) \right] =$$


$$= \int dx_1 \int dx_2 \dots \int dx_N \left[H \sum_{k_1} \sum_{k_2} \dots \sum_{k_N} C(E_1, E_2, \dots, E_N, t) \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N) \right]$$

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So, this is the expression that we have got and the wave function we already agreed that a general correlated wave function, a wave function of a correlated system of particles is written as product of these n single particle states weighted by the coefficients which contain the statistics okay. So, this is your left hand side, track the time derivative which is on the left hand side which is this partial derivative with respect to time.

It is written over here and on the right hand side you have got the Hamiltonian which contains the kinetic energy operators and the potential energy operators which may depend on the coordinates of two particles okay. So, this is your expression that you get on carrying out this integration. (Refer Slide Time: 16:40)

$$\begin{aligned}
& i\hbar \int dx_1 \int dx_2 \dots \int dx_N \left[\frac{\partial}{\partial t} \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N) \right] = \\
& = \int dx_1 \int dx_2 \dots \int dx_N \left[\frac{\partial}{\partial t} \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N) \right] \\
& \int dx_k \psi_{E_i'}(x_k)^\dagger \psi_{E_j'}(x_k) = \delta_{E_i E_j} \\
& i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \\
& = \int dx_1 \int dx_2 \dots \int dx_N \left[\frac{\partial}{\partial t} \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N) \right]
\end{aligned}$$


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So, let us write it to the top of this next slide here. And now we are aware that these single particle states are essentially orthonormal okay. So, we work in a basis of orthonormal single particle states and we exploit the orthonormal conditions so this integral will be given by a Dirac delta in the case of continuous functions or Kronecker deltas in the case of discrete functions.

So, in general it is a delta function and whether this is a Kronecker delta or a Dirac delta can be plugged in according to the context in general we will simply use it as a Kronecker Delta. But in general it could include the continuum states as well okay. So, you have got this orthonormal condition orthogonality condition. And we exploit this orthogonality because when you are having this integration okay.

This coefficient C can be factored outside the integration because this does not depend on the coordinates x1, x2 etcetera. And then you have got the integrals of this kind and wherever you have orthogonality you can get this delta function. And then when you sum over these E1 prime, E2 prime, En prime. So, if you were to take consider this term, the only term that would survive is the one corresponding to E1 prime = E1 or like that right.

Whichever is being considered there? So, you can exploit the orthogonality condition and what you have on the left hand side is C after contracting these integrals exploiting the kronecker deltas and the orthogonality of the wave functions. You get iħ cross then you have the time derivative of the time dependent coefficient C which contains the statistics. So, now you have got the iħ cross del C by del t on the left hand side.

After exploiting the orthogonality on the left hand side there is only one term that will under all of those integrations right. That will be the coefficient C corresponding to a particular set

which is E1, E2, E3 which is the unprimed set that we used in the previous set right. So, that is the only term that will survive on the left side on the right side I have written the term just the way it was without any further modification.

So you have got integration over all of these n coordinates or four n coordinates if you like and then you have got this adjoint product of single particle states. Then you have the Hamiltonian here and then you have got the complete wave function inclusive of the time-dependent coefficient which has got the statistics built into it okay. (Refer Slide Time: 19:49)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \int dx_1 \int dx_2 \dots \int dx_N \left[H \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \psi_{E_1'}(x_1) \psi_{E_2'}(x_2) \dots \psi_{E_N'}(x_N) \right]$$

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \int dx_1 \int dx_2 \dots \int dx_N \left[\psi_{E_1'}(x_1)^\dagger \psi_{E_1}(x_1) \dots \psi_{E_N'}(x_N)^\dagger \times H \psi_{E_1}(x_1) \psi_{E_2}(x_2) \dots \psi_{E_N}(x_N) \right]$$

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', E_2', \dots, E_N', t) \int dx_1 \int dx_2 \dots \int dx_N \left[\psi_{E_1}(x_1)^\dagger \psi_{E_1}(x_1) \dots \psi_{E_N}(x_N)^\dagger \times \left[\sum_{k=1}^N T(x_k) + \frac{1}{2} \sum_{\substack{k=1 \\ l=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \psi_{E_2}(x_2) \dots \psi_{E_N}(x_N) \right]$$

$$H = \left[\sum_{k=1}^N T(x_k) + \frac{1}{2} \sum_{\substack{k=1 \\ l=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k, x_l) \right]$$

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So, this is what we have got and we will now look at the right hand side carefully. On the right hand side you have got the Hamiltonian okay. And the Hamiltonian for a many particle system is the sum of all these kinetic energy operators and a two center interaction. This is the general form of a typical Hamiltonian.

So, you substitute this Hamiltonian by its explicit form consisting of the kinetic energy operators and the potential energy operators which is coming from interaction between every 2 pairs of particles okay. So, this is your general form of the many particle Hamiltonian. (Refer Slide Time: 20:21)

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) &= \\
&= \sum_{k_1}^N \sum_{k_2}^N \dots \sum_{k_N}^N C(E_1', E_2', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\psi_{k_1}(x_1)^\dagger \psi_{k_2}(x_2)^\dagger \dots \psi_{k_N}(x_N)^\dagger \times \right. \\
&\quad \left. \left[\sum_{i=1}^N T(x_i) + \frac{1}{2} \sum_{\substack{i=1 \\ i \neq j}}^N \sum_{\substack{j=1 \\ j \neq i}}^N V(x_i, x_j) \right] \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N) \right] \\
i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) &= \\
&= \left[\sum_{k_1}^N \sum_{k_2}^N \dots \sum_{k_N}^N C(E_1', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\psi_{k_1}(x_1)^\dagger \dots \psi_{k_N}(x_N)^\dagger \times \right. \right. \\
&\quad \left. \left. \left[\sum_{i=1}^N T(x_i) \right] \psi_{k_1}(x_1) \dots \psi_{k_N}(x_N) \right] \right] + \\
&\quad + \sum_{k_1}^N \sum_{k_2}^N \dots \sum_{k_N}^N C(E_1', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\psi_{k_1}(x_1)^\dagger \dots \psi_{k_N}(x_N)^\dagger \times \right. \\
&\quad \left. \left[\frac{1}{2} \sum_{\substack{i=1 \\ i \neq j}}^N \sum_{\substack{j=1 \\ j \neq i}}^N V(x_i, x_j) \right] \psi_{k_1}(x_1) \dots \psi_{k_N}(x_N) \right]
\end{aligned}$$



Now this is what we are getting from the Schrodinger equation for the N particle correlated system okay. So, we have now built in all the correlations the statistical correlations are there which are sitting in the coefficients C. And any correlations over and above the statistical correlations like the Coulomb correlations are also sitting in the fact that you have got a infinite set of these products of single particle states.

Which have gone into your total wave function? So, all of them have been covered. So, now this is $i\hbar \text{cross del } C \text{ by del } t$ on the left hand side, and on the right hand side you have got two terms one coming from the kinetic energy term and the other coming from the potential energy term.

So, it is the same two terms but I have written them as the first term corresponding to the kinetic energy term. And a second term corresponding to the potential energy term, so I have only separated them because that makes it easy to handle them because you already have so many terms and you do not want to mess with too much everything at the same time. (Refer Slide Time: 22:03)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) =$$

$$= \left[\sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\psi_{E_1}(x_1)^\dagger \cdot \mathcal{H}_{E_2} \psi_{E_2}(x_2) \times \left\{ \sum_{k=1}^N T(x_k) \right\} \psi_{E_1}(x_1) \cdot \mathcal{H}_{E_N} \psi_{E_N}(x_N) \right] \right] +$$

$$+ \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\psi_{E_1}(x_1)^\dagger \cdot \mathcal{H}_{E_2} \psi_{E_2}(x_2) \times \left[\frac{1}{2} \sum_{k=1}^N \sum_{l=1}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \cdot \mathcal{H}_{E_N} \psi_{E_N}(x_N) \right]$$

Integration of the one-particle terms over independent degrees of freedom

$$\frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} \left[\frac{C(E_1', \dots, E_N', t) \times \int dx_1 \psi_{E_1}(x_1)^\dagger T(x_1) \psi_{E_1}(x_1) \int dx_2 \psi_{E_2}(x_2)^\dagger \psi_{E_2}(x_2) \dots \int dx_N \psi_{E_N}(x_N)^\dagger \psi_{E_N}(x_N) \right] +$$

$$+ \sum_{E_1'} \sum_{E_2'} \dots \sum_{E_N'} C(E_1', \dots, E_N', t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{l=1}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \cdot \mathcal{H}_{E_N} \psi_{E_N}(x_N)$$

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So, this is what you have got now let us look at the kinetic energy term, the first term. And you are carrying out integration over x_1, x_2, x_n etcetera. And all of these integrations can be carried out independently of each other. The kinetic energy operator depends only on one coordinate at a time right. So, all of these integrations can be carried out on each coordinate separately okay. We will deal with the potential energy term a little later.

So, first let us take the kinetic energy terms and the kinetic energy term the one which depends on the argument key will have the operator $T(x_k)$ sandwiched between $\psi_{E_1}^\dagger$ and ψ_{E_2} with the arguments x_k over here as well as over here and you have an integration over x_k okay.

All the other integrals will not have any operator and you will simply have the orthogonality integrals $\int dx_1 \psi_{E_1}(x_1)^\dagger \psi_{E_1}(x_1)$ this is integration over x_1 $\int dx_2 \psi_{E_2}(x_2)^\dagger \psi_{E_2}(x_2)$ and you will have orthogonality integral between E_1 and E_1' coming from here. And then when you sum over E_1' you can exploit the kronecker deltas okay.

So, that is going to make all these very many chance that you are dealing with you will be left with very few because of the orthogonality condition. Again we will carry forward our discussion on the potential energy term to a later part. And continue our focus on the single particle kinetic energy terms for the time being.

So, you have got the single particle matrix element of the kinetic energy operator here and the orthogonality integral over here as well as here and so on okay right, all the way over x_1 to x_n . So, there are n integrals out of these n integrals $n - 1$ integrals will be the orthogonality integrals. Only one of them will contain the matrix element of the kinetic energy operator in single particle states.

(Refer Slide Time: 24:40)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) =$$

$$= \sum_{k_1'} \dots \sum_{k_N'} \sum_{l=1}^N \left[C(E_1', \dots, E_N'; t) \times \int dx_1 \psi_{E_1}(x_1)^\dagger \{T(x_1)\} \psi_{E_1}(x_1) \times \int dx_2 \psi_{E_2}(x_2)^\dagger \psi_{E_2}(x_2) \dots \times \int dx_N \psi_{E_N}(x_N)^\dagger \psi_{E_N}(x_N) \right] +$$

Orthogonality and summation over E_j etc.

$$+ \sum_{k_1'} \dots \sum_{k_N'} C(E_1', \dots, E_N'; t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \dots \psi_{E_N}(x_N)$$

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So, I have written this same expression on this slide because in the previous slide this expression was little primed up in a small space. So, this is a magnification of the same expression so that you can look at these things T_m terms better. This is a matrix element of the single particle kinetic energy operator in single particle states which depend on the coordinate's x_k and you have got integration over k okay.

This is integration over dx_k and of course you have a summation over all k is going from 1 to n . And the rest of the integrals are all of these orthogonality integrals. The potential energy interaction is just the same okay. So, that term is not touched. So, you can exploit the orthogonality carry out the sum.

(Refer Slide Time: 25:45)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) =$$

$$= \sum_{k_1'} \dots \sum_{k_N'} \sum_{l=1}^N C(E_1', \dots, E_N'; t) \int dx_1 \psi_{E_1}(x_1)^\dagger \{T(x_1)\} \psi_{E_1}(x_1) \int dx_2 \psi_{E_2}(x_2)^\dagger \psi_{E_2}(x_2) \dots \int dx_N \psi_{E_N}(x_N)^\dagger \psi_{E_N}(x_N) +$$

Orthogonality and summation over E_j etc.

$$+ \sum_{k_1'} \dots \sum_{k_N'} C(E_1', \dots, E_N'; t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \dots \psi_{E_N}(x_N)$$

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{k_1'} \dots \sum_{k_N'} C(E_1', \dots, E_N'; t) \int dx_1 \psi_{E_1}(x_1)^\dagger \{T(x_1)\} \psi_{E_1}(x_1) +$$

$$+ \sum_{k_1'} \dots \sum_{k_N'} C(E_1', \dots, E_N'; t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k, x_l) \right] \psi_{E_1}(x_1) \dots \psi_{E_N}(x_N)$$

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Contract the Kronecker deltas over these terms. And once you exploit it what are you are left with, you are left with summation only over E_k prime okay. That is the only term over which

you need to carry out a summation, you do have to carry out the summation over all the coordinates x going from, k going from 1 through n you have got the coefficients C as before.

But the coefficient C will have the argument T as before but all of these single particle quantum numbers E_1 prime up to E_n prime will all become the unprimed labels because of the Kronecker delta except the one, except the label which goes into the matrix element for the kinetic energy operator okay. So, that is the only one which will remain so you are left with a summation over E_k prime.

There is no summation over other single particle quantum numbers that is just what single summation over E_k prime. Then there is a summation over k going from 1 through n you have got the coefficient C but the arguments are all unprimed except the k th 1 which is E_k prime.

Then you have got this matrix element of the kinetic energy operator in the single particle states corresponding to the coordinate x_k . And then the rest of them have given you from the Kronecker delta a factor of unity which you have multiplied throughout. Again the potential energy term is left untouched that remains to be tackled with okay. So, this is what you get from the kinetic energy term.

(Refer Slide Time: 27:38)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{E_k'} \sum_{k=1}^N C(E_1, \dots, E_k', \dots, E_N, t) \int dx_k \psi_{E_k'}(x_k)^\dagger T(x_k) \psi_{E_k'}(x_k) +$$

$$+ \sum_{k=1}^N \sum_{l=1}^N C(E_1, \dots, E_N, t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{l=1}^N \sum_{k \neq l} V(x_k, x_l) \right] \psi_{E_k}(x_1) \dots \psi_{E_l}(x_N)$$

writing W instead of E_k'

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_W \sum_{k=1}^N C(E_1, \dots, E_{k-1}, W, E_{k+1}, \dots, E_N, t) \int dx_k \psi_W(x_k)^\dagger T(x_k) \psi_W(x_k) +$$

$$+ \sum_{k=1}^N \sum_{l=1}^N C(E_1, \dots, E_N, t) \int dx_1 \dots \int dx_N \left[\frac{1}{2} \sum_{k=1}^N \sum_{l=1}^N \sum_{k \neq l} V(x_k, x_l) \right] \psi_{E_k}(x_1) \dots \psi_{E_l}(x_N)$$

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So, I have written it here at the top of the slide and now instead of E_k prime I use the letter W just focus attention on that. Because it is a particular state over which you must sum over right. E_k prime is the dummy label you can change it to anything you want and just to remind us that this is the one which is being summed over. We write it as W , I am actually following the notation from Fetter and Walecka's book. Which I have referred hints for this discussion.

So, I am using the same notation as Fetter and Walecka. So, I use W instead of Ek prime, so here instead of Ek Prime I have a W other than that everything else is the same. So, all of these coefficients up to W which are coefficients from E1 to Ek – 1, they remain the same. And all the coefficients, all the single particular quantum states after the kth 1 beginning with Ek + 1 up to En they remain the same and there is of course a time dependence. (Refer Slide Time: 28:54)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{\substack{W \\ k=1}}^N C(E_1, \dots, E_{k-1}, W, E_{k+1}, \dots, E_N, t) \int dx_k \psi_{E_k}(x_k)^\dagger T(x_k) \psi_W(x_k) +$$

$$+ \sum_{\substack{k' \\ k'=1}}^N \dots \sum_{\substack{E' \\ E'=1}}^N C(E_1, \dots, E_N, t) \int dx_1 \dots \int dx_N \left[\psi_{E_1}(x_1)^\dagger \dots \psi_{E_N}(x_N)^\dagger \times \left\{ \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N V(x_k, x_l) \right\} \psi_{E_1}(x_1) \dots \psi_{E_N}(x_N) \right]$$

Now, focus on the 2-particles term:

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) =$$

$$= \sum_{\substack{W \\ k=1}}^N C(E_1, \dots, E_{k-1}, W, E_{k+1}, \dots, E_N, t) \int dx_k \psi_{E_k}(x_k)^\dagger T(x_k) \psi_W(x_k) +$$

$$+ \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{E'} \sum_{E''} \left\{ C(E_1, \dots, E_N, t) \times \left[\int dx_1 \dots \int dx_N \left[\psi_{E_1}(x_1)^\dagger \dots \psi_{E_N}(x_N)^\dagger V(x_k, x_l) \psi_{E'}(x_k) \psi_{E''}(x_l) \right] \right\}$$

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So, this is what we have got and now we consider the two particle terms the potential energy terms. So, we had differed our discussion on the two particle terms which we take up now. Now the two particles part of the Hamiltonian is this half double sum over k in l. And put and an interaction term V which depends on the coordinates x and l and this interaction we do not want to count twice.

So, it is half of this double sum okay and you must exclude k = l okay. This is the two particle interaction so this has been written explicitly now, as this and you can write this half sum over k and l outside these summations signs okay. So, they are moved all the way to the left and the rest of the terms you have got the summation over E1 prime up to En prime which is written over here.

You have got the coefficient C which is here, so this coefficient C has been written here along with the time dependence and then you have got the two particle interaction terms which are being integrated out okay. Because you will have to carry out integration or all of these coordinates x1 upto xn.

Now this two particle interaction connects only the coordinates of xk and xl. So whatever is neither xk not xl is independent of this particular interaction and those integrals can be factored out they will give you essentially orthogonality integrals okay.

(Refer Slide Time: 30:47)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) =$$

$$= \sum_{\mathcal{W}} \sum_{k=1}^N C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \int dx_k \psi_{E_k}^*(x_k) T(x_k) \psi_{\mathcal{W}}(x_k) +$$

$$+ \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{k'} \sum_{l'} \left\{ C(E_1', \dots, E_N', t) \times \right.$$

$$\left. \times \int dx_k \int dx_l \left[\psi_{E_k}^*(x_k) \cdot \psi_{E_{k'}}^*(x_{k'}) V(x_k, x_l) \psi_{E_l}(x_l) \cdot \psi_{E_{l'}}(x_{l'}) \right] \right\}$$

Due to orthogonality of single particle wavefunctions integrations over all coordinates except x_k and x_l give Kronecker deltas....

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{\mathcal{W}} \sum_{k=1}^N C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \int dx_k \psi_{E_k}^*(x_k) T(x_k) \psi_{\mathcal{W}}(x_k) +$$

$$+ \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{k'} \sum_{l'} C(E_1', \dots, E_N', t) \int dx_k \int dx_l \psi_{E_k}^*(x_k) \psi_{E_{k'}}^*(x_{k'}) V(x_k, x_l) \psi_{E_l}(x_l) \psi_{E_{l'}}(x_{l'}) \delta_{E_k, E_{k'}} \delta_{E_l, E_{l'}}$$

integrations over x_k and x_l

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So, we will exploit that now. So, only the terms which have got coordinates in x_k and x_l they will be handled separately and those are, so you have got a two center integral integration over k and integration over l dx_k and dx_l . And then you have got this is an integral of a certain integrand, that integrand is the matrix element of the potential energy operator between Ψ_{E_k} dagger Ψ_{E_l} dagger okay, with arguments x_k and x_l respectively okay.

And then on the right you have got E_k prime and E_l prime respectively with arguments x_k and x_l and the rest of the integrals over all the other coordinates will give you these kronecker deltas. And then you can carry out the summation over E_1 prime E_2 prime up to E_N prime and contract the summations so that you are left with very few terms.

(Refer Slide Time: 32:02)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{\mathcal{W}} \sum_{k=1}^N C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \int dx_k \psi_{E_k}^*(x_k) T(x_k) \psi_{\mathcal{W}}(x_k) +$$

$$+ \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{k'} \sum_{l'} C(E_1', \dots, E_N', t) \int dx_k \int dx_l \psi_{E_k}^*(x_k) \psi_{E_{k'}}^*(x_{k'}) V(x_k, x_l) \psi_{E_l}(x_l) \psi_{E_{l'}}(x_{l'}) \delta_{E_k, E_{k'}} \delta_{E_l, E_{l'}}$$

summing over $E_1',$ and $E_2',$ etc. & exploiting $\delta_{E_1, E_1'}$ etc.

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_{\mathcal{W}} \sum_{k=1}^N \left\{ C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \times \right.$$

$$\left. \times \int dx_k \psi_{E_k}^*(x_k) T(x_k) \psi_{\mathcal{W}}(x_k) \right\} +$$

$$+ \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{k'} \sum_{l'} \left\{ C(E_1', \dots, E_k', \dots, E_l', \dots, E_N', t) \times \right.$$

$$\left. \times \int dx_k \int dx_l \psi_{E_k}^*(x_k) \psi_{E_{k'}}^*(x_{k'}) V(x_k, x_l) \psi_{E_l}(x_l) \psi_{E_{l'}}(x_{l'}) \right\}$$

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So, let us exploit the orthogonality integrals okay. So, left with a two center integral which is this which is the matrix element of the interaction depends on the k th and the l th coordinate

x_k in x_l . This is an integral between the states Ψ_{E_k} and Ψ_{E_l} with coordinates x_k and x_l . And here you have got the adjoint Ψ_{E_k} and Ψ_{E_l} with the coordinates x_k and x_l . So, this is the 2 center integral integration being over x_k and x_l .


And this double integral is then multiplied by a bunch of Kronecker deltas and when you carry out the summation over all of the E_l and up to E_n most of these will drop out because of the orthogonality. So, let us exploit that the only thing that does not get dropped out are those with summations E_k and E_l .

Which are the ones which are under the integration of this two center term, this potential energy term? So, you are left with the summation only over E_k and E_l whereas over here you had a summation over all the end quantum states. Now you are left with a summation earlier over two of them okay. But each is a set of 4 quantum numbers mind you okay or 4 or it could even be more.

Because depending on the number of degrees of freedom the particle has and how many compatible measurements you can carry out you will get those many number of single particle labels so it could be 4 or more. So, you have got this double summation you have got the half of this double summation over k and l , k not equal to l .

And then you have got this coefficient C as before this coefficient C is coming from here, this is the two center term, this term over here is the kinetic energy term which we have already discussed earlier. So, we are now focusing our attention on the potential energy term which has got this coefficient time dependent coefficient which contains those statistics. And then you have got this integral of the potential energy term.
(Refer Slide Time: 34:35)

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) &= \sum_{\mathcal{W}} \sum_{k=1}^N \left\{ C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \times \right. \\
 &\quad \left. \times \int dx_k \psi_{E_k}(x_k)^\dagger T(x_k) \psi_{\mathcal{W}}(x_k) \right\} + \\
 &\quad + \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{E_k'} \sum_{E_l'} \left\{ C(E_1, \dots, E_k', \dots, E_l', \dots, E_N, t) \times \right. \\
 &\quad \left. \times \int dx_k \int dx_l \psi_{E_k}(x_k)^\dagger \psi_{E_l}(x_l)^\dagger V(x_k, x_l) \psi_{E_k}(x_k) \psi_{E_l}(x_l) \right\} \\
 &\quad \text{writing } \mathcal{W} \text{ instead of } E_k', \text{ and } \mathcal{W}' \text{ instead of } E_l' \\
 i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) &= \sum_{\mathcal{W}} \sum_{k=1}^N \left\{ C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_N, t) \times \right. \\
 &\quad \left. \times \int dx_k \psi_{E_k}(x_k)^\dagger T(x_k) \psi_{\mathcal{W}}(x_k) \right\} + \\
 &\quad + \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_{\mathcal{W}} \sum_{\mathcal{W}'} \left\{ C(E_1, \dots, E_{k-1}, \mathcal{W}, E_{k+1}, \dots, E_{l-1}, \mathcal{W}', E_{l+1}, \dots, E_N, t) \times \right. \\
 &\quad \left. \times \int dx_k \int dx_l \psi_{E_k}(x_k)^\dagger \psi_{E_l}(x_l)^\dagger V(x_k, x_l) \psi_{\mathcal{W}}(x_k) \psi_{\mathcal{W}'}(x_l) \right\}
 \end{aligned}$$


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So, we have written this at the top of the next slide which is this and just as we label this summation over Ek prime as W, we now focus attention on the summation over Ek prime and El prime and to underscore this point we label Ek prime as W prime, Ek prime as W and El prime as W prime okay. So, that we know that the W's are the special ones over which the summation is left to be carried out.

All the other summations have been carried out already. So, it is the same expression rewritten here except for the fact that instead of Ek prime we have used a W here and instead of El prime we have used a W prime here. And you have that the coefficient C as well because the coefficient C had an Ek here and an El here.

So, they get be placed respectively by W and W Prime okay. Likewise in the integral you have got the coefficients Ek Prime and El prime here and these get replaced by W and W prime over here okay. So, it is just the same expression which is rewritten with the W's instead of the E's.

(Refer Slide Time: 36:04)

$$i\hbar \frac{\partial}{\partial t} C(E_1, E_2, \dots, E_N, t) = \sum_W \sum_{k=1}^N \left\{ C(E_1, \dots, E_{k-1}, W, E_{k+1}, \dots, E_N, t) \times \right. \\ \left. \times \int dx_k \psi_{E_k}(x_k)^\dagger T(x_k) \psi_W(x_k) \right\} + \\ + \frac{1}{2} \sum_{\substack{k=1 \\ k \neq l}}^N \sum_{\substack{l=1 \\ l \neq k}}^N \sum_W \sum_{W'} \left\{ C(E_1, \dots, E_{k-1}, W, E_{k+1}, \dots, E_{l-1}, W', E_{l+1}, \dots, E_N, t) \times \right. \\ \left. \times \int dx_k \int dx_l \psi_{E_k}(x_k)^\dagger \psi_{E_l}(x_l)^\dagger V(x_k, x_l) \psi_W(x_k) \psi_{W'}(x_l) \right\}$$

statistics : $i \rightleftharpoons j$
 $C(E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N, t) = \pm C(E_1, E_2, \dots, E_j, \dots, E_i, \dots, E_N, t)$
 + *Bosons* - *Fermions*

Our immediate interest is in: *Electrons* (Fermions)
 $C(E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N, t) = -C(E_1, E_2, \dots, E_j, \dots, E_i, \dots, E_N, t)$
 $i \rightleftharpoons j$

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Now plug in the statistics and we have agreed that it is contained in the symmetry of the coefficient C. If the coefficient C are symmetric you have bosons and if the coefficient C are anti-symmetric you have the fermions. So, I will now discuss the case of electrons because that is where most of the interest in atomic physics is.

Because you deal with the system of N electrons, so I will first discuss the fermions. And for fermions if you interchange these two labels Ej and Ei then the coefficient C must change its sign okay these are forming particles.

(Refer Slide Time: 36:51)

Electrons (Fermions):

$$C(E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N, t) = -C(E_1, E_2, \dots, E_j, \dots, E_i, \dots, E_N, t)$$


If $E_j = E_i$, $C(E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N, t) = 0$

Ordered sequence: $E_1, E_2, \dots, E_i, \dots, E_j, \dots, E_N$

Ordering denoted by: $E_1 < E_2 < \dots < E_i < \dots < E_j < \dots < E_N$

Coefficient: $C(E_1 < E_2 < \dots < E_i < \dots < E_j < \dots < E_N, t)$

all information about which one-electron states are occupied is contained in a coefficient:

$$f(n_1, n_2, \dots, n_i, \dots, n_j, \dots, n_N, t) \text{ where } n_i = 0 \text{ or } 1$$


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Of course if two of these labels happen to be the same if E_j is equal to E_i then this coefficient must vanish okay. This is nothing but a statement of the Pauli's exclusion principle. But for fermions for electron you cannot have the same state occupied by two particles. So, what we do is we consider an ordered sequence of these single particle states. This is not necessarily in increasing order of energy okay.

So do not get carried away by the letter E okay, E is a set of 4 quantum numbers remember okay. It includes the energy quantum number but it could also have other quantum numbers okay. Some of these may be degenerate for example the 1s up and the 1s down in the helium atom they have the same energy in the ground state okay. So, some of them may be degenerate.

So, obviously some of these energies will be actually equal to each other. But this inequality is an indication of the ordering and not a relationship between energy. So, do not get carried away by the letter E. It is not representing an energy it represents a particular quantum states and these quantum states you can always order in a certain way in a predetermined order. You decide how you want to do it okay.

You can put spin up before the spin down or vice versa it does not matter. But you decide what that order is and once that order is decided do not touch it, do not tamper with it okay. And that ordering is what is indicated by this inequality sign, it is not that this is any energy or angular momentum less than that of the next.

It only means that this set of quantum numbers will come before the next set of 4 quantum numbers which will come before the next set before the third set and so on. So, there is a certain ordered sequence of single particle quantum numbers. And these coefficients are also

having these arguments, the single particle quantum numbers E_1 through E_n . And they are also arranged in the same order.

So, all the information about the single particle states is now contained in a coefficient which tells us which single particle states are occupied and which are empty okay. This is where the importance of the occupation number formalism comes in because some of the single particle States will be empty okay.

You have considered infinite possibilities but only n out of these infinite possibilities are occupied because each single particle fermions state can be occupied by only one particle. There are n number of particles, so out of these only n are occupied the rest of them are vacant. And now if you write occupation numbers n_1 which is the number of fermions in state E_1 the number n_2 which is the number of fermions in state E_2 .

And each of these numbers for fermions will be either 0 or 1. For bosons it could be anything it could be 0, 1, 2 many or okay. So, you can have a number of different possibilities that we will first focus our attention on fermions and we find that the fact that which one is occupied and which one is not. This information is completely equivalent to the information which is there in the coefficients C .

So, there is a one to one mapping between the physical information which has gone into the coefficient C and the physical information which goes in this function f which is a function of all of these infinite single particle quantum numbers. Out of which only n will have a value 1 and the remaining will have a value 0.

But which one will have will depend on which of these single particle states are occupied all the others being vacant. So, this is where all this information is contained.
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$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, x_2, \dots, x_N, t) = H \Psi(x_1, x_2, \dots, x_N, t)$$

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{E_1} \sum_{E_2} \dots \sum_{E_N} C(E_1, E_2, \dots, E_N, t) \psi_{E_1}(x_1) \psi_{E_2}(x_2) \dots \psi_{E_N}(x_N)$$

$$f(n_1, n_2, \dots, n_1, \dots, n_n, t) \equiv C(E_1 < E_2 < \dots < E_i < \dots < E_j < \dots < E_N, t)$$

Many-electron wavefunction:

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{n_1=0}^1 \dots \sum_{n_2=0}^1 \dots \sum_{n_n=0}^1 f(n_1, n_2, \dots, n_n, t) \Phi_{n_1, n_2, \dots, n_n}(x_1, x_2, \dots, x_N)$$

Time-dependence

$$\Phi_{n_1, n_2, \dots, n_n}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{E_1^0}(x_1) & \dots & \psi_{E_1^0}(x_N) \\ \dots & \dots & \dots \\ \psi_{E_N^0}(x_1) & \dots & \psi_{E_N^0}(x_N) \end{vmatrix}$$

Slater determinant is time-independent

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So, this coefficient F which is a function of these occupation numbers and time is completely equivalent to the coefficient C which is a function of the single particle occupied states and time. Now you have a many electron wave function and this many electron wave function which you can write as the product of these single particle states.

So you plug in the statistics in it so you have got a Slater determinant which we have discussed in our earlier discussions and also in the previous course at great length, we dealt with the Slater determinant especially in the context of the Hartree Fock formalism. So, your n particle fermions state is given by these elements of the Slater determinant.

This is a normalized Slater determinant as you can see given the fact that we are dealing with single particle normalized states. So these elements of the Slater determinant are single particle normalized states of some, one particle operators. So, essentially what you are doing is you are superposing one Slater determinant over a second one, over a third one, over a fourth one the coefficients contain information about which are the occupied states.

The corresponding Slater determinant is used over here and you have as many Slater determinants as are important to describe the correlations. The correlated many-electron system will then be written as a superposition of very many Slater determinants in principle infinite okay. But in most practical cases only one may be important.

And in some others may be 5 or 6 or 10 a 20 are important or maybe a few hundred or even a few thousand okay. So, the Slater determinant is made up of these elements which are time independent single particle states all the time dependence is in the coefficients C and hence in the coefficient F okay.

So, the Slater determinant itself is independent of time the time dependence is in the coefficient F (Question time: 44:30—not audible) sorry yeah this is a particular Slater determinant that I consider okay. Which is the zeroth one but then you may have another one okay. So, just to indicate that this is a particular Slater determinant I have used the superscript zero.
(Refer Slide Time: 44:58)

Fermion occupation number state vector:


$$|\Psi(t)\rangle = \sum_{n_1=0}^1 \dots \sum_{n_r=0}^1 \dots \sum_{n_n=0}^1 f(n_1, \dots, n_r, \dots, n_n, t) |n_1, \dots, n_r, \dots, n_n\rangle$$

It is operated upon by
Fermion (electron) creation and destruction operators

fundamental anti-commutation rules
for fermion operators:

$$[a_r, a_s^\dagger]_+ = \delta_{rs} \quad [a_r^\dagger, a_s^\dagger]_+ = 0 \quad [a_r, a_s]_+ = 0$$

anti-commutator $[A, B]_+ = AB + BA$

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So, now we go over to a Fermion occupation number vector. So, the N particle system can now be described by a vector in something like a Hilbert space. But this space is what we shall call as an occupation numbers vector space. So, these are vectors very similar in properties you can define their norms, you can define their orthogonality relations.

You can define their completeness very similar to how you dealt with single particle vectors in a Hilbert space. And we now introduce the Fermion occupation number state vector which has this information. This occupation number for single particles can be either 0 or 1 and for each n1 both the possibilities are there. So, you should sum over n1 going from 0 to 1 okay.

And the fundamental properties of the Fermion particles is contained in what are known as creation and destruction operators. So, a is the destruction operator, a dagger is the creation operator and the statistics is completely defined by these operators. These are what are known as fundamental anti commutation rules.

The statement of these anti commutation because this is a comma a dagger which is a a dagger + a dagger a. So, A, B with a + subscript after this rectangular bracket is the anti commutator AB +BA at this anti commutator you have got for a at a dagger equal to delta rs this is the Kronecker delta, so it is equal to 1.

When r is equal to s otherwise it is 0 and for 2 creation operators the anti commutator is 0 and also for 2 destruction operators the anti commutator is 0 okay.
(Refer Slide Time: 47:21)

Boson occupation number state vector:

$$|\Psi(t)\rangle = \sum_{n_1} \dots \sum_{n_m} f(n_1, \dots, n_1, \dots, n_m, t) |n_1, \dots, n_1, \dots, n_m\rangle$$


$$\sum_i n_i = N$$

It is operated upon by
Boson creation and destruction operators

fundamental commutation rules
for boson operators:

$$[b_r, b_s^\dagger]_- = \delta_{rs} \quad [b_r^\dagger, b_s^\dagger]_- = 0 \quad [b_r, b_s]_- = 0$$

commutator: $[A, B]_- = AB - BA$



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So, now you have the Boson occupation number state vectors which are also defined in a very similar way except for the fact that the creation and destruction operators have got different properties but now there is no such constraint that these numbers n_1, n_2 etcetera are either 0 or 1. They can be anything they can be 0, 1, 2, 3, 10, 100 many right.

But the summation over all of these occupation numbers must add up to the total number of bosons that you are talking about okay. So, that is the only constraint and these occupation number vector states will be operated upon by creation and destruction operators which have a different set of rules. And these are given by the Boson creation and destruction and commutation rules AB with a - is $AB - B$.

This is the usual commutator that we work with especially when we deal with the position momentum operators okay, is the same commutator. But in the case of the Fermi operators you have the anti commutator. So, where is the statistics it is contained in the wave function in the first quantized formalism? The wave function is either symmetric or anti-symmetric under the interchange of two particles.

Then we found that the statistics was contained in the coefficients C okay. And the information in C is the same as the information in F which is in the occupation numbers. So, how do the creation and destruction operators operate in succession okay? That is where this statistics is contained. So, all the statistical information is now contained in these creation and destruction operators which are why they are different for Fermi particles as for the Bose particles.

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Fermion (electron) creation and destruction operators

Properties $|\Psi(t)\rangle = \sum_{n_1=0}^1 \dots \sum_{n_1=0}^1 \dots \sum_{n_x=0}^1 f(n_1, \dots, n_1, \dots, n_x, t) |n_1, \dots, n_1, \dots, n_x\rangle$

fundamental anti-commutation rules


for fermion operators:

$$[a_r, a_s^\dagger]_+ = \delta_{rs} \quad [a_r^\dagger, a_s^\dagger]_+ = 0 \quad [a_r, a_s]_+ = 0$$

$$a_s^\dagger a_s^\dagger |0\rangle = ? \quad a_s^\dagger a_s^\dagger = \frac{1}{2} \times 2 a_s^\dagger a_s^\dagger = \frac{1}{2} \times [a_s^\dagger a_s^\dagger + a_s^\dagger a_s^\dagger]$$

$$= \frac{1}{2} \times [a_s^\dagger, a_s^\dagger]_+ = 0$$

Pauli exclusion: you cannot create another fermion in a state occupied already!

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So, you have got the Fermi particles here that we are working with. Let us ask this question what would happen if two creation operators for the Fermi particle in s state operate in succession one after the other? What would happen? You are expected to go to 0, but that is from your knowledge of Fermi Dirac statistics, from first quantization. You should arrive at the same conclusion on the basis of the anti commutation rules for the Fermi operator's okay.

Because this is what we have defined which we have now introduced and these are the focal points of interest in the context of the statistics that all the statistics is contained in the anti commutation properties of the creation and destruction operators. So, using the anti commutation properties alone you should arrive at the same conclusion okay without referring to anything else.

So, if you did that the two operators, the two creation operators for the quantum state s operating in succession of each other. A succession one after the other, so it is half of twice of this right, twice of this is the sum of these. And the sum of these is just the operator as dagger as dagger anti committed with the same and what is that, that goes to zero right. And that goes to zero not from your previous knowledge of the Pauli Exclusion Principle.

But from the property of the anti commutation property of the creation operators so all the information the statistical information is now contained in the anti commutation relation. So, using this property you find that these two operators, then operate operated in succession give you zero which means that you cannot create a Fermion in a Fermi state which is already occupied this is the Pauli Exclusion principle.

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Eigenvalue of Fermion 'number' operator: $n_s = a_s^\dagger a_s$
fundamental anti-commutation rules :

$$[a_r, a_s^\dagger]_+ = \delta_{rs} \quad [a_r^\dagger, a_s^\dagger]_+ = 0 \quad [a_r, a_s]_+ = 0$$

$$[a_s, a_s^\dagger]_+ = 1 \quad n_s = a_s^\dagger a_s = 1 - a_s a_s^\dagger$$

$$(a_s^\dagger a_s)^2 = (1 - a_s a_s^\dagger)(1 - a_s a_s^\dagger)$$

$$= 1 - a_s a_s^\dagger - a_s a_s^\dagger + a_s a_s^\dagger a_s a_s^\dagger$$

$$(a_s^\dagger a_s)^2 = 1 - a_s a_s^\dagger - a_s a_s^\dagger + a_s (1 - a_s a_s^\dagger) a_s^\dagger$$

$$= 1 - a_s a_s^\dagger = n_s \quad \therefore n_s^2 = n_s$$

i.e. $n_s(n_s - 1) = 0$
operator identity *eigenvalues of n_s : 0 or 1*

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So, likewise you can understand other properties of the number operator. So, these are the fundamental anti commutation rules and if you know have the same state as and as dagger then this for r equal to s will be equal to 1. So, now if you write the operator as dagger as what do you get from this expression? From this expression you get that as dagger as which is the number operator is 1 – as as dagger okay.

Now this being the fact if you now take the square of this okay, if you take the square of this you have got 1 – as as dagger followed by 1 – as as dagger. Now you expand all of these so you get 4 times 1 – as as dagger. Then you get another as as dagger from this and then you get these two minus signs give you a plus sign. And then you get as as dagger again is as as dagger that is what you get right.

So, far for charms over here now out of these 4 terms you can anticommute these two. Because as dagger, if you want to move as behind as dagger you will get 1 - as as dagger right. So, I have exploited the anti commutation between in as and as dagger and using that anti commutation I get these two terms 1 - as as dagger. From this you get as multiplied 1 multiplying as dagger with a + sign.

So, you get as as dagger + which cancels one of these and you are left with only this which is 1 – as as dagger right. From the residual term you have got as dagger as dagger which we saw in the previous discussion already goes to zero. So, you get only 1 – as as dagger which is nothing but the operator ns itself.

What does it tell you that the square of ns is the same as ns right? And if that is the case then, these being an operator identity the only two possible Eigen values the occupation number

operator can have are either 0 or 1 okay. Now this we already knew because of our familiarity with the Pauli's exclusion principle.

But we are now able to actually deduce it from the anti commutation properties which has got all the statistics built into it including the consequences of statistics such as the Pauli Exclusion Principle okay. So, this is the power of the anti commutation rules for fermions and you have got the same power for the boson commutation properties.
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fundamental anti-commutation rules :

$$[a_s, a_s^\dagger]_+ = \delta_{rs} \quad [a_s^\dagger, a_s^\dagger]_+ = 0 \quad [a_s, a_s]_+ = 0$$

$n_s = a_s^\dagger a_s \quad \therefore n_s^2 = n_s$ $a^\dagger a$: Number operator eigenvalues of n_s : 0 or 1

Number 0 'zero'

$a^\dagger |1\rangle = 0$ $a|0\rangle = 0$

$a^\dagger |0\rangle = |1\rangle$ $a|1\rangle = |0\rangle$

a^\dagger : Creation operator a : Destruction operator

Vacuum state: $|0\rangle$
No particle

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So, you have got these properties the square of the occupation number is the same as n_s . And you will find that the creation operator, if it tries to create a particle in a state which is already occupied, then you get 0. Because you cannot create a particle in which you already have occupancy nor can you destroy a particle from a vacant state from a vacuum state.

Marea yuve ko kya marna right if there is no state in it already you cannot destroy a particle out of it. So, a , the destruction operator operating on the vacuum state will give you the number 0. So, keep track of the difference between the number zero and the vacuum state. The vacuum state is a vector in the occupation number state. The number zero is the arithmetic zero which ancient Hindu mathematicians invented okay.

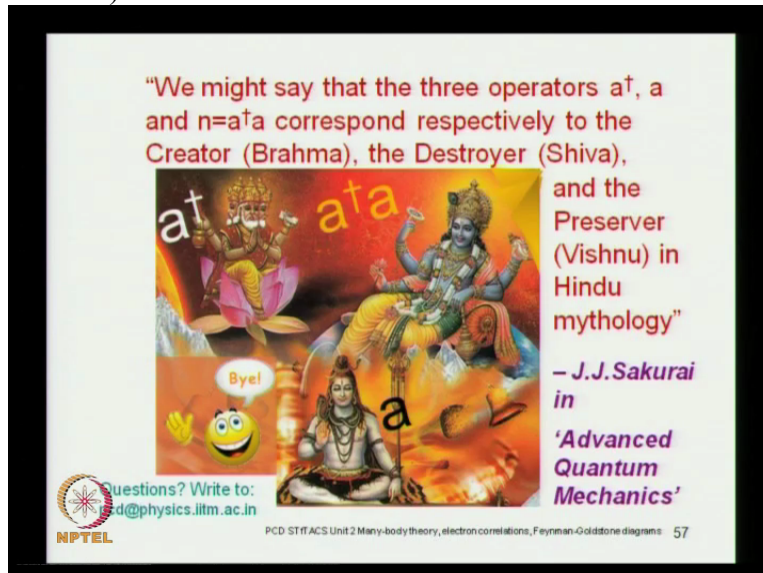
So, these are two different things, so these are your fundamental properties and they explain to you why this should be called as the destruction operator? Why it should be called as an annihilation operator? Why the its adjoint should be called as a creation operator? And why this operator a^\dagger , should be called as the number operator.

So all of these operators acquire a particular significance in the context of the properties they attained from the anti commutation properties of these operators. So that is where the physics

is, that is where the statistics is okay. And they tell you which single particle states are occupied and which are not occupied.

All properties like Pauli exclusion and principle etcetera are contained in the properties of these creation and destruction operators. And this is a good point to take a break here and continue from this point in our next class.

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And on the lighter wane, I will like to quote Sakurai from his book Advanced Quantum Mechanics, Sakurai has got two excellent books one is Modern Quantum Mechanics which you have used the other is Advanced Quantum Mechanics which also some of you would have used which I strongly recommend which is very good.

And in this book Sakurai has got a rather interesting quote, he says that we might say that the three operators a dagger a, and a dagger a, correspond respectively took the creator, the destroyer the Brahma, the Shiva. On the preserve Vishnu okay. So, these are the creation destruction and number operators. This is where the physics is sitting okay. That is what our interested okay.

All the physics is sitting over here in the properties of these creation and destruction operators. And we will continue from here in the next class and see how this formalism helps us deal with correlation that is our fundamental interest okay. In the absence of correlations we already know how to deal with the n particle electron system that is the Hartree Fock theory.

But they do not include any Coulomb correlations when you want to include the Coulomb correlations when you want to go beyond the Hartree Fock then you must have a many body

correlation formalism which is why you have a superposition of all of these Slater determinants. And because it is so messy to work with these factorial n terms in the Slater determinant it is now going to be very convenient to deal with these numbers.

Because now you just have to deal with two numbers either 0 or 1 it is all binary okay. So, it is the whole physics, the same physics but we are going to have an operational convenience. So, it is not like a fundamental step in quantization as we take from classical mechanics to quantum mechanics that is a big step that step involves dispensing with causality.

And determinism of classical mechanics and replacing it with the uncertainty principle and measurement and the idea of compatible measurements and so on okay that is a very big jump. Whereas in this case it is just a formalism which you are moving over from the first quantization formalism to a second quantization formalism which is going to make it very easy.

So, it is convenient mathematical convenience, mathematical elegance and not like a fundamental step involved in quantization. So it is called a second quantization because now you have got the wave functions which get quantized, I will deal with that little later. But actually the creation and destruction operators become quite significant in the context of relativistic formalism.

Because in relativity you have matter and energy which you can convert from each other, so you can actually create particles when no particles existed okay or you can annihilate an electron against a positron and create energy right. So, you can actually destroy or create particles in this relativistic formalism and then second quantization becomes really necessary to describe those processes.

But in the absence of those terms and that is not the domain of interest in atomic physics because our interest in atomic physics is at low energies okay. Now these processes do not take place at low energies, you have to go at least above the rest mass energy of two electrons okay. So, which is about a million electron volts, so that is not the domain of atomic physics the structure in spectroscopy that we do work with in atomic physics.

But for us it is mathematical elegance, it is mathematical convenience and a great convenience at that. Any question (Question time: 1:02:03 –not audible) we can call it the number operator only because of the first two I mean a dagger, because its square is equal to itself, that is an operator identity which tells you that its Eigen values can be only 0 or 1 okay.

Eigen value of the number operator is either 0 or 1 that is the number which tells you whether a single particle state is occupied or not. And in the case of fermions either it is occupied or it is not occupied there is nothing in between. So, that is what justifies it named as the number operator because its Eigen values can be either 0 or 1.

In the case of Boson it actually gives you the number of Bosons in that particular state, n is an occupation number vector, you can do algebra in occupation number space, you can construct a linear superposition of two occupation numbers vectors just the way you can do a superposition of two Hilbert space vectors right. And you can add a null vector to another vector which gives you the same vector.

But it is a vector in the Hilbert space whereas the number 0 is not a vector in the Hilbert space it is the arithmetic zero. (Question time: 1:03:47- not audible) yeah when we have a electron in a particular state and we are trying to create an electron in that space we are not getting a vacuum state, we are getting $n=0$ what I mean that is not, we are not getting it zero state, just a zero.

You do not get a vacuum state; you do not get a vacuum state by trying to destroy a particle in a vacuum state. What this equation is telling you is that you cannot do that. It is not that you get vacuum by destroying a particle in the vacuum state because there is no particle on the vacuum state. So, you just simply cannot do it that is the number zero. So, on this note we will stop here for now and then we will continue the discussion from the next class.