Advanced Condensed Matter Physics
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Lecture – 04
Second quantization II

So, we named this as equation 1.

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$$\Psi = |\lambda_1, \lambda_2 \ldots \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} n_\lambda!}} \sum_K p^{(1-\operatorname{sgn} K)/2} |\lambda_{K_1}\rangle \otimes |\lambda_{K_2}\rangle \otimes \ldots\ldots |\lambda_{K_N}\rangle \quad (1)$$

$\operatorname{Sgn} K = 1$ or -1

$+1$: for even number of transpositions

-1 : for odd number of transposition.

$\frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} n_\lambda!}}$: normalization

$p^{(1-\operatorname{sgn} K)/2}$: Symmetrizes the wave function.

And to remind you that we have this factor which is 1 divided by root over of N factorial. And then there is a product of n lambda factorial and lambda really goes from 0 to infinity. So, this is our normalization factor and these normalization factor normalizes the many body wave function psi which is written in equation 1; the left hand side of equation 1.

And the, this quantity which is P to the power 1 minus S g n K divided by 2; it symmetrizes the wave function. So, what we mean by symmetrizing the wave function is that as been told earlier that for the Fermions any change in the position of the particle or transposition of two particles would bring in a negative sign. And if that is done twice then it brings back another negative sign which means it becomes positive whereas, for Bosons it is always positive no matter how many times the transposition is done.

So, this is our many body wave function that we are going to talk about now let us look at a typical many particle state as this.

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Many particle state

$$|1,1,1,1,2,2,3,3,3,4,6,6\cdots\rangle$$

$$\equiv |4,2,3,1,0,2,\cdots\rangle$$

Many particle state $\Rightarrow$ how many particles occupy position i. for fermions, the numbers will take values 0 and 1. for Bosons, they can be any.

occupation representation $\equiv$ Fock Basis (after Russian Scientist V.A. Fock)

So, we are giving an example of a many particle states let us say that it is written with a ket which is 1, 1, 1, 1 and then 2, 2 and then 3, 3, 3 and then its 4 and then it is 6, 6 and etcetera. So, what is meant by this notation is that at the real space that is i equal to 1 as the position space ah; for i equal to 1 there is one particle the for i equal to 2; there is another one again one particle then at i equal to 3 then there is another one particle i equal to 4 one particle, i equal to 5 two particles i equal to 6 two particles and so, on.

Now, this notation for a many particle system can be simplified; if we simply write this as 4 and then 2 and then 3 and then 1 and 0 and 2 and so, on. So, in going from this many particle state on the top from in the written in the position basis we have gone to a many particle state where we have simply written down the number of particles that is at position. So, so these are there are 4 number of particles at the first 4 positions rather. So, there are 4 occupancy in the first 4 sites or locations and then it is 2, then there are 3 and 4 1 and there is no 5. So, if we put a 0 and then there is there are 2; 6 and so, on.

So, now this is written in a basis which is called as the Forck basis. So, what is the Forck basis; so, we have written down this many particle state or the wave function in. So, telling that how many particles occupy. So, occupy position i; so, for Fermions of course, we know by the exclusion principle Paulis exclusion principle.

So, the numbers will take values the numbers that is written here the numbers will take values 0 and 1 and for bosons, they can be any because. Bosons do not have any exclusion principle embedded there. So, as many as possible or as many as number of particles are there, they can occupy the same energy level unless it is been or rather constrained by any other principle or any other you know symmetry argument.

Now, this writing it in the occupation basis or the particle number basis is called as the Forck basis. And we will call this as a occupation representation and this is same as the Forck basis or Forck representation. And this is after the name of Russian scientist after Russian scientist of V. A. Forck.

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forck basis as $\mathcal{F}$

The many body state is written as,

$$|\Psi\rangle = \sum_{n_1, n_2 \cdots n_N} C_{n_1, n_2 \cdots\cdots} \underbrace{|n_1, n_2 \cdots\cdots\rangle}$$

$$\boxed{\sum_i n_i = N}$$

Total fock space is written as,

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^N \qquad \bigoplus : \text{Direct Sum.}$$

$\mathcal{F}^0$: vacuum necessary to include in the family of basis states.

So, now, we will write this Forck basis as. So, this is written with a curly F a curly F like this and so, the many body state would be written as in this occupation number is this I am writing it with a ket we could have written this with the ket as well. So, so this is equal to some n 1 n 2 and so, on and then there is a n n and this C n 1 n 2 and all of that and then its n 1 n 2 and so, on.

So, that is some many body state where C n 1, n 2 etcetera are the coefficients and these are the Forck basis. So, the occupation number basis. So, we have occupation n 1 at a given side and then occupation n 2 and occupation n 3 and so, on. So, n 1 and n 2 will all be equal to either 0 or 1 for Fermions whereas, for Bosons there could be any number.

Now, in the; so, in general we have n i equal to N. So, the total number of particles is equal to N; however, in a grand canonical sense we can relax this constraint and we can say that we have a Hilbert space which is large enough to accommodate infinite number of particles. So, then the total Forck space is written as Forck space is written as it is equal to a notation that I will use I will just tell in a while its n equal to 0 to infinity and this is equal to the power N where this is known as the direct sum.

Now this Hilbert space must necessarily include F 0 which is vacuum means that it does not contain any particle and it necessarily should be to include in the family of basis states. So, now, we have a state which is given by this and written in the occupation basis or the Forck basis and in the Forck basis; the total Forck space is written in terms of the this F to the power N and written as a direct sum for from n equal to 0 to infinity. And we do not have this constraint of this one any longer that is sum over N i which is basically the occupancy of each state has to be equal to some finite number n that is not there any longer.

So, what is this occupation number representation useful for? So, what is the benefit derived from starting from a representation which we have written in the position basis. And then we have tried to go on to the occupation number basis or the Forck basis what is the benefit of doing that. In fact, it of course, as you can see that this looks much more simpler as compared to the representation that has been used earlier that is the position representation.

However, in the position representation there is an enormous summation involved here in equation 1 which is a sum over K and then there is a P to the power 1 minus S g n k by 2; it is been told earlier and its written here as well that S g n k is either equal to k plus 1 or minus 1 and when it is equal to plus 1 then there is no sign that is this factor is equal to 1. However, when there is a S g n k is equal to minus 1 then we have sign. So, that is the becomes P equal to 1 where P is equal to plus 1 for Bosons and P equal to minus 1 for the Fermions.

And from there we wanted to go to this occupation number basis and even though it looks simpler, but this enormous sum that appears here how is it going to be taken care of. And remember that this sum is important for the symmetrization of the state and this symmetrization gives the slater determinant for the Fermions which is the anti symmetric property of that matrices are encoded in transposition of particles; for Fermions which would pick up a negative sign. As one does a transposition or changes the position of one particle.

So, how that is going to be encoded into this occupation number basis? And in principle we are need to be worried because we are talking about 10 to the power 23 number of particles and transposition of them leading to the right symmetrization for a particular wave function need to be taken into account. So, this is done very elegantly in the using a second quantized formalism.

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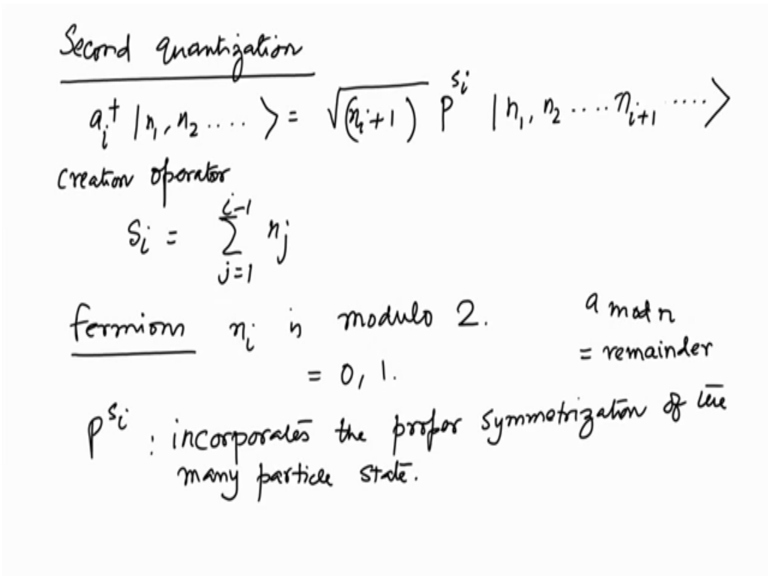

So, this is where the second quantization is important and will tell you how it is important. So, let us define a creation operator which is acting on a many particle system such as this. So, a i dagger acting on n 1 n 2 etcetera and that by definition we are now using a definition that we are going to we are introducing introducing it for the first time. And this is n i plus 1 and then there is a P si and then there is a n 1 n 2 and n i plus 1.

And so, what it does is that a i which is a creation operator. So, this is the definition of operation of a creation operator. So, creation operator acts on the ith particle and raises the occupancy of the ith particle from n i to n i plus 1; brings in a coefficient which is root over n i plus 1 additionally to take care of the symmetrisation requirement brings in another factor which is P to the power S i and where S i is equal to summation over j from 1 to i minus 1 and n j. So, we will have to sum over all the occupancies up to that ith side just before the ith side and that ith side of course, the occupancy is raised by one.

Now, it is important to note that; so, in a fermionic system. So, for Fermions this n i is is modulo 2; so, what we mean by modulo two is that when you divide a number a by n it is called as a modulo n and what it means is that; when you divide a by n the answer is the remainder of this division. So, for Fermions the division will leave a number which is either 0 or 1 because i am dividing by 2. So, n is equal to 2 here and so, n i is modulo 2 means that automatically it means that it can acquire values 0 or 1. And that is the reason or rather that takes care of the fact the that the occupancy of Fermions at each side could be either 0 or 1 and so, that emphasizes the Paulis exclusion principle.

Now, let us take a; so, basically; so, P to the power S i; it makes accommodates or rather incorporates the symmetrisation, the proper symmetrization of the many particle state.

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$$a_3^{\dagger} |n_1, n_2, n_3 \cdots\rangle = \sqrt{n_3+1}\; P^{(n_1+n_2)} |n_1, n_2, n_3+1 \cdots\rangle$$

$$P \text{ takes } \begin{cases} +1 & \text{for Bosons} \\ -1 & \text{for Fermions} \end{cases}$$

$P^{(n_1+n_2)}$: takes care of Symmetrization of the state

$$|n_1, n_2 \cdots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} \left(a_i^{\dagger}\right)^{n_i} |0\rangle \qquad (2)$$

Two particles $a_i^{\dagger}, a_j^{\dagger}$ $\qquad a_i^{\dagger} a_j^{\dagger} |0\rangle = |2\rangle$ $\quad i \neq j$

$$\left(a_i^{\dagger} a_j^{\dagger} - P a_j^{\dagger} a_i^{\dagger}\right) = 0$$

So, let us give an example take a many particle state which n 1; n 2, n 3 and so, on. And let us operate by a creation operator which operates on this third occupation and then we can write this as root over of n 3 plus 1 and P to the power n 1 plus n 2 and we have n 1, n 2, n 3 plus 1 and so, on ok.

So, this the operation of the creation operator acting on n 3. So, as usual a P takes a value P takes plus 1 for Bosons and minus 1 for Fermions and so, this P s i here n 1 plus n 2 this takes care of care of symmetrization of the state; which means that if n 1 plus n 2 is equal to 1. Then we have an anti symmetric state because for Fermions it is an anti symmetric state because it is minus 1 whole to the power 1; however, if n 1 plus n 2 is equal to 0 then we have a symmetric state or n 1 plus n 2 equal to 2; we have a symmetric state. And so, this is how the in this Forck basis; the symmetrization of the many particle state is encoded and it is very elegantly done in the second quantized formalism you will get more glimpse of it as we go along.

So, now let us then write down a wave function many particle wave function in the Forck basis as this which is a product of and this is a n i factorial and there is a a i; n i acting on a vacuum let us call this as equation 2. And if you remember that we have insisted of having this vacuum or that F 0 that we had written which is null state or a particle without any particles as an important element in the family of the of the Forck basis.

And this is we actually create a many particle state by successively operating the creation operator on the vacuum and so, this complicated permutation entanglement; which is there in equation 1; here by this summation over K and P 1 minus S g n k by 2; now that is encoded here and how would it be encoded? It will be encoded through the commutation relation of these operators. And that is why this formalism of second quantization is so, helpful for dealing with many particle systems. So, so, this basically tells you that there is an enfold application of this operator a dagger on the vacuum state to build a many particle state.

Let us try to understand that how the symmetrization is built in by the commutation relation of this operators; let us take only two particles to begin with. So, we have two particles and say they are located at a i or rather i and j and they are; so, we just write them as a i dagger and a j dagger as the creation operator for these two particles. So, as if they are acting on vacuum.

So, a i dagger and a j dagger acting on vacuum gives me that state which is what I want to consider. Let us call it just a two particle state and let us look at the commutation relation of these two particles. And needless to say here that i is not equal to j because for Fermions it is anyway forbidden to have i equal to j you cannot have two particles being formed at the same side or being created at the same side.

So, let us define the commutation relations by this a i dagger, a j dagger minus P a j dagger; a i dagger and equal to 0. So, what I have done is that; I have written them as i and j and then in the next term; I have written with a minus i mean with a j and i in addition to that we have a minus P.

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Where $P = 1$ denotes Commutation relation

$= -1$ denotes anticommutation relation.

$$[a_i^\dagger, a_j^\dagger]_P = 0$$

$$[A, B]_P = AB - PBA.$$

$$[A, B]_{P=1} = AB - BA. \longrightarrow$$ Commutation relation of A & B.

$$[A, B]_{P=-1} = AB + BA. \longrightarrow$$ Anticommutation relation.

$$[a_i^\dagger, a_i^\dagger] = 0.$$

And so where P is equal to where P equal to 1 will stand for denotes commutation relation and P equal to minus 1 denotes anti commutation relation.

Let us see clearly; what it means is that we have a i dagger a j dagger and I will write a P sub script here which is equal to 0. So, the notation is that if I have two operators A and B and written with a P as a sub with a square bracket and this is equal to A B minus PBA. So, for commutators; this relation is P equal to 1 which is equal to A B minus B A and for anti commutation.

So, this is the commutation relation of A and B and this is the anti commutation relation for A and B. So, if this commutator is equal to 0 then we say that this two operators commute. And when two operators commute it is usually correct that they have same set of Eigen functions they have common Eigen functions. And if they do not commute then that does not hold and these this is the anti commutation relation of since the anti commutation relation ok. And if we go back to our a i dagger a i dagger then that is equal to 0 because the identical operators would commute.

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Summarizing,

$$\forall\, i, j \quad [a_i^\dagger, a_j^\dagger]_P = 0$$

$$\mathcal{F}^N \rightarrow \mathcal{F}^{N+1}$$

annihilation operators, $\mathcal{F}^N \longrightarrow \mathcal{F}^{N-1}.$

$$[a_i, a_j^\dagger]_P = \delta_{ij}\ ; \ [a_i, a_j]_P = 0;\ [a_i^\dagger\ a_j^\dagger]_P = 0.$$

And so, if we summarize; here these relations for all i and j a i dagger; a j dagger equal to P equal to 0. So, ah; so, similarly we have we can write this as. So, for both P equal to 1 and P equal to minus 1 and just like the similarly if we want to write it for the annihilation operator; just like that a creation operator takes N component Forck state from this to this F N to F N plus 1; we can also talk about annihilation operators on which we will take my Forck state N to N minus 1.

And we have relationships similar relationships; commutation relationships for the annihilation operators as well and they are written in a compact form by this relation which is equal to this and a i; a j P equal to 0 and a i dagger a j dagger P equal to 0.

So, the enormous complex the complexity of the of the many particle space and the complexity that is related to symmetrization of the many particle wave function; is taken care of in the Forck basis by choosing or rather from the commutation relations or the anti commutation relationships of the operator. And this is a phenomenal improvement of the situation as we can see in the next discussion.