Introduction to Statistical Mechanics

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Lecture – 28
Creation and Annihilation in Fock Space- I

So, today let us begin a new topic, so this is continuing in the same vein as the other topics that I just covered, so these would fall under the category of advanced topics, so I would not be testing you on these topics in the examination, so but still these are sufficiently important that you should know them so, it is debatable whether you want to classify this strictly as being part of statistical mechanics or not.

But certainly, you know, see physics is a unified discipline that you cannot really have sharp boundaries in physics, so the topic that I am going to discuss today namely the creation and annihilation operators in many particle systems or many body physics is quite important for modern condensed matter physics and particle physics and so on.

So, it is important for you to learn what second quantization means especially in the context of solid state physics okay, so trying to tell you roughly what I am talking about, so you see just as we could you know if you take a simple harmonic oscillator which is described you know in terms of position and momentum variables, so you could do quantum mechanics in the Schrodinger picture by writing the momentum operator as minus ih bar d by dx.

And writing down a Schrodinger's wave equation and finding the stationary states, so alternatively what you could do is you could create and annihilate quanta of the model, so basically you describe the creation and annihilation operators in terms of the position and momentum but what happens is that in many cases, so in that context; in the context of harmonic oscillator, you can create and destroy basically excitation.

So that means, you have a ground state and you can create an excited state from the ground state by adding a quantum of excitation but then what happens is that in many particle physics, it is frequently the case that the number of particles in a given system can also change, so that means not just the; I am not talking about the quanta which correspond to the excitations but the particles themselves can be created and destroyed.

So, if that is the case, then we really need a formalism that this can describe you know what happens to a system which has a certain number of particles whether they are fermions or bosons and how to describe them if I add one more particle or remove a particle from the system, so that requires a slightly different perspective from whatever in discussing till now but it still uses the idea of creation and annihilation operators.

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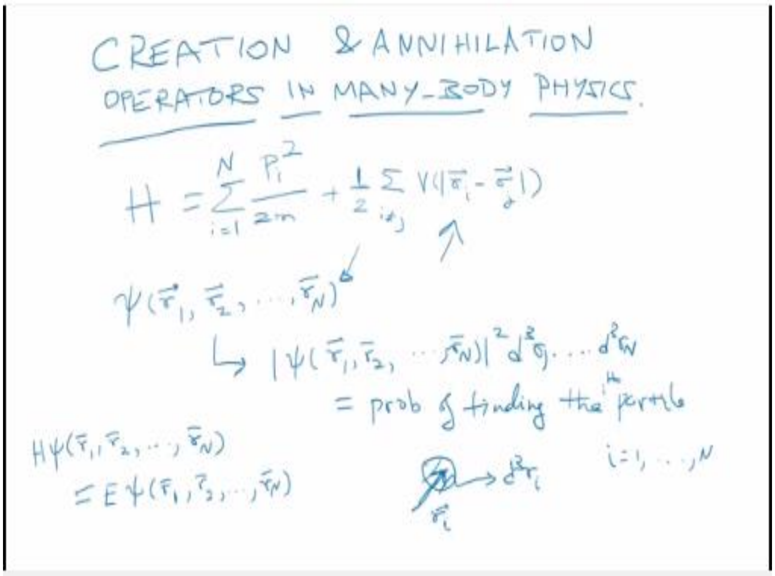

So, let me go ahead and tell you how I do it, so imagine let us start off by describing a system which is of this nature, there is you have say N quantum particles, I will tell you well, right now we will not commit ourselves to either fermions or bosons but later we will have to commit ourselves right now, we just know that they are one of the 2 and they are quantum particles.

So, now imagine that I have a situation where I have these N quantum particles and naturally they have kinetic energy but they also have a mutual potential energy that means that they interact mutually pairwise, so there is a pairwise potential energy which is described by with this v here, okay. So, how would Schrodinger have dealt with this problem?

See, what Schrodinger would have done is that he would have said that well the best way to deal with this problem is to list all the stationary states namely that I would be looking for you know a wave function of this type, so I am going to say that there is an complex valued function I am sorry, there is a complex valued function of this type, so this represents; so what is the physical meaning of this?

So, this means that this quantity, right is the probability, this is the probability of finding the particle; finding the ith particle I should say, finding the ith particle in this region, so basically this is your ri and this volume is basically d cubed ri, so the probability of finding the ith particle in a volume d cubed ri around the point ri, so and where i goes from 1 to n, so that means the probability of it is the joint probability of finding the first particle at r1 within a volume of d cubed r1.

Second particle at position r1 within a volume of d cubed r2 etc., etc., so that is what this means, so the question is how would you compute these stationary states, you would naturally go ahead and solve this type of equation and you would be able to write down a whole bunch of; so you will have many solutions to this corresponding to each Eigen, so there will be several eigenvalues, so this is an eigenvalue problem.

So, you will have many eigenvalues and so the point is you see now, you have to ask yourselves if the underlying particles are bosons or fermions, so where does that information go into this formalism? Basically, it goes into the formalism by virtue of imposing or realizing that there is a further constraint on the nature of this wave function.

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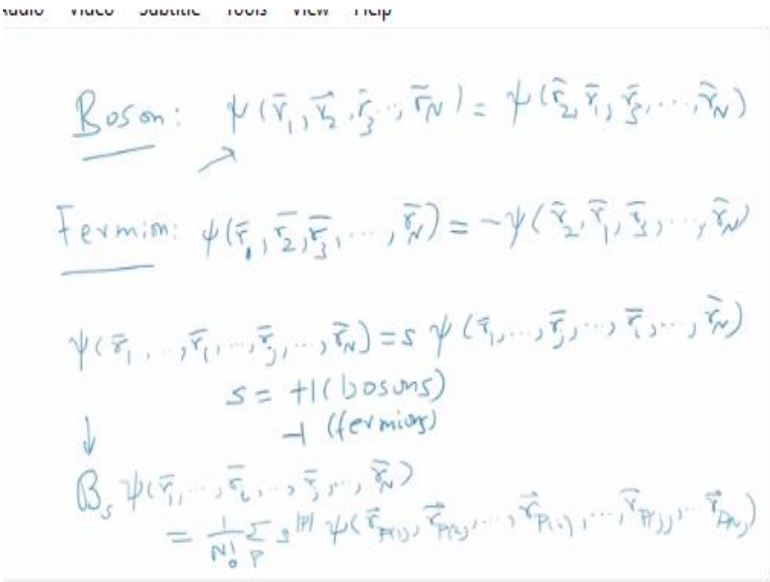

So, the constraints I am going to list here, so if it is boson, the constraint is that if I take, so let us take for example r1 and r2, so if I interchange r1 and r2 and keep all the other things fixed, okay. So, r3 is unchanged, so I interchange r1 and r2, right and keep all others fixed, so I should get back the same wave function. So, if it is symmetric under exchange of any 2 particle; does not have to be 1 and 2, it can be 4 and 8 or 1 and 7 or 1 and 12.

So, it can be any pair so, if I interchange any pair I should get back the same wave function so, if the wave function is you know you impose such a constraint on the wave function and also go ahead and solve this equation, so that would describe to you a stationary state of a many boson system; so N boson system specifically in this context but suppose, you want to describe the stationary states of a N fermion system, what would you do?

What you would do is; you would impose a different constraint, you would say that the constraint imposed is basically, the one which flips the sign as we exchange or interchange pairwise, so if I interchange r1 with r2, the wave function changes sign. So, if you do; then you call that of N fermion system. So, just both boson, N boson systems and N fermion systems have to obey the stationary state Eigen value equation, this time independent Schrodinger equation specifically that is what it is called here.

So, I am going to write this compactly in the following way, so I am going to generalize this so, if I interchange i and j for example say, ri, rj so, interchange rj so, I am going to write this as s times r1 rj ri rN, so s is either plus 1 for bosons or minus 1 for fermions okay. So, this is s1 for bosons, is minus 1 for fermions. So, now I am going to continue to develop some formalism which will enable me to you know avoid this rather clumsy approach.

See notice what is clumsy about this approach is that I mean there is nothing conceptually or mathematically inadequate or insufficient about this approach but what is clumsy about this approach is that you see it requires you to solve a Schrodinger equation with you know N particles, where N could be macroscopically large, so imagine the number of electrons in a typical solid, it will be you know 10 raised to you know something like a 20 or 30 more or less.

So, for typical sized sample, so but then that is you know solving a Schrodinger equation with that many variables is quite silly and you want to bypass that type of requirement and see if you can simplify your formalism which will enable you to sidestep having to actually solve you know the time independent Schrodinger equation. So, in order for me to accomplish this, I need to develop some formalism, so which is what I am doing right now.

So, I am just pointing out to you that these; so by following a certain sequence of steps, I will be able to eventually sidestep having to solve time independent Schrodinger equation. Look, if you find some solution to the time independent Schrodinger equation namely this that there is no guarantee that solution will either describe N fermions system or N boson system.

So, a typical solution will be, it will not respect any particular symmetry, so it could be quite unsymmetrical, so it could; it describes neither bosons or fermions, so the first task that we have in front of us is to develop or introduce an operator that would help us in restoring proper symmetries to these wave functions. So, if you have a wave function that does not obey any particular symmetry, I want to introduce an operator that forces a certain kind of symmetry on the wave function.

So, let me introduce that operator right now, so that is called the symmetrisation operator in the case of boson or the anti-symmetrisation operator in the case of fermions. So, the operator is basically described by the script B with subscript s corresponding to plus 1 for bosons and minus 1 for fermions and I am going to define it like this, so this is the definition of the; this is the ith particle and this is the jth particle.

So, now I am going to define it in this fashion, so I permute over all the particles and so okay, so that is what that is. So, this is; this would what does the so it looks very formidable, so let me tell you what is going on here, so basically the idea is that if you have a wave function that is not guaranteed to be symmetric or anti-symmetric what you do is that you force it to become one or the other.

So, if s is plus 1, what this is going to do is that it is going to you know permute the sequence, so you see if you have a sequence of N objects, you can have N factorial permutations, so every permutation has a certain index, so that means okay, so let me describe to you what I mean by that.

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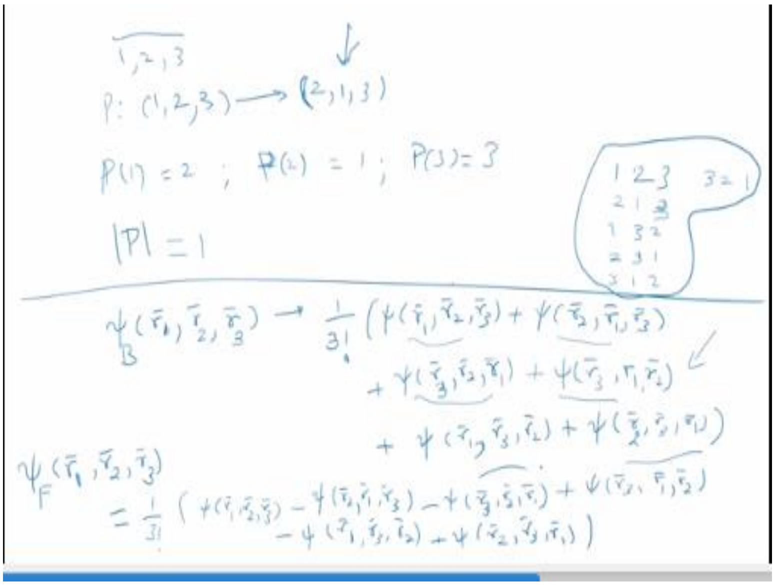

Suppose, you have 3 particles; 1, 2 and 3 okay, so you can have a permutation where the permutation can be that I take 1, 2 and 3 and jumbled it up and make it 2, 1 and 3, so this is the; this is my permutation so, I can ask myself what would be the image of 1 under this permutation. So, the image of 1 under this permutation is basically, 2, the image of 2 under this permutation that means 1 becomes 2, 2 become 1 and 3 remains 3.

So, this is what it is, so this is my permutation okay, so now I define something called mod P which is a number which tells me the number of pairwise interchanges I need in order to bring this jumbled up sequence back to the original sequence namely 1, 2, 3. So, in this case I need precisely one such interchange, so if I take 2 and 3, I interchange 1 with 2 and 2 with 1, basically I interchange 2 and 1.

So that is sufficient for me to send this back to its canonical form namely 1, 2, 3, so in other words this mod P in this context is 1, so similarly you can if you have many more particles, so you can have a mod P which is something else, so the point is that notice that here it is s raised to mod P, so the only thing that matters is whether mod P is odd or even. So, if s is 1, it does not matter at all, it is independent of mod P completely.

But if s is minus 1, in other words if you are describing fermions, it really does matter, so if it is; if the number of interchanges you require to bring the jumbled up sequence back to the original one is odd, then you pick up a minus sign, if it is even you pick up a plus sign, so that is in the context of fermions but if for bosons it is always plus 1. So, now I have to convince you that this, wave function.

So, even though this notice that this psi, even though this did not have any particular symmetry after acting by this symmetrisation operator, it is going to obey the symmetry described by this index s. So, if it; if s is plus 1, it is going to describe a system of N bosons and if s is minus 1, so this whole object after acting on the script B is going to describe a system of N fermions, if s is minus 1 okay.

So, question is how do you convince yourself of that and so let me give you a simple example, so this looks very formidable, so I do not want to scare you with general forms. So, let us take a very simple example say for example, 2 is too simple, so let us try with 3, so just like I told you earlier. So, you have 3 particles, so you have; so imagine you have a system of 3 particles and you want to convert that to a system of 3 bosons.

So, what you would do is that so, if initially this does not respect any symmetry, you can convert this to a system of 3 bosons by doing this, so what you do is capital N is 3 and s is plus 1 because you want a system of 3 bosons, so then 1 raised to mod P is always 1, then you have to sum over all the permutations. So, how many permutations of 1, 2, 3 are there? So, there are 3 factorial, which is 6 permutations.

So, what this is saying is basically you take this and so you start listing all the permutation, they are 6 of them, so I am going to list all of them like this. So, if I interchange 1 and 2, then I interchange 1 and 3 yeah, I interchange 1 and 3, then I interchange 2 and 3, I am just going to list them, write 1 2 3, 2 1 3, write 1 3 2, 2 3 1, then 3 1 2, then 3 2 1, I think we have, yeah listed 1, 2, 3, 4, 5, 6 these are all.

So, 1 2 3, 2 1 3, 3 2 1, then 3 1 2, okay and what did I leave out; psi 1 3 2 + psi 2 3 1, okay, so I think 1, 2, 3, 4, 5, 6 okay, so this makes sense so, I have this is my whole story. So, this is what I get but now this would describe a 3 boson system, okay but suppose I want to describe a 3 fermion system what would I do. So, notice that this does not have any particular symmetry but put together, it has symmetry.

So, let me convince you that it has this requisite symmetry, so imagine that I take this whole thing and I interchange 1 with 2, suppose I inter change 1 with 2, what is going to happen is that this goes to this and this goes to this okay, so these 2 go to each other, so together they remain unchanged. So, similarly if I interchange 1 with 2, these 2 go to each other and they remain unchanged.

And similarly, here if I interchange 1 and 2, this goes to this and this goes to this, so together they remain unchanged. So, overall the whole thing remains unchanged if I exchange 1 and 2, same with any other pair, so that is the reason why this works. So, now let us imagine I want to describe a system of 3 fermions, so the question is how I would do this.

So, I have to just make sure that I do not add up all these contributions rather I add them up with alternating signs depending upon whether the number of permutations required to you know restore the sequence the jumbled up sequence to the canonical form is even or odd, so if it is even it is plus 1, if it is odd, it is minus 1. So, the question is; how do I decide that it is very easy all I do is; I write it down like this.

So, I have interchanged 2 and 1, so that is one permutation which requires, so I have to have a relative minus sign there okay, so let us look at this. So, if I interchange 1 with 3, I get the canonical form, so that is a minus sign, and 2 remains in the middle and 1 and 3 get interchanged to get the canonical form and similarly here I need to interchange 1 with 3, okay and then 3 with 2 in order to retain the canonical form.

So, that is 2 interchanges, so that is even, so the sign remains plus okay, so what about this penultimate term; the penultimate term is again a minus sign because I need to interchange 2 and 3 in order to obtain a canonical form, so it is going to be r1, r3, r2 and then here the very last term I need to interchange twice because I need to interchange you know, 1 with 3 and then 1 with 2 in that order.

So that means, this remains a plus, so that 3 pluses and 3 minuses basically okay, it is the 3 pluses and 3 minuses, so this would describe a 3 fermions system, so if you; you know, if you went here and solve your time independent Schrodinger equation with 3 particles and you obtain some solution which describes a legitimate stationary state, it would still not be acceptable as the physical wave function until you have properly either symmetrized it in order to describe a 3 boson system or properly anti-symmetrized it to describe a system of 3 fermions okay.

So that is the whole idea, so now let me describe to you this particular simple example was simply to convince you of the utility of this operator, so this operator that I was talking about namely the, this symmetrisation operator or the anti-symmetrisation operator as the case may be, so the utility of this has been right now clarified through this example. So, now let me go ahead and introduce what I would call annihilation operator.

It annihilates a variables from the wave function, it does not necessarily, it does not physically describes an annihilation of a fermion or boson yet.

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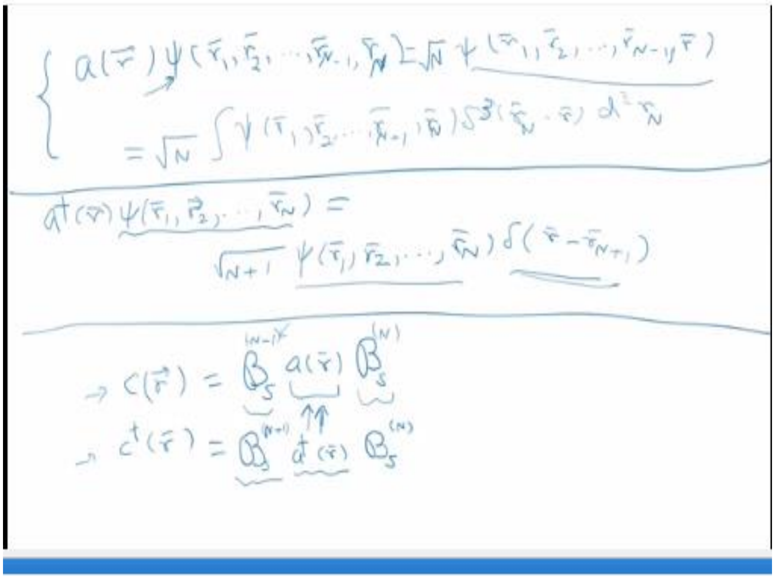

So, right now, so imagine an operator, there is an operator a which I define to be this, so imagine now you have a wave function which is you know as before neither boson or fermion, it has not been properly symmetrized, it could describe a properly symmetrized wave function also but it need not. So, let us imagine a general wave function which just as some kind of a solution of a Schrodinger equation or it does not have to be that either.

So, it just describes a complex amplitude you know which describes the wave function of particle 1, particle 2 etc., so I define this operator a which has an argument called r vector to be basically the following. So, the idea is that; so let me write it more explicitly, so I am going to; so you have N variables starting from r1, r2 all the way up to r N minus 1, rN, so that is the last variable.

So, what this operator does is basically it freezes the last variable and makes it just; so notice that r1 and r2 are the locations of the particles in the particles are dynamical and they can be anywhere they want to be, so but what this operator a of r does is; it just freezes one of the variables, it prevents that which it is as if that particle has been kind of turned into stone, you know you just take the Nth particle and turn it into stone and freeze it at the location r, so that is what this operator does.

So, it takes the Nth particle and freezes it and gets rid of rN altogether and becomes r, so now that number of dynamical variables has been reduced by 1 namely earlier there were N dynamical position variables namely, r1, r2, r3 all the way up to rN now, there are only N minus 1 dynamical variables namely r1, r2, rN - 1 and rN is no longer there, it has been replaced by r.

And of course, there is also I forgot there is a factor of square root of N, for reasons that I will explain later square root of N, so you could also write this in this instructive way, you can write this as an integral over the original wave function which had N variables and then you freeze the Nth variable by integrating with the help of a Dirac delta function, so in other words the Dirac delta function does the job of freezing that variables to rN to r, okay.

So, this would correspond to annihilating a particle, so not necessarily either a boson or fermion because we have not been careful about symmetrisation and notice that if even if your earlier variables say if your earlier wave functions which contain N particles were properly symmetrized to begin with. So, suppose it was symmetrized or anti-symmetric to begin with, the moment you annihilate the Nth particle you are immediately spoiling the symmetry of the system of that wave function.

So, the wave function that survives which describes N minus 1 particles is now not going to have any particular symmetry, so the symmetry gets spoiled, so it gets spoiled and what you have to do is you have to use your as symmetrisation script B operator which I described here in order to restore the appropriate symmetry, so that is the reason why I introduced this operator.

Because it is going to be useful in restoring symmetries which have been destroyed by you know this annihilation operator which is partial towards the Nth variable, so this is the operator that destroys the Nth variable and not anything else, so it is obvious therefore that the end result will not have any particular symmetry, so now that we know how to define the annihilation operator.

Now, we can describe its counterpart namely the creation operator, so how would you go about creating a particle, so this how you'll destroy a particle so, if you have N particles in your system, you destroy a particle this way, so how do you create a particle, you would create a particle by rather than multiplying my delta function and integrate which will freeze one of the variables, you introduce a new particle through a delta function.

So, this is how you do it, so this is naturally how you do it and you take the Nth particle and you would; so this is the 3 dimensional Dirac delta function, if you are in 3 dimensions and so on. So, you add new variable called rN + 1 and then you freeze it to be r, so in other words okay sorry, so a dagger r acting on; so if you have a wave function with N particles and you act the wave function of N particles by the creation operator, you end up with a very function with one more particle namely rN + 1.

And the wave function also I mean the end result of course also depends on R, so what this describes is that you are placing another particle at the location r, so that is what you are doing, you are taking another particle that was not there before, so the original set had only N particles, so you are taking the one more N + 1 particle and you are placing at location r, so the end result is a wave function which is the original wave function times the product with the Dirac delta function that indicates that you are placed it at that location.

So, this is fine except that it does not really respect these symmetries like I was telling you so even if you are started off with a wave function which has N particles that is properly symmetrized to describe either bosons or fermions, the moment you either create or destroy a particle in this way, you are spoiling the symmetry of the wave function. So, in order to restore the symmetry of the wave function, so what I am going to do is; I am going to introduce a new operator called c of r which has this property that it is a of r times B of s.

So, what it does is that so let me tell you what this does so, it is basically it is the same annihilation operator but what it does is it makes sure that whatever comes to the input wave function, if it is not properly symmetrized is properly symmetrized first so, it is like preprocessing you know it is processed food type of thing okay. So, you first process it by you take an input wave function, you symmetrize it to describe either bosons or fermions first.

Then, you do this annihilation thing which spoils the symmetry but it physically annihilates the Nth particle but then you do not want to give partiality to Nth particle, so there is no nothing special about Nth particle it could have been anyone so, in order to restore impartiality what you do is; you further anti symmetries the remaining particles, so because this is this would correspond to the N, this would correspond N – 1.

Because I mean this, like you are symmetrizing or anti-symmetrizing a wave function containing N particle and then you are annihilating with a which would reduce the number of particles by 1 and then you would then go ahead and again symmetrize or anti symmetrize, so therefore you will be symmetrized with respect to 1, less number of particles.

So, this is; this would then correctly describe an operator that either describes the destruction of a fermion in the system, if s is minus1 or it describes the destruction of boson in the system is if s is plus 1, see a itself does not describe the destruction of; it just describes the destruction of some quantum particle which has ambiguous statistics but c of r correctly describes the destruction of either bosons or fermions depending upon the value of s, okay.

And now, I am going to stop here and in the next class, I will continue this discussion and I will try to explain to you; you know I will give you an example which explains why the c of r does what I claim just now through a simple just like in the early case with 3 particles, I am going to use 3 particles wave function to convince you that it indeed does what I just described.

And having done that I am going to establish that c of r obeys a certain closed commutation rule with the corresponding, so let me write down the other thing which I forgot to write which is so similarly, just like you can write down the creation, just like you can write down the annihilation of a fermion or a boson, you can describe the creation of a fermion or a boson in this fashion.

So, you will be creating a particle, so you will be first symmetrizing it properly, then you will be creating an ambiguous I mean, a quantum particles with ambiguous statistics at location r, then in order to you know eliminate the ambiguity, you would be further you know symmetrizing or anti symmetrizing the wave function which now who remember has one more particle as opposed to one less particle as I did here.

So, here it had one less particle upon annihilation and upon creation, it has one more particle, so other than that it is pretty much the same so, in the next class I am going to establish that c and c dagger and c and other types of c's of a certain commutation or anti commutation rules depending upon whether they are bosons or fermions. So, I am going to stop here and hope you will join me for the next class.

And I am quite confident that you will be benefiting from this description quite a lot if you are going to be you know interested in specializing for example, in condensed matter physics and so on later on in your career, okay. Thank you.