Introduction to Statistical Mechanics

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Lecture - 30
Green Functions in Many Particle Systems

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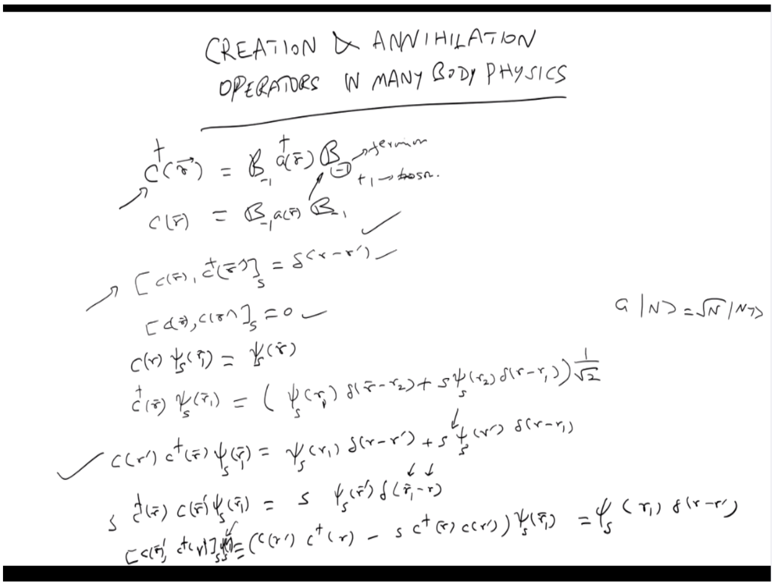

Okay so let us continue our discussion of creation and annihilation operators in many body physics. So, if you recall in the earlier lectures, I had defined quite carefully what it means to create a boson or a fermion. So, suppose you wanted to create a fermion at a certain point in space, what you would have to do is basically you have to sandwich the generic creation operator in between 2 projection operators that basically anti-symmetrize the wave function.

So, the implication therefore is that if you or what this creation operators C of r does is basically it creates a fermion at a certain point in space called r. So, in order to do that what it does first is that when it is supplied with a wave function of say N particles, so it has to add a particle, another fermion at a location r, so what it does is first it ensures or it kind of forces the anti-symmetry or the properly anti-symmetrized wave function is first generated through by an application of this anti-symmetrization operator called script B is subscript – 1.

So, this is the one here. So, there is a projection operator that anti-symmetrizes the wave function and then there is this generic creation operator that adds. Suppose you have N position label starting from r1, r2 all the way up to rN, you add the last one and which is the next one after rN which is rN + 1 but then having done that you again spoil the symmetry of the wave function.

And you are forced to ensure that it is again properly symmetrized or in this case anti-symmetrized by a further application of the anti-symmetrization in projection operator. So, having done all this, so similarly for the annihilation operator, so the whole idea was to then show that C of r acting the anti-commutator was delta's, so these are called canonical commutation rules of bosons or fermions.

So, this is for fermions. So, if this was + 1, it would be boson, so this would be fermion and this will be boson. So, the point is that so this is somewhat easy. So, I am going to skip this. So, I am going to focus on this first. So, I am going to try and see if I can prove this. So, in order to do that I am going to take the simpler example that suppose I take a wave function of one particle, so it does not matter if it is one particle, it is already properly symmetrized.

So, now I am going to create a particle at position r okay, so I am going to create not a particle, properly specifically a s particle. So, if s is – 1, I am creating a fermion. If s is + 1, I am creating a boson, so I am following with an s particle. So, I am going to create a particle with statistics s. So, this s does not appear here, it appears there. Anyway, so how would I do that? So, remember that how you create a particle is you know you first but it is already properly symmetrized.

So, first you create the second one here, so that means you create r r2 but then you know this is not properly symmetrized under the exchange. So, what you do is you basically you add an s and you interchange r1 and r2. So, you end up doing this okay. So, you create a wave function, which is now properly symmetrized. So, now if you interchange r1 and r2, basically you are going to get s times the original wave function.

So, if s is – 1, you get the negative of it and if s is + 1, you get back the same thing. So, now I am going to see if I can, now look I am now going to do this, I am going to ask myself what is this. So, I am going to see if I can annihilate a fermion. So, notice that this is already properly symmetrized. So, all I have to do is just annihilate the last particle here which is this, the second one okay.

So, just freeze the value of the second one to r dash. So, r2 is now frozen to be r dash okay. So, when a acts on a state, you get square root of N times N – 1. So, there is the square root of N. So, remember here there are 2 particles, so I pick up a square root of 2 there. So, that square root of 2 cancels with this and I end up annihilating the particle here, r2 becomes r dash and s r2 becomes r dash r – r1 okay, so that is what it is.

So, now I am going to do the reverse. So, this is fine but suppose I do the reverse, so if I want to first annihilate a particle that is even easier because there is only one particle and how do you annihilate this just you know freeze the value of that variable to whatever it is that wherever it is that you want to annihilate it at, so that is all there is to it. So, C of r acting on psi s r1 is basically going to be psi s of r.

Now, if I now go ahead and so okay, so I am going to do r dash because this is r dash, so now if I ahead and create a particle, so how would I do that? So, I am going to create a particle at a new location called r1. So, now again because it is finally only 1, so this is a state with no particles at all, but now from a state with no particles at all if I create a particle, there is only 1 particle, so I do not have to worry about the symmetry of that wave function.

So, I end up creating a particle at r. So, that is the end of story. So, now what I am going to do is I am going to multiply this by s and subtract. So, I am going to do the following. I am going to first multiply the second equation by s and I am going to subtract. So, when I do that I end up getting, so notice that this particular, so when I multiply by s, this cancels out with this, so these two get cancelled out and what remains is s of r1 times delta of r – r dash.

So, you see, so this is nothing but the s commutator of C dagger r subscript s acting on your wave function okay. So, when you act this s commutator on your wave function, you end up getting the delta function times, so that is what you get. So, you get the delta function times the wave function that you put in here okay. So, that sort of it is not really a proof because it is just one of those, it is just a proof through example.

So, it is not really a convincing proof, but it just tells you that it is plausible okay. So, that is how it works. So, I am going to defer the general proof you know to perhaps home works or you know you can think about it at leisure or you know look it up somewhere. There are not very many good books that explain how to prove this very rigorously, they probably also just like me relegated to exercises and so on.

So, you are on your own as far as the general proof is concerned, but I have told you the plausibility argument here alright.

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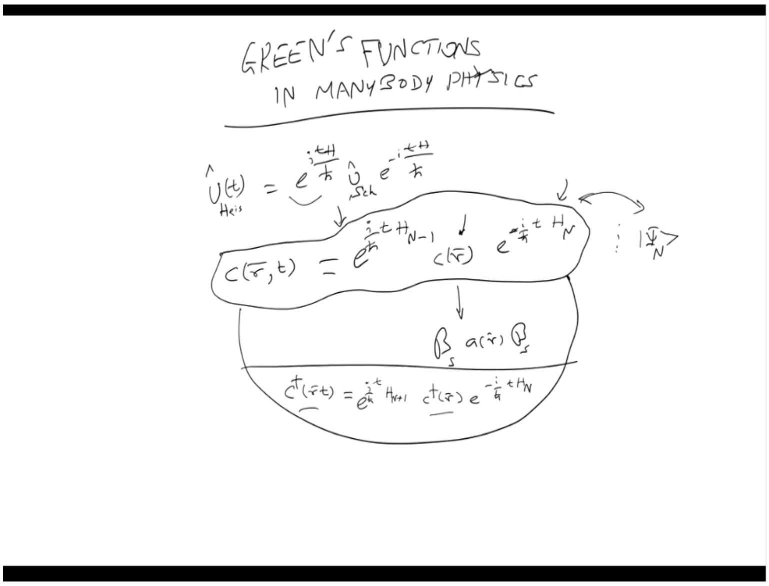

So, now I am going to start discussing a new topic called Green's function in many body physics. So, what are Green's functions? Green is of course the name of a mathematician. So, Green with a capital G okay, before I define Green's functions, so remember that in the Heisenberg picture of quantum mechanics, you know you can think of the wavefunction as being independent of time whereas the operators depend on time and they evolve by through a unitary transformation.

So, in the Heisenberg picture, operators are time dependent whereas wave functions are time independent. So, this is the Heisenberg operator and this is the Schrodinger version, so this is the Schrodinger and Heisenberg. So, the Schrodinger operator and Heisenberg operators are related in this fashion. So, the Schrodinger operator is strictly time independent, but the Heisenberg operator can be time dependent in this fashion.

So, we are going to use the Heisenberg picture and try and see if I can make sense out of an operator such as this. So, remember that I made sense out of the Schrodinger version of that namely this. So, if you recall that this was nothing but you know that symmetrization times a of r times again symmetrization that is what that was.

So, having made sense out of this, now I am going to see if I can make sense out of the, so I like to do something similar to what I did here but then there is a catch in the following sense that you see this is a funny operator C, you know it is not just unlike other operators in quantum mechanics, which say depend on position or momentum and that sort of thing but this operator does something far more drastic.

It actually changes the number of particles in your system altogether. So, in which case, you know when you are talking about Hamiltonians, you clearly are required to keep track of how many particles there are. So, if it say if free particles, if your N particles in your system and there is only kinetic energy, you are required to take the summation of P squared or 2m, PI squared or 2m where PI is the momentum of the Ith particle and then you are required to sum over all the I's from 1 to N where N is the number of particles.

So, clearly that Hamiltonian keeps track of how many particles there are in your system. So, as a result, I am going to introduce a subscript to the Hamiltonian which reminds me how many particles there are in my system. So, what happens is here that you know namely I would expect to do this. So, imagine I originally start off with N particles, so whatever state comes on the right, imagine the N particles in which case I am going to be using the Hamiltonian with N particles to act on that state.

Because otherwise it does not make any sense, then I am going to annihilate a particle, which is the C of r. So, I start off with some state; let us imagine there is some state called psi which has N particles. So, if it has N particles, this unitary evolution acting on the state with N particles makes perfect sense, but now having done this. Now, this continues to remain a state of a different state or containing N particles.

But then that different state is now acted upon by an annihilation operator. So, when you act it upon an annihilation operator, it reduces the number of particles by 1 unit. So, as a result, the resultant state is no longer going to be in a state containing N particles. It is going to be a state containing one fewer particles than N. So, that is N – 1. So, now if I want to make sense out of the remaining unitary term here, so I have to put a subscript of N -1.

Because that Hamiltonian now refers to 1 less particle, so this is the correct meaning of you know the Heisenberg time evolution of an annihilation operator. So, it is that you know the Hamiltonians here are different that this has N particle this is 1 less particle okay, there is no t dash, this is just t okay, well with creation operator is different because, so with creation operator, so what you are doing is you are starting with the Heisenberg, well this is just the Schrodinger picture and the Heisenberg picture.

And you are going to start which of course you always start with N particles, but then when you create a particle, you are going to end up with a state with one more particles. So, you are going to be writing this. So, you are going to get 1 more particle okay. So, this is the meaning of time evolution of creation and annihilation operators in many body physics. So, now having made sense out of this, now I am going to define what is called the Green's function in many body physics and that is the following.

So, I am going to first define what is called the whole Green's function. Firstly, let me describe the particle Green's function.

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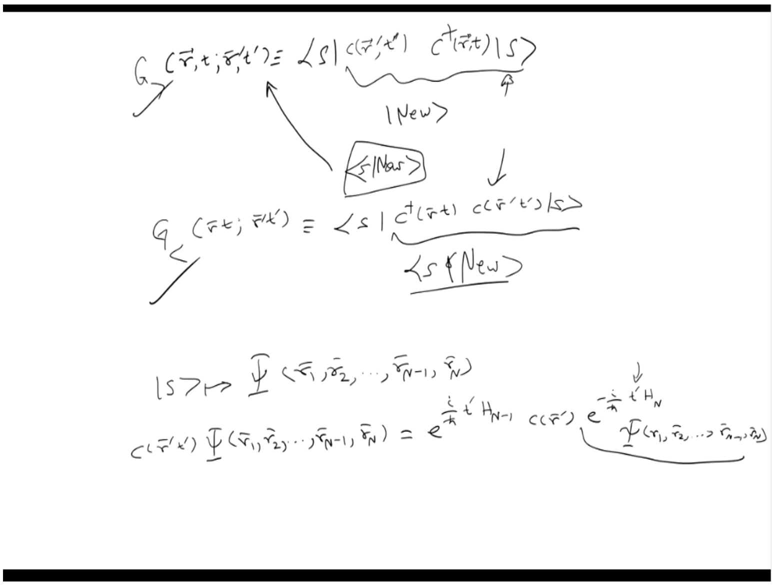

So, the particle Green's function is denoted by G greater, so it is denoted by r vector, t; r dash, t dash. So, imagine there is some reference state as starting state. So, I start with a state s, then I decide to do the following. I create a particle, so it is called the particle Green's function or the particle propagator. So, I create a particle at position r at time t and then at a different time, I decide to annihilate the particle with the same statistics.

So, notice that in quantum mechanics, particles are all indistinguishable. So, you cannot say, you cannot really keep track of a certain particle, you cannot follow it around, so that you can annihilate or create the same particle contrary. First, create a particle and then follow it around and destroy the same particle because all the other particles are in the system are of the same type as this.

So, they are indistinguishable and they kind of merge and then you will never be able to figure out which is which, so basically all you have to do is you create a particle, then annihilate a particle with the same statistics. So, the question is how do you do this is the question. So, what you do is you create a particle at position r, t and then you annihilate it at a different time at a different position.

And then you ask yourself, so as a result, you will get a new state, you know call this state something else. So, we call it a new state or new, I am going to call it new, so this is a new state. So, this is your starting state. So, you create a particle at position r at time t, then at a different time, at a different time called t dash you annihilate the particle with the same statistics as before but at a different location called r dash.

So, having done that you end up with a new state because so you remember what is going to happen that if you take a state and you add a particle to it at some location, it is at a certain time, you basically significantly disturbing that system because it you know the old system has already come to terms with the fact that it has N particles in it and it has properly anti-symmetrized its wave function and all of a sudden a new particle is being added to the mix.

And then all of a sudden you know it has to rearrange its wave function in such a way that is again properly anti-symmetrize. So, that is likely to be a very violent process in the sense that it is going to significantly disturb the state that you started off with, but then later on what once that process is taking place then you decide all of a sudden at some other time called t dash to again remove a particle.

So, that itself will again create more rearrangements. So, which will result in a new state which we do not know what it is but we can certainly ask the question what are the chances or what is the probability that new state is the same state as before. Of course, I mean there is no particular reason to ask this question, but suppose you do ask this question and what we end up doing is calculate this quantum mechanical overlap.

So, you calculate this overlap and this overlap is called a Green's function of the system. So, specifically it is called the one-particle Green's function because it firstly is the particle propagator because you are first adding a particle and then removing it. It is also called the one-particle Green's function because you are adding just one particle and then removing one particle, but you could also have two-particle Green's functions where you add one particle at a point at a time, then you add another particle at a different point at a different time.

And then, you again remove these particles one by one or some other types of those, I mean the same type of particles 2 of them you remove at a later time or a different time one by one. So, that would constitute a two-particle Green's function, but this is an example of a one-particle Green's function.

So, similarly you could define something called the hole propagator which is denoted by subscript G less which is r, t; r dash, t dash which is going to be s times C of r, t. So, you first annihilate, so that means you first annihilate a particle. So, if you annihilate a particle, you are basically creating a hole, so you are leaving behind a void, a gap in that system. So, you can think of it as a hole, so that is why it is called a hole propagator.

So, you create a hole or basically destroy a particle. So, if you destroy a particle at r dash, t dash and then at a later time you reintroduce a particle with the same statistics, but at location r then again you are going to create a new state which I am going to again denote it by new, it is not the same new as before but it is new in the sense that is different from the original state s. So, now you can ask the same question what is the overlap between this state and the original state.

And that would correspond to what we call the hole Green's function, so this is called a hole Green's function. So, you started off with particle Green's function and then you have the hole Green's function. So, these 2 are the important what are called the one-particle Green's function of a many-body system. So, you see the point of doing this is that many of the interesting physical quantities that we are interested in are actually expressible in terms of these one-particle Green's functions.

So, let us learn some properties of these one-particle Green’s functions. So, specifically before I do that I am going to tell you why we are calculating these Green’s functions. First of all, you know if you think of a system with N particles, the completely correct way of handling this system, a quantum mechanical system of N particles is to just solve you know the time dependent Schrodinger equation for N particles with appropriate initial conditions.

And if you could do that, it is then there is nothing like it, I mean that is the end of story because that contains the complete information. Then, practically you will never be able to do that because that end that you are thinking of could be microscopic, that means it could be, it could correspond to the total number of electrons in a metal for example if that is what you are describing or it could be you know N boson cold atoms that are trapped in some cloud and harmonic trap which could also be pretty huge.

So, in which case it is not practical to write down the wave function for N particles, so you need a simpler method to handle this and that simpler method is basically by evaluating by not insisting that you evaluate these wave functions themselves but rather you evaluate something simpler which is called the one-particle hole Green's function and one-particle Green's function.

So, as a result see then immediately raises the question is there some connection between these Green's function which are of course also complex numbers with wave functions of many particle systems which you also know are complex numbers. So, the question is what is the relation between these complex numbers which are G greater and G less and also the complex numbers which correspond to the N particle wave function.

So, indeed there is such a relation and I am going to describe what that is. So, okay so notice that in order to describe this, so imagine that this state s actually is described say by a wave function of this form. So, imagine that is described by a wave function with r2, rN – 1, rN. So, imagine the N particles and this is what it is. So, now I am going to see if I can make sense out of, so I am going to first start describing the hole propagator.

So, I am going to first annihilate, I am going to annihilate a quantum particle with appropriate statistics at location r dash at time t dash from this state called psi. So, when I do that what am I going to get is the question. So, what I am going to get is this is going to become so if you remember, recall the definition of the Heisenberg time evolution of the annihilation operator in terms of its Schrodinger equivalent, it is going to be this t dash HN – 1 C of r dash, so that is what that is.

So, now notice that this state is nothing but the ordinary, you know time evolved wave function, so it is just this evolved up to time t dash. So, you started off with this, you evolve, you just simply wait until time t dash has elapsed. So, this is how you started off with, this state you started off with and then you simply wait. Of course, I am assuming my Hamiltonians are explicitly time independent here.

So, otherwise I have no right to write this, but let us assume that my Hamiltonians are explicitly time independent okay. Thank you.