Introduction to Statistical Mechanics
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Lecture – 31
Second Quantised Hamiltonians

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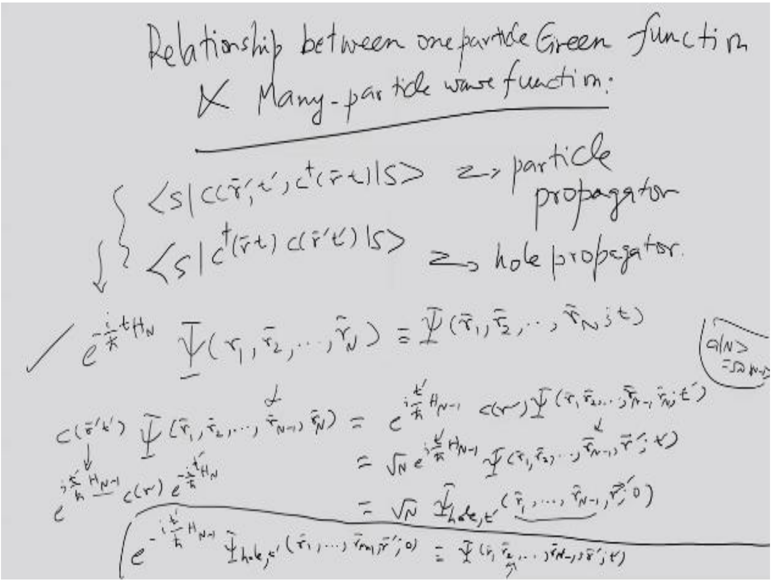

Okay, so I am going to continue from where I left off. And so if you recall in the earlier discussion I had introduced a notion called the single particle or one particle greens function. So that involves something called a particle propagator which could be something like this or it could involve a whole propagator which would; so this would correspond to a particle propagator, and this would correspond to a whole propagator.

So the point is that given the fact that these notions are somewhat unfamiliar to people have not studied the subject but those who have studied the subject will of course be familiar through their prerequisite there would be familiar with the notion of the many particle wave function of the system, so there would be more familiar with an object such as this that so if you have n particles in your system, you know what this means.

So in the Schrodinger picture this would be time-dependent and if you want to evolve this you know from a given time to a later time this would be the solution of the time-dependent Schrodinger equation. Okay. So people are going to be familiar with this and this is somewhat unfamiliar. But it would be therefore desirable to link these two, you know to be able to say how these notions are related to this motion, so that is what I have been trying to do.

So in order to do this, so I am going to start with my one particle or the many-body wave function so let us imagine I start like this, okay so all the way up on the end and then I imagine that I decide to annihilate a particle. And this is going to basically mean this; so let us imagine this is properly symmetrize to begin with like I was saying, so firstly this involves writing this.

So you have an n particle wave function, Hamiltonian is described by H subscript n signifying that it is the Hamiltonian of n particles. And then once you annihilate the resulting state has one less particle so you should be evolving with respect to one fewer particle, okay so that is going be T - there so that is what that is. So this basically means that you are going to be doing this.

So it is going to be CR -, so then I am going to freeze them because; well first I'm going to; first I am going to evolve and then I am going to freeze, so I am going to freeze the last term there. And remember that when I annihilate I pick up a square root of n because you know the annihilation is basically square root of n times n - 1, so I am going to pick up a square root of n, and I'm going to freeze the last variable. Okay.

So now I am going to call this, this entire thing I am going to call this Psi of whole parametrized by t dash but acting so it is a parametric type of wave function it is parametrized by t dash but the interpretation is going to be that it is actually the wave function at time T=0; but then it is parametrized by t dash and it has one fewer variables than n, so that means it is; the number of dynamical variables is only n-1.

So what is the physical meaning to the action of the time evolved annihilation operator on the original in many particle wave function is this beast here. So the question is how do I interpret this? So the way I interpret this is that the whole wave function is one which has the property that if you evolve the whole wave function from t=0 all the way up to t=t dash, you get a wave function which is the same as this wave function.

So this is the interpretation which makes it easier to understand what is going on. So you just write it like this so, so this is going to be this is going to be Psi of r1, r2 r n-1, r dash t dash. So we know what this is, see what is this. This object is easy to understand what this is. So basically it is just the time evolved version of the; well it is firstly you time evolved this way original wave function then you annihilate a particle that is what this is. So you time evolve it and then you annihilate a particle.

So but the whole wave function is that wave function where you start off with one less particle to begin with but it is as already parameterize by T dash and R dash okay so there is some state parameterize by r dash and t dash but it also describes this state with n-1 particles but parameterize by r dash and t dash, that is your starting state and you evolve that for a period of time called t dash until you reach a new state.

And so if that new state is called is exactly the same as this state which is the, you know the time evolved original state followed by annihilation. So if these two are the same states then you call this the whole wave function it parameterized by t dash. So I understand that it is a little hard for you to grasp because it is kind of; see all I am trying to do is I am trying to translate what is really a complicated mathematical notion into ordinary English, so that is likely to be quite ambiguous and probably unwise.

But then, you know this is how I would look at it if I wanted to interpret it, you know using words. But then I will allow you to do it yourself whichever way you want. So the equations are very transparent they say whatever they want to say and how you translate it into words is entirely up to you. So the point is that having known what this whole wave function really means. So let me go ahead and try to explain what this object is in terms of the wave function.

So namely I am going to explain what the whole propagator is. So I am going to write down a formula for the whole propagator in terms of my many-body wave function, so that is something very desirable.

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$$G_{<}(\vec{r}t;\vec{r}'t') \equiv \langle S|\, c^{\dagger}(\vec{r}t)\, c(\vec{r}'t')\,|S\rangle$$

$$= \int [d\vec{r}]\, \Psi^{*}_{S}(\vec{r}_1,\ldots,\vec{r}_N)\, c^{\dagger}(\vec{r}t)\, c(\vec{r}'t')\, \Psi_{S}(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$$

$$= \int d^d r_1 \ldots d^d r_N \left(c(\vec{r}t)\, \Psi_S(\vec{r}_1 \ldots \vec{r}_N) \right)^{*} \left(c(\vec{r}'t')\, \Psi_S(\vec{r}_1,\ldots,\vec{r}_N) \right)$$

$$= N \int d^d r_1 \ldots d^d r_N\, \Psi^{*}_{hole,t}(\vec{r}_1,\ldots,\vec{r}_{N-1};\vec{r},0)\, \Psi_{hole,t'}(\vec{r}_1,\ldots,\vec{r}_{N-1};\vec{r}',0)$$

$$\Psi_{part,t}(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N,\vec{r}_{N+1};\vec{r},0) = e^{\frac{i}{\hbar} t H_{N+1}}\, \underset{\substack{+1\ (boson)\\ -1\ (fermion)}}{\beta_S}\, \delta(\vec{r}-\vec{r}_{N+1})\, e^{-\frac{i}{\hbar} t H_N}\, \Psi_S(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$$

So in order to do this so let me start off by defining my whole wave function which is denoted by this G subscript less symbol. So it is going to be denoted like this. So now in terms of many-body wave functions clearly and this is what this is.

Well, whole bunch of all the R's that are there and times, my many-body wave function which describes this state called S, I mean this is the capital S that statistical parameter S, this is the state S, okay. This is the uppercase s. So r1 all the way up to rn, so this is what that is; I mean this is the meaning of that. So I am going to be able to write this in the following way, so this also makes equally good sense namely, you know I am just explicitly writing this out.

So notice that I can always think of, you know I can always write it like this. Okay, I see notice that I have I just first I have taken the trouble to explain to you what this object which is the annihilation of a particle with well-defined statistics of course at a time t dash at position r dash is when it acts on given many-body wave function. So I have told you what that is, so that is basically this object called the whole wave function parameterize by R dash and t dash.

So now so as I research this is nothing but having known what that means so this is basically nothing but n because there is a square root of n coming from this annihilation and another square root of n coming from this annihilation, so the net result is a factor of n and this remains as it is. And I am going to end up with this whole wave function parameterized now in this case by T and R.

And like I told you a whole wave function by definition has one fewer number of particles. So the number of dynamical variables is n-1 rather than n. So it is parameterized by this R and this T because this R and T is the location at which you annihilate the particle. So you can see now we have made sense out of the whole Green's function in terms of the many-body wave function.

So it is basically what it does is in essence; it is a kind of overlap between the many-body wave functions. You find the overlap between two different many-body wave functions. And you integrate over all variables except two of them and you freeze those two variables to be the values at which you are going to create an annihilate, but then you have to also make sure that you properly evolve the state to the times that are required before you do this, before you evaluate the overlap integral.

So that is the reason why you should first make sense out of this object called the whole wave function parameterized by r dash and t dash before you interpret it this way. So this is going to be your wave function description of the whole propagator. So similarly, you can define the wave function description of the particle propagator so let me describe to you the particle wave function; you just cut a long story short just like you have a whole wave function, you can have something called a particle wave function again parametrized by T.

But notice that unlike a whole wave function which has one fewer number of particles a particle wave function has one more number of particles, so that means that you start; if your original system contains n particles then you end up stopping not at n but you add one more particle, okay. So that's going to be continued to be parameterized by r and t and the meaning of this is basically you first evolve your original wave function up to time T and then you add a particle which is the n+1nth particle because already n particles here.

If you add one more particle you are going to add it here at the location R. But then this state is no longer properly symmetrized remember. So what you should be doing is then go ahead and properly symmetrize I mean this is my statistical parameter S which could be +1 if it is goes on or it could be -1 if it is fermium, okay. So now you are going to properly symmetrize this and then you kind of do the anti evolution because I told you that, you know the interpretation is that you push this to this side and that gives you the interpretation.

So this wave function is that wave function which when evolved with this Hamiltonian for a period of time T becomes the same as this so, so that is the meaning of this particle wave function just as it was in the case of the whole wave function. So having defined the particle wave function in this fashion so then you can go ahead and define.

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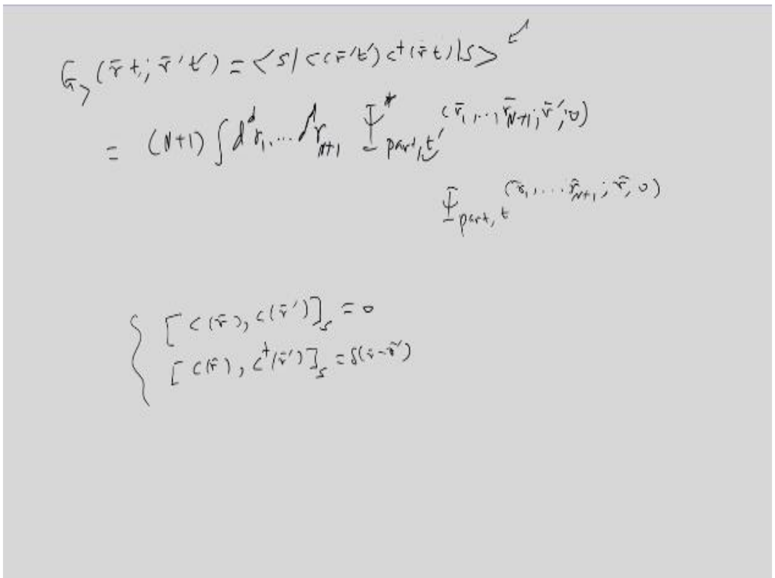

The particle propagator which is nothing but; so you first create and then you annihilate. So this is going to end up becoming this. Notice now that there because you have created there going to be one more number of particles so that means the total number of particle n+1, so you got a deal with that. So this is parametrized by t dash and it has one more particle and it has r dash but then this continues to be it time t0 because you know, so we interpret this as the parametric dependence on time.

So the parametric dependence is now T in in the other case and this has just as before it has one more particle and 0. So this is the definition of the particle greens function in terms of the many-body wave function of the system which presumably you are more familiar with.

And in fact most of us are more familiar with wave function because that is how we learn quantum mechanics, now we will learn the Schrodinger's version of quantum mechanics which talks about wave functions and then when we have many particle system like we start off by discussing helium atom and that sort of thing and then we discussed wave function with two electrons and that sort of thing then we become familiar with wave functions with more than one particle and that is very familiar to us.

And so when you encounter a completely new notion like the particle greens function or the whole greens function then it is certainly very desirable to link it to some notions such as many-body wave function many particle wave function that you are already familiar with, so that is precisely what we have accomplished now. Okay.

So the next topic having understood what many-body wave functions are. So now that you know what it means. Now you also know therefore why we are calculating it because you the whole point is that the wave function of a many-body system is contains a whole lot of information that we probably do not care about, it would be nice if we could write it down fully but most of the time you cannot.

So what you end up doing is instead define some object in terms of the many-body wave function which contains far fewer variables, so in this case precisely two vectors and two numbers like t and t dash. So even though the many-body wave function contains a huge number of variables such as r1, r2 up to rn. So in this definition you basically integrate over all of them. So whatever remains is just 2 or 3 like that.

So the implication therefore is that it is going to be; so you will have to develop techniques where it is far easier to evaluate such an object then it would be to evaluate the entire wave function. So that is the claim and that is the implication. So in order to verify this claim or you know make that convincing that claim convincing I will have to first rewrite my Hamiltonian also in terms of these creation and annihilation operators.

Because remember that we took that trouble to explain that these operators or were these types of commutation equal time commutation rules. So they obey this equal time commutation rules. Okay. So now the point is that, now these operators; they do things amongst themselves so we know how they, you know commute or do not amongst each other; we know exactly how they the algebra amongst themselves.

So it is nice to now go ahead and start expressing every other operator we are familiar with in terms of these creation and annihilation operators then we will be able to study all these many body systems purely in terms of these operators. So as opposed to for example position and momentum that you are kind of grew up with.

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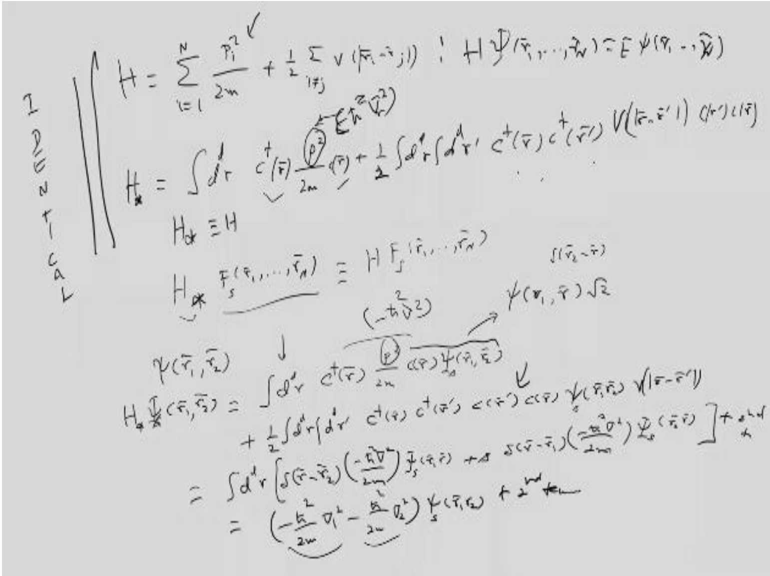

So let me start with that Hamiltonian that you grew up with namely this. So you grew up with this sort of Hamiltonian that just describes the two body wave function, okay. Typically, it only depends on the distance between two objects, so I am going to start with this the simple; you know n body system with two body mutual interactions between the particles. So now the claim is that this is not exactly the same as this object.

So I am going to claim that this object is the same as; so I am going to claim that it is exactly this. See, one advantage; okay first let me write it down and so it is going to be this. So this is the same view there as before. Okay, that's fine. So this is; the claim is that these two are identical. So these two are identical there is the same operators. So now let us stare at both and see what are the advantages and disadvantage of doing this.

See firstly, this really -H bar squared del squared. I mean this is this operator del R, del with respect to R, okay. All right. So what is the advantage of doing this? Firstly, here you see that this really does contain capital N number of variables. So if I wanted to solve Schrödinger equation this would really read this so I will be solving E Psi. But then stare at this you will see that instead of containing n variables is just I mean I am just making do with just one R and at most two of these R's here.

So it seems miraculous that as original Hamiltonian which contain n variables has now completely transformed to another operator which we are claiming is identical to the earlier one but nevertheless contains only two variables integrated over and so on. So of course that is an illusion because the definition of C and C dagger is involves these many-body wave function which actually contains information about the number of particles in your system.

So it contains the information about how many particles there are; so that is implicit in the definition of C and C dagger. So now how do I go about proving that these two are equal? So the easiest; I mean the only way actually is to just show that the action of H, you know I am going to call this H* maybe. Finally, I am going to show the H* as identical to H. So the claim is that see I have to show that H* acting on some wave; and not just wave on anything not just; I am not talking about this is as a Eigen state of H or anything it can be any anything which is properly symmetrized.

So any function of n variables that has the proper permutation symmetry. So the claim is that this H* acting on such a wave function is the same as H acting on that wave function. So if I can show that for every S- FS then I can show that this claim that these two operators are the same is convincing. So in order to do this so of course I am not going to do this in full rigor,so I am going to use a plausibility argument but I am going to start with a simple function of two particles which have the proper symmetry.

So now I am going to ask myself what is this? Okay. So what is this? This is going to be clearly this. Okay. So that is what that is. So now let us see if we can simplify this further. So notice that this acting on Psi of R, it just annihilates a particle, so I can just go ahead and rewrite this as Psi of r1, r with a square root of 2 because there are 2 particles to begin with and then I annihilated it, okay.

You know I have to first do this; this is -h bar square dash square, then having done that I have to create a particle at location R, okay. So this is one particle, so I have to create one more particle at location R. But then keep in mind that once I create one more particle I am going to have two particles in my system and then I have to take care to properly symmetrize that. So the implication is that it comes properly symmetrized.

So I have to leave it properly symmetrized, you know the way that our teachers are expected to, you know leave the blackboard clean; when we exit the classroom because it was clean when we entered, so that is how it works even here. So if it is properly symmetrized when it was given to you, you should leave it properly symmetrized when you are done with it. So how does that work?

So basically when you create so you are going to create by adding a particle again at location R but then you have properly symmetrize that, okay. So when I do that I end up; so this first term I am talking only about the first term. The first term is going to look like this. So I am going to add a particle at R2 but this is always there but then there is this which has been chosen here. And there is the S symmetry.

So I have to flip the r1 and r2 and put an s factor, this small s which can be +1 or -1, Psi s r2 r, okay. So this is going to be clearly because of the delta functions it is going to become -H bar squared over 2m delta 1 squared - H bar squared over 2m delta 2 squared of Psi s r1 r2, so that is the first term. So that is + second term + second term which I have not done; there is the second term with this one.

So I will come to the second term later Okay, so the only the first term is just this. So you can see that, that is same as this. So this is just the kinetic energy of the first particle + kinetic energy of the second particle which should be corresponding to this. So if there are only two particles so it is; so we have convinced ourselves that this second quantized form of the kinetic energy is exactly what we would get if we had you know explicitly listed all the particles in terms of position and momentum T squared. So now let us come to the second term which is the potential energy of the system.

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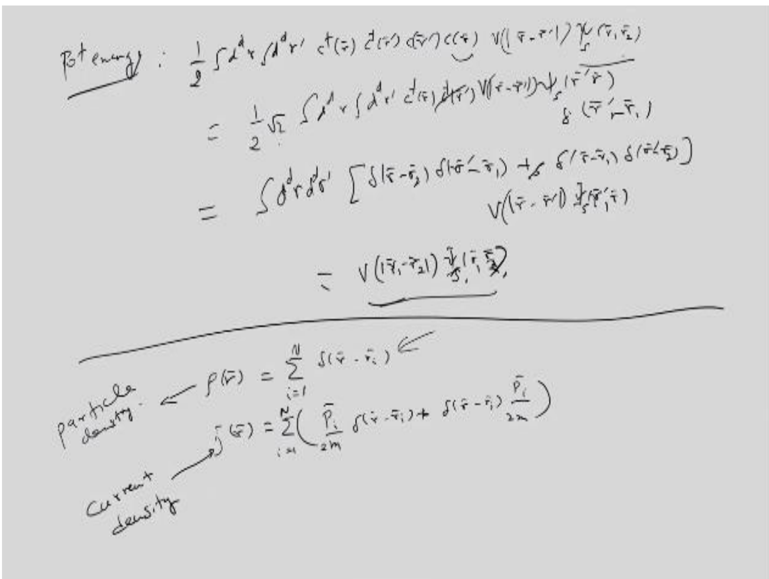

So this potential energy is going to look like this, so the potential energy operator I am going to act on that two particle wave function and see what comes out. So when you take a wave function and you operate it on a wave function to particles so I am just going to write a sequence of steps which you can I am sure I understand what I am doing. There is going to be a square root of 2 because once you annihilate so you notice that first you are going to annihilate a particle, so it is going to end up looking like this.

Okay so you are going to annihilate two particles. So I am going to do that in one shot because once you annihilate you end up with a wave function of just one particle; if you have a wave function with one particle annihilating one more is a trivial activity and I am going to do this in one shot instead of you know making two steps for it. Now I am going to start adding particles. So annihilating is easy because all it means is freezing the variables to whatever it is wherever it is we want to annihilate.

But then adding a particle involves adding a new dynamical variable and then properly anti-symmetrizing or symmetrizing. So let us do that. So if I do that I am going to skip some steps and I am going to allow you to think about it. So if I add one more then there are no particles to begin with adding is easy. It is just a delta function. But then having added this so this is going to go away and it is going to become r- - r1 so that is what it is going to become.

But then now I have to add one more, so if I add one more so it is going to be; the square root of 1+1 because if it is a state with one particle and I add one more so creation gives me square root of 1+1. So that is another factor of square root of 2 that gets multiplied with this square root of 2 which cancels with this 1/2 and then I end up with this result. Okay, end up with this result because of the requirement of properly symmetrizing and I am doing this.

So that is what that is. So you see that this is precisely what you would expect from here, so if you have two particles you know if it is just r1 and r2, I is not J so it is either 1 and 2 or 2 and 1 so you add them up and then they are the same thing so that gets cancelled out here so, so if you have a, you know the potential energy of two particles you just take I=1, I is not = J and I can be either 1 or 2; so either I is 1 and J is 2 or I is 2 and J is 1.

So for both these the answer is the same. So when you add them up that cancels with this 2 here and you get V of r1- r2 which is precisely; this times the wave function that you acted this operator on. So you can see that we have now convinced ourselves that this operator is same as Sigma i=1 to n; Pi square by 2m and this operator this whole operator is nothing but this one right there. So it is just the potential energy of the system. So in the next class I am going to explain how to write down the density operator which is defined like this.

So this is the local density of particles at location I or the current density you could describe something called the current density which is basically the velocity of the particle which is momentum divided by mass. But then notice that in quantum mechanics P and R do not commute so what you should be doing is as you know rendering it Hermitian by, you know taking a symmetric combination and taking the average of the symmetric combination.

So this would be the current density so this would be called a current density and this is the particle density. So this is the particle density of the system and this is the current density at location R. So just like we did here so we express the conventional description of the kinetic energy and the conventional description of the potential energy in terms of the second quantize of the creation annihilation description.

So we would like to express the density which is expressed using the traditional variables r1, r2 up to Rrn also in terms of creation and annihilation operator and similarly, the current density which is expressed in terms of the conventional variables phase which are r1, r2 up to rn and P1, P2 up to Pn also in terms of creation and annihilation operators. So that is what I am going to do in the next class. I hope you will join me for that. Thanks.