## Dynamics of Classical and Quantum Fields: An Introduction Prof. Girish S. Setlur Department of Physics Indian Institute of Technology, Guwahati

## Creation and Annihilation Lecture - 34 Particle and Hole Green functions

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Here  $H_N$  is the Hamiltonian of an N-particle system and  $H_{N-1}$  is the same Hamiltonian but with one less particle. For instance, if there are two body forces:  $H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{j \neq j=1}^{N} V(r_i - r_j)$ (8.82)  $H_{N-1} = \sum_{i=1}^{N-1} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i=1}^{N-1} V(\mathbf{r}_i - \mathbf{r}_j),$ (8.83) so that for every s-symmetrized function of N variables  $\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$  we may write,  $c(\mathbf{r}',t')\Psi(\mathbf{r}_1,..,\mathbf{r}_{N-1},\mathbf{r}_N) = e^{\frac{i}{\hbar}t'H_{N-1}}c(\mathbf{r}')e^{-\frac{i}{\hbar}t'H_N}\Psi(\mathbf{r}_1,..,\mathbf{r}_{N-1},\mathbf{r}_N)$  $=e^{\frac{1}{2}t'H_{N-1}}c(\mathbf{r}')\Psi(\mathbf{r}_{1},..,\mathbf{r}_{N-1},\mathbf{r}_{N})t') = \sqrt{N} e^{\frac{1}{2}t'H_{N-1}}\Psi(\mathbf{r}_{1},..,\mathbf{r}_{N-1},\mathbf{r}';t')$  $\equiv \sqrt{N} \Psi_{hole,t'}(\mathbf{r}_{1},..,\mathbf{r}_{N-1},\mathbf{r}';0) \qquad (8.84)$ where  $\Psi_{holes'}(\mathbf{r}_1, ..., \mathbf{r}_{N-1}, \mathbf{r}'; 0)$  is that wavefunction at time T = 0 of N-1 variables  $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N-1}$ , which when evolved from this time T = 0 to time T = t' using  $H_{N-1}$  becomes a function identical to the function  $\psi(\mathbf{r}_1, ..., \mathbf{r}_{N-1}, \mathbf{r}'; t')$  (which 202 Field Theory is nothing but the original  $\Psi(r_1,...,r_N)$  time evolved from time T = 0 to T = t and then replacing  $r_N$  by t' (antihilation)). If the starting state is represented in position space as  $|S > \rightarrow \Psi_S(r_1,..,r_N)$ , then the Green function may be receptrested in a mixed language of operators and wavefunctions as follows  $(d^d[r]) \equiv d^d r_1 d^d r_2...d^d r_N)$ .

So, today, let us continue our discussion of the Definition of Creation and Annihilation Operators in Many-Body Physics.



So, specifically we want to utilize that to define what are called Green's function. So, I have already introduced you to you the concepts of particle and Hole Green's functions in the last class. So, but one thing I failed to do was I did not explained to you how to consider these operators as being time dependent. Because normally you associate the concept of operators being time dependent with the Heisenberg picture rather than the Schrodinger picture.

So, I want to be able to first properly define what it means for an operator to change with time. So, that is of course, straight forward if you think about it from the perspective of a system with fixed number of particles. So, then it is just the unitary evolution times the operator times the inverse. So, it is as simple as that. But here also there is something similar, but there is a subtle variation in interpretation.

So, the reason is because, you see if you want to define the time evolution of an operator such as the annihilation operator, it is not that straightforward because you see the annihilation operator changes the number of particles in the system itself. So, that is a very drastic thing that it does.

So, it actually removes a particle from the system. So, that is an unusual circumstance. You see in, if you just think about it you will not be able to recollect any example in your undergraduate or MSc class, where you studied a quantum mechanical system, where a particle was actually removed from the system. Of course, you might think of you know grand canonical statistical mechanics. But that is statistical system, that is not what I am talking about.

So, if you have a closed system, somebody coming and you know picking out a particle and throwing it away, and asking what the dynamics will look like from then onwards. You would not have studied that problem. Although, you have to admit that is an interesting question to study.

So, the reason why those questions were not addressed. Of course, one is would be the lack of time. The other would be that you probably really need this formalism or this sort of machinery and that I am discussing in these classes, in order for you to address those questions in a compact and convincing way.

So, the thing is that if you do not use these tools of creation and annihilation operators, answers to such questions become very unwieldy and lengthy and confusing. So, the reason why we introduced these operators precisely to make the answers to such questions very transparent, ok.

So, let me continue my definition of the annihilation operator and how it changes with time. So, the way it changes with time clearly is has to be nearly the same as what we normally expect. Namely, if you have an operator in the Heisenberg picture that changes with time, by definition it is that operator which is sandwiched between the evolution operator on the right and its inverse.

But then, keep in mind that the evolution operator clearly involves the Hamiltonian of the system. But the Hamiltonian of the system has a fixed number of particles. I mean if you have to specify the number of particles before you specify the Hamiltonian. So, clearly that Hamiltonian is a function of the number of particles which is why I have written a subscript capital N signifying the number of particles.

But then you see the moment you annihilate, so you are supposed to first evolve the system. So, if you want to find the time dependence of the annihilation operator, you are

supposed to first evolve the system up to time t dash using a Hamiltonian that contains N particles. And then, you are supposed to annihilate a particle at position r dash.

But then keep in mind that the moment you annihilate a particle, you are reducing the number of particles from N to N minus 1. So, now, when you operate it operate that state by an inverse of this evolution operator, that inverse now begins to look quite funny. Because now you see we are supposed to use the Hamiltonian again to perform the inverse of the evolution operator, but which Hamiltonian.

You see now that you have annihilated a particle it has one fewer particle than before. So, that means, you are supposed to now use the Hamiltonian that corresponds to a system with one fewer particles. So, which is why I have done this. So, this is not what you normally expect when you think of evolution of operators in the Heisenberg picture. It is the same thing here and here.

But this is the only exception that when you are dealing with an operator that changes the number of particles. You have to keep track of how many particles there are in your system. So, you should remind yourself that you have to use the Hamiltonian that contains the right number of particles.

So, just to drive home this point, I have specifically explicitly written down the Hamiltonian containing N particles here and another Hamiltonian containing one fewer particle. But then keep in mind here I have arbitrarily chosen to omit the last particle that. So, the p N and r N are removed from the system.

I could have chosen to remove p 1 and r 1 instead and that would be perfectly valid and in fact, that would also correspond to a system with one fewer particles. So, similarly I could have chosen to remove p 2 or r 2. So, basically I could have chosen to remove any particular particle.

But I purposely chose to remove the last one, just to remind you that you have to do this, you have to remember to do that. That means, you have to remember to remove a particle. But now comes the point. So, the point I just made namely that which one should you be removing is now addressed here.

So, now suppose I want to make; so, the question is how do you make sense of this operator acting on wave after all you know any operator is basically by definition characterized by how it acts the behavior of the operator is determined by how it acts on some state. So, state is characterized by a wave function.

So, the answer clearly is the following. Suppose you have a wave function with N particles, then you act this wave function by a annihilation operator. So, that annihilation operator which has been evolved to a time t dash is clearly determined by the unitary time evolution with N particles and then it is inverse with one fewer particle because there is an annihilations in between, ok.

So, now when you act this on the wave function containing N particles. So, clearly this has a very familiar interpretation. And namely that is it is; so now, this becomes the wave function in the Schrodinger picture which has been evolved from time t equal to 0 up to time t equal to t dash. So, that is the that is how you transit from the you know Heisenberg to the Schrodinger picture, if you recall your undergraduate quantum mechanics.

Because now this has a clear interpretation of the wave function of a system of N particles. But this does this has a wave function of system of N particle which has been evolved from time t equal to 0 up to time t equals t dash.

But then what do you do with that wave function? You annihilate a particle at position r dash. So, I am going to assume that these wave functions have already been properly symmetrized. I mean it just lengthens our calculations if it has not been done. So, because you are supposed to hit the wave functions with the symmetrisation H time to ensure that they get properly symmetrized. So, it makes perfect sense to assume that has been done before hand.

So, given that it has been done beforehand, you are supposed to now annihilate a particle at r dash. And if it has already been done beforehand, it its does not matter which one you annihilate, because you know I told you that the symmetrisation operator which has already been carried out on this wave function democratizes all the coordinates in such a way that it does not make a difference which one you annihilate. So, as a result I am going to without loss of generality choose to annihilate r N. So, if I annihilate r N, it is now becomes r dash. So, having done that then I am now called upon to; so that is the transition here. So, this becomes the Schrodinger interpretation and now r N gets annihilated by r and it becomes this.

Now, what I am supposed to do, you see now you stare at this. What is this wave function? It is a wave function with one fewer particles; that means, it had N particles to begin with, but it has one fewer particle. Now, what you do is you undo what you did.

And what did you do? Earlier you evolved, you evolved the system from time t equal to 0 to t equal to t dash using the Hamiltonian containing N particles. Now, you undo that, that means, you devolve. But then in order to de devolve we have to use the same Hamiltonian, but now all of a sudden you see there is one fewer particle in your system. So, that means, you are supposed to now devolve using a Hamiltonian which has one fewer particles.

So, which is in other words this one which is the reason why I chose to omit the last one, because see once you democratize using the symmetrisation operator, it makes no difference which one you annihilate. So, I preferentially chose the last one without loss of generality and then I have end up doing this.

So, you see now clearly this particular; so, once you devolve you end up with a wave function and that wave function has a very specific physical meaning. And that is basically the what I call the hole wave function; that means, it is a wave function, ok. So, let us let us read this off here.

So, it is basically says the interpretation, so that means, if you decide to annihilate a particle at position r dash at time t dash on a state, which had initially N particles, you end up with a hole wave function. And what is the meaning of that hole wave function?

It is that wave function at time t equal to 0 of N minus 1 variables r 1 r 2 up to r N minus 1 which when evolved from this time to t equals t dash, so that means, it is that wave function which when evolved from this t equal to 0 to t equal to t dash right, becomes identical to this function.

So, and what is this function? This is basically the original function evolved from t equal to 0 up to t equal to t dash, and then replace the last one and by r dash. So, basically that is what it is. So, I am making a big fuss about something that is rather simple to understand if you just think a little bit.

So, basically I am just trying to put this in words. I am just trying to you know verbalize these equation, which is not always a good idea, but. So, basically this is what it is. It basically represents a system with a hole. But then that hole has been propagating. So, the point is that is a hole is a function of time t dash. So, it depends on at what time you create the hole. So, it is parameterized by t dash.

So, basically you are creating a hole in your system and that hole is parameterized by t dash because that is a; that is a time at which you are creating a hole. And that hole wave function clearly contains one fewer particle than what you had earlier because you have annihilated, ok. So, now, that I have rigorously justified what it means to evolve creation and annihilation operators with time, that is the Heisenberg picture.

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sented in position space as  $|S \rightarrow \forall S(\mathbf{r}_1,..,\mathbf{r}_N)$ , then the Green function be reexpressed in a mixed language of operators and wavefunctions as fo  $(d^d[r] \equiv d^dr_1 d^dr_2...d^dr_N)$ .  $G_{<}(\mathbf{r},t;\mathbf{r}',t') = < S|c^{\dagger}(\mathbf{r},t)c(\mathbf{r}',t')|S >$  $= \int d^{d}[r] \Psi_{S}^{*}(\mathbf{r}_{1},..,\mathbf{r}_{N})c^{\dagger}(\mathbf{r},t)c(\mathbf{r}^{'},t^{'})\Psi_{S}(\mathbf{r}_{1},..,\mathbf{r}_{N}).$ (8.85) We may also rewrite this as  $G_{\leq}(\mathbf{r},t;\mathbf{r}',t') = \int d^d[r] \Psi_S^*(\mathbf{r}_1,..,\mathbf{r}_N) c^{\dagger}(\mathbf{r},t) c(\mathbf{r}',t') \Psi_S(\mathbf{r}_1,..,\mathbf{r}_N)$  $= \int d^{d}r_{1}d^{d}r_{2}...d^{d}r_{N-1} (c(\mathbf{r},t)\Psi_{S}(\mathbf{r}_{1},..,\mathbf{r}_{N}))^{\dagger}(c(\mathbf{r}',t')\Psi_{S}(\mathbf{r}_{1},..,\mathbf{r}_{N}))$  $= N \int d^{d}r_{1}d^{d}r_{2}...d^{d}r_{N-1} \Psi_{holes}^{*}(\mathbf{r}_{1},..,\mathbf{r}_{N-1},\mathbf{r};0) \Psi_{holes'}(\mathbf{r}_{1},..,\mathbf{r}_{N-1},\mathbf{r}';0).$ (8.86) (8.86)The last step follows when we insert the last step of Eq. (8.84) into the penultimate step of the above equation. Notice that we have converted the effect of the creation operator into the effect of an annihilation operator followed by a Hermitian conju-gate. This automatically makes one variable, namely  $\mathbf{r}_{N}$ , disappear. However, it is possible to get the same answer more directly, but this is left to the exercises. Thus the important identity relating to the hole propagator is,  $\langle S|c^{\dagger}(\mathbf{r},t)c(\mathbf{r}',t')|S \rangle$  $= N \int d^d r_1 d^d r_2 ... d^d r_{N-1} \ \Psi^*_{hole,i}(\mathbf{r}_1,..,\mathbf{r}_{N-1},\mathbf{r};0) \ \Psi_{hole,i'}(\mathbf{r}_1,..,\mathbf{r}_{N-1},\mathbf{r}';0).$ (8.87)  $^{(8,87)}$ The reason for the extra factor N (that follows rigorously from the definitions) may be understood by realizing that the quantity  $\int d^d r < S[c^{\dagger}(r,t)c(r,t)]S \geq E$  N is the total number of particles. Succinctly, Eq. (8.87) says that the operator definition of the hole propagator is equivalent in the wavefunction language to evaluating the overlap of two functions obtained using the following procedure. (i) First evolve the initial (s-symmetric) wavefunction to some time, then (ii) replace one of the

So, now I am perfectly justified in making statements, such as these which basically tell you the definition of the hole and particle Green's function. So, this is the Hole Green's

function because I am first creating a hole and then filling the hole with a particle. So, that is what 8.85 is.

So, now you see I can actually make physical sense out of the Hole Green's function itself by inserting the definitions of the time evolved, creation and annihilation operator so, which is what I have done here. So, if I do that, you see this now has the definition of the overlap between the hole wave functions at r and r dash.

And the hole wave functions remember are parameterized by the time at which the holes are inserted into the system. So, it is as if, so the hole wave the hole Green's function is basically the quantum mechanical overlap between a hole wave function where you insert a hole at position r dash at time t dash and when you insert the hole instead at position r at time t.

So, see when you insert at r and time t you get a certain hole wave function. But if you insert at r dash at time t dash, you get a different hole wave function. So, the hole Green's function is basically the quantum mechanical overlap between these two states so, which is what this is.

So, quantum mechanical overlap means, you take the complex conjugate of a; of the second wave function multiplied by the first and then integrate over all the dynamical coordinates. Namely, the positions of the particles r 1, r 2 up to. Remember that having created a hole, you have one fewer particle than what you started off with.

So, you had N particles to begin with now you have N minus 1. So, that is the reason why you are supposed to now instead of integrating over all N of them, you are supposed to only integrate up to N minus 1 because you have created a hole and there is one particle missing, ok.

So, that is the physical interpretation of the hole Green's function. So, you can just pause a moment to think about what this means. So, basically, it means that see this hole Green's function therefore, has a very intuitive physical meaning. It is just the quantum mechanical overlap between two situations, one is when you create the hole at r at t, the other is when you create the hole instead at r dash at t dash. So, it asks you know how close are these wave functions I mean, how close are these two states you know. So, that, so it is a measure of the closeness of these two operations. So, clearly you can imagine that if you create a hole at time at r at time t, and if you create a hole at instead at r dash at t dash, and if r and r dash are very far apart or if t and t dash are very different, then you can imagine that the answer would be something not at all close to unity.

Because you see the system would have evolved a lot. So, the two are not the same, right. So, because you are creating at very wildly different times or wildly different positions. So, it kind of is a measure of the havoc that hole creates in in a system, ok. That is pretty much what it measures.

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So, similarly, you can define the particle Green's function as a similar interpretation that is the wave function of system of N particles, to begin with and you create a particle; that means, you insert a particle at position r at time t. And then, suppose you instead insert at position r dash at time t dash, the quantum mechanical overlap between these two states is basically what the particle Green's function is. Because now you will have to having inserted a particle, you will have one more dynamical variable position variable that you have to integrate over. So, instead of up to r N, you have to integrate over up to r N plus 1, ok.

| (iv) de-evolve using the Hamiltonian H <sub>N+1</sub> back to time T = 0. The   | e particle Green                                   |
|---|--|
| function is then the overlap between two such functions.  |  |
| $G_{>}(\mathbf{r},t;\mathbf{r}^{'},t^{'}) =  =$   |  |
| $(N+1)\int d^{d}r_{1}d^{d}r_{N+1} \Psi^{*}_{t', nrtel}(\mathbf{r}_{1},,\mathbf{r}_{N+1};\mathbf{r}',0)\Psi_{t,prtcl}(\mathbf{r}_{1},$   | $(\mathbf{r}_{N+1}; \mathbf{r}, 0).$               |
| J . U.M.  | (8.89)   |
| Now we examine how we may reexpress Hamiltonians that are ori<br>of positions and momenta using these operators.  | iginally in terms                                  |
| 8.4 Hamiltoniane Using Creation   |  |
| 8.4 Hallintomans Using Creation   |  |
| and Annihilation Operators  |  |
| As before, consider the Hamiltonian,<br>$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V( \mathbf{r}_i - \mathbf{r}_j ).$   | $\int \int ds = 1 e^{\frac{3}{2}} e^{\frac{3}{2}}$ |
| We wish to show that this can also be written as (in this section d   | <b>tr</b> is the volume                            |
| element (d-dimensional) and $\delta(\mathbf{r}-\mathbf{r}')$ is the d-dimensional Dirac d   | delta function),                                   |
| $H = \int d\mathbf{r} c^{\dagger}(\mathbf{r}) \frac{p^2}{2m} c(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' c^{\dagger}(\mathbf{r}) c^{\dagger}(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}') V( \mathbf{r}' ) d\mathbf{r}'$ | r = r' ), (8.91)                                   |
| To do this we have to show that $H_1F_s(\mathbf{r}_1,,\mathbf{r}_N) = H_2F_s(\mathbf{r}_1,,\mathbf{r}_N)$   | $N$ for any $F_s =$                                |
| $\mathfrak{P}_s F$ and $H_1$ is the expression in Eq. (8.90) and $H_2$ is the expression<br>Consider  | on in Eq. (8.91).                                  |
| $H\psi(\mathbf{r}_1, \mathbf{r}_2) = \int d\mathbf{r} c^{\dagger}(\mathbf{r}) \frac{p^2}{2m} c(\mathbf{r}) \psi(\mathbf{r}_1, \mathbf{r}_2)$  |  |
| $1 f \cdot f \cdot t + c + c + c + c + c + c + c + c + c +$   |  |
| $+\frac{1}{2}\int d\mathbf{r}\int d\mathbf{r} c'(\mathbf{r})c'(\mathbf{r})c(\mathbf{r})c(\mathbf{r})V( \mathbf{r}-\mathbf{r} )\psi(\mathbf{r}_1,\mathbf{r}_2)$  | 2). (8.92)   |
|   |  |
|   |  |

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So, this is as far as making contact with more familiar starting points such as the Schrodinger picture and so on. So, I have interpreted you know this creation and annihilation operator and its time evolution using the familiar examples of quantum mechanical overlap of wave functions which are familiar from the Schrodinger's approach to quantum mechanics.

So, having done this now I am equipped to show you that you see, ok; now the question was what is the utility of this technique. So, remember, what is the, suppose you ask the same question for the original problem that I started off with in this chapter namely one mass tied to one spring. What is the utility of using creation and annihilation operators there?

The utility clearly is that if you there are many uses one of them, one very obvious important use is that if you rewrite the Hamiltonian of the system in terms of creation and annihilation operators rather than working with position and momentum, you would clearly be able to read off the eigen values of the Hamiltonian.

So, you would be able to read off the energy levels of the system, just by staring at that Hamiltonian written down in terms of creation and annihilation operators. You would not have to struggle, you do not have to solve Schrodinger equation, you do not have to struggle with Hermite polynomials. I mean unless you want the wave functions, you do not have to struggle at all. So, the eigen values just drop out of the calculations all by themselves.

So, even if you do not want them they there. So, that is the main advantage of working with creation and annihilation operators. It simply you know gives you the eigen values of the Hamiltonian just like that. So, for the same reason, we now want to be able to express a system of N particles in terms of creation and annihilation operators of particles themselves rather than excitations.

But rather than, in terms of the original picture original description in terms of position and momentum. So, you see if the original description was like this as shown in equation 8.90, now I am going to try and convince you that this Hamiltonian is nothing, but this I mean these two are the same. So, long as this operator acts on the on a Hilbert space containing N particles because you see this is sort of this Hamiltonian is agnostic to the number of particles.

Agnostic means like it does not care about how many particles there are in the system. It is only when you act this operator on a state containing a fixed number of particles, then that dependence on the number of particles then shows up in the result of that action.

So, therefore, I have to now so the claim is that 8.91 and 8.90 are operator identities. Mean they correspond to the same operators provided; see here there are already N particles. So, I am not, I do not have to further qualify this by saying that this 8.90 has to have N particle that is apparent just from the definition.

But here it is not apparent. So, I have to specify that when 8.91 acts on a Hilbert space containing N particles it is only then that these two become the same operator. So, the operator described in terms of creation and annihilation operator becomes precisely the same as the operator that is described in terms of position and momentum, ok.

So, now I feel is a good time for me to stop because in the next class I am going to prove this rather startling, but important claim. So, it is not at all obvious that you can do that. You see the superficially this seems incredibly simple compared to this. So, 8.91 seems incredibly simple for the following reason. Because you see here there are only two vectors r and r dash. But here you see how many vectors are there, there N vectors and then N could be macroscopically large.

So, if you have a system, say if you have a typical gas or if you say electrons in a metal. you would have lot more than this, ok. So, you would have this many. So, this Hamiltonian has that many electrons and that many r vectors, r 1, r 2 up to that many 10 raise to 30 R's.

But then, this is formidable unwieldy. However, this even though the same information is contained in both the number of vectors that you have to deal with are only two. Of course, that is I mean you might think that seems implausible because then where is the information contained.

Clearly, there is a hidden assumption that you are going to act this, finally, on the appropriate number of; you are going to act it on a state containing the appropriate number of particles which kind of. So, that is where that information is hidden.

But nevertheless it is really; so, you can imagine that from a formal stand point for calculational purposes 8.91 is likely to be far more convenient in doing practical calculations than 8.90 because of the sheer number of vectors that you have to handle here. Because they are all mutually interacting by implication. So, these are, this is two body potential energy.

So, they are mutually interacting, so it is quite formidable. But here even though they are mutually interacting, the number of vectors that you have to handle are a lot fewer, ok. So, I am going to stop here now. And in the next class I am going to prove this claim to you in significant detail, ok.

Thank you. So, hope to see you in the next class.