Advanced Condensed Matter Physics
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Lecture – 12
Wick's theorem and normal ordering

We have introduced Green's function at 0 temperature and we have also provided an expression what the Green's function looks like. So, the Green's function is a time ordered product of a creation and an annihilation operator and it has to be. So, this is the unperturbed Green's function that I am talking about and expectation value of these time ordered product of one creation and one annihilation operator has to be computed with respect to the non interacting ground state which is assumably known.

Now, we will have to understand how to compute full Green's function that is Green's function for interacting systems. In fact, that is one of the main aim of introducing Green's function. So, in order to calculate Green's function for the interacting system will have to understand one theorem which is very important in this context.

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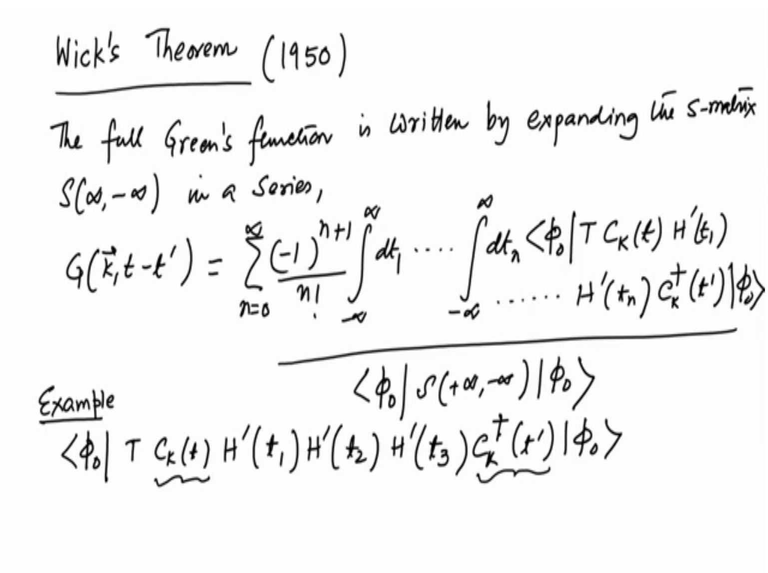

It is called as a Wick's theorem. So, this was introduced by Wick's in 1950 and before we go that go to that of how to use Wick's theorem in the context, let us write down the full greens function. So, the full Green's function and why we are using the word full Green's function is because we have computed the non-interacting or the unperturbed greens function.

So, the full Green's function is written by expanding the s matrix that has been introduced earlier and the s matrix in this particular case is s infinity minus infinity in a series and it acquires a form. Now we are writing it a little more specifically for a translationally invariant system where the momentum k is a good quantum number it is equal to sum over n equal to 0 to infinity minus one whole to the power n plus one divided by n factorial.

And all these summations from minus infinity to plus infinity d t 1 and so on and from minus infinity to plus infinity a d t n a phi 0 and t that is a time ordering C k t and then all these series of interaction terms at time t 1 all the way till h prime t n and then we have a C k dagger at t prime and this has to be taken within 5 0 divided by the denominator that we have seen earlier which is s infinity minus infinity phi 0.

Now, it does not matter even if we forget the denominator because it just acts as a normalization we can ignore that and still we will have the numerator to compute and the numerator can be written as for a particular case say we go up to t 1, t 2 and t 3 that is we include 3 orders of the interaction term at a distinct times t 1, t 2 and t 3, then we will have to compute a ground state expectation of the time ordered C k t h prime t 1 h prime t 2 and h prime t 3 and will have to will have another coming from the greens function. So, there will be a term which is C k dagger t prime and a phi 0.

So, this is an example that we are considering in which case in this series that we have written above in the numerator there 3 distinct times that are taken t 1, t 2, t 3 and we have written down the Green's function the full Green's function including these 3 terms. So, remember that there will be one annihilation operator at the left and there is one creation operator at the right and this time ordering will take care of all the combinations of times of t v, t 1, t 2, t 3, t prime and will ultimately put the time which is largest at the left.

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Assume, $H'(t_1) = \frac{1}{2}\sum_{q} \frac{4\pi e^2}{q^2}\, c^{\dagger}_{k+q,\sigma}\, c^{\dagger}_{k'-q,\sigma'}\, c_{k'\sigma'}\, c_{k\sigma}\; e^{it_1(\xi_{k+q}+\xi_{k'-q}-\xi_{k'}-\xi_{k})}$

How many creations and annihilation operator in G?

Each $H' \rightarrow$ 2 creation, 2 annihilation

$3H' \rightarrow$ 6 " , 6 " } operator

$G^0 \rightarrow$ 1 " , 1 "

= 7 " , 7 " operators

Time indices – t, t_1, t_2, t_3, t'

So, let us assume that the interaction term that we are going to consider has a coulomb form. So, we will write down a coulomb interaction at t 1 is equal to half this is a coulomb interaction same as e square over r where r is the distance between the 2 particles and; however, it is written now in k space. So, we use a term which is 4 pi e square over q square and a C k plus q dagger sigma as a spin C k prime minus q sigma prime dagger and C k prime sigma prime and a C k sigma.

And followed by will have an exponential i t 1 and this is my, the terms that are the energies and k minus q minus k prime minus k. So, these are the that Fourier transform. So, that we are writing it in. So, these are the terms for h prime given at a time t 1 and similarly there will be 3 terms which are h prime t 1 t 2 and h prime t 3 all will have to be written because it is an interaction term expectedly it will have to creation and 2 annihilation operators.

So, how many creations and annihilations operator we have operators in g each one of the h primes will give. So, each h primes will give 2 creation and 2 annihilation and how many of them are there. So, there are 3 of them are there. So, a 3 h prime will give 6 creation and 6 annihilation operators and the Green's function itself has or the in non-interacting Green's function has one creation and one annihilation.

So, these two will have to be added and will have seven creation operators and seven annihilation operators and each of them will have different times I mean in the sense that the h primes will have one time t 1 the other h prime will have t 2 and t 3 etcetera. So, all these fermionic operators C and C dagger will have will correspond to times t 1, t 2, t 3 and then there is a t and t prime which are coming from the non interacting greens function. So, there are 4 or rather 5 time indices that are appearing here namely. So, they are the time indices are. So, a time index in these cases a t t 1, t 2, t 3, t prime.

And when we consider a higher order problem that is a, suppose, we have 5 h primes. So, we go up to the fifth order in order to compute the full h prime the full sorry the Green's function then will have more number of time indices we need to be ordered now keeping track of all these time orderings become a problem and because of that taking all sort of time combinations that is t greater than t 1 and. So, these are t t 1 t 2 t 3 and t prime. So, we can have combinations such as t greater than t 1, but less than t 2 less than t 3 greater than t prime and so on and so forth.

So, this keeping track will be difficult. So, computing a full Green's function often can be big problem a problem that is becomes formally quite complicated and messy; however, things are not that difficult and a solution is provided by the Wick's theorem and this is what we are going to talk about, but before we go into Wick's theorem let us also see that.

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Equal no. of creation and annihilation operators.

$$\langle \phi_0 | T\, c_1(t)\, c_1^{\dagger}(t_1) \cdots\cdots c_n(t_n)\, c_n^{\dagger}(t_n) | \phi_0 \rangle$$

Unequal number of creation and annihilation operators will yield zero expectation value.

Creation operator creates a particle in $|m\rangle$, the annihilation operator must destroy the state $|n\rangle$, such that $|m\rangle = |n\rangle$

<u>Example</u> $\langle \phi_0 | T\, c_\alpha(t)\, c_\beta^{\dagger}(t') | \phi_0 \rangle = 0$ unless $\alpha = \beta$

$$\langle \phi_0 | T\, c_\alpha(t)\, c_\beta^{\dagger}(t_1)\, c_\gamma(t_2)\, c_\delta^{\dagger}(t') | \phi_0 \rangle = 0$$

unless $\alpha = \beta$, $\gamma = \delta$ or $\alpha = \delta$, $\gamma = \beta$.

We should have equal number of creation and annihilation operators in a greens function. So, this is basic requirement because suppose we write a time ordered of C 1 t a C 1 dagger t 1 and going up to C n t n and C n dagger t n and a phi 0.

This should only exist an unequal number of a creation and annihilation operators will yield 0 expectation value now why is that. So, suppose we have unequal numbers that is there is one C dagger which is extra which is not being compensated for and that will act on the non-interacting ground state and will create a state which will have 0 expectation or 0 overlap with the non-interacting ground states.

So, that is why this there has to be equal number of the creation and annihilation operators further the job of the creation operator is to create a particle in a certain state. So, creation operator creates a particle in state say m the destruction operator or the we are talking about annihilation let us call it annihilation though they mean the same thing.

Operator must destroy the state m state n such that m has to be equal to n. So, that the system is returned back to the ground state and it has finite expectation with respect to the ground state ok. So, say for example, we have a phi 0 T C alpha T C beta t dagger t prime and a phi 0 has to be 0 unless alpha equal to beta.

And if alpha is not equal to beta then it is equal to 0 and if alpha equal to beta this will correspond to a Green’s function g t minus t prime and similarly another example can be given which is a larger term inside the expectation term. So, this is C beta dagger t 1 and a C gamma t 2 and a C delta dagger t prime and this is phi 0. So, just to avoid confusion so, this is a equal to again equal to 0 unless alpha equal to beta gamma equal to delta or alpha equal to delta gamma equal to beta.

So, it has to returned to the ground state to have a nonzero expectation in the ground state because if a state is created by acting an operator on the phi 0 if that state is not destroyed that particular, the new state will not have an overlap with the original state of the problem or the ground state of the problem.

So, that is why it has to vanish and so, there are in when you have larger number of such terms inside the phi zeros then you will have a many such orderings that are going to appear and each ordering will then have to be dealt separately and not only that the main question still lies that how do we actually compute a Green's function which is given here.

So, a Green's function such as phi 0 the time ordered of C k t h prime t 1 h prime t 2 h prime t 3 C k dagger t prime and phi 0, how will they have be how will they be calculated and to bring to a form that makes sense. So, then this is done by the Wick's theorem and Wick's theorem uses a concept which is known as normal ordering. So, let us learn what normal ordering and then will see what Wick's theorem does.

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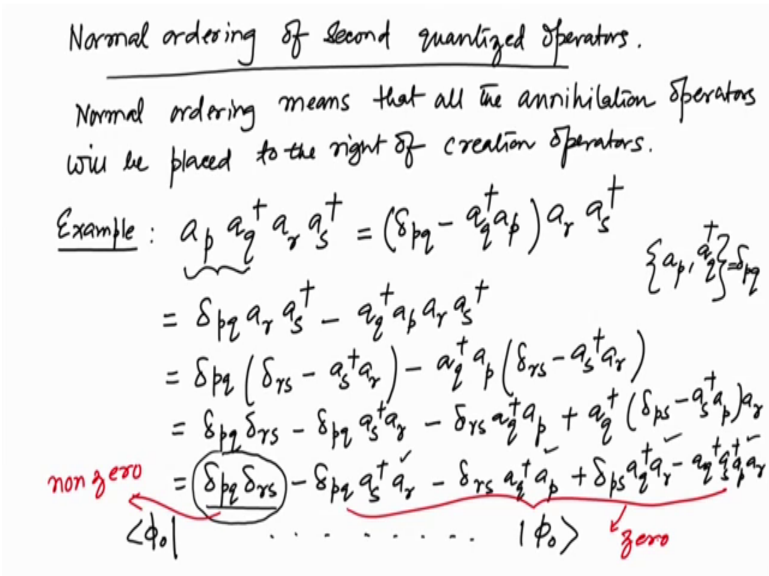

So, normal ordering; so, normal ordering means that all the annihilation operators will be placed to the right of the creation operators.

So, this is the process in which you will use the anti-commutation relations of the fermion operators and place all the creation all the annihilation operators to the right of the creation operator. So, all the creation operators will be on the left and all the annihilation operators will be in the right.

So, take an example and let us call it a p a q dagger a r a s dagger where p q r s are some states which are the some quantum numbers which are valid quantum numbers for a given problem. So, this can be written as now as I said that all the annihilation operators will be to the right. So, first start with this a p a q dagger if I have to move a p to the right of a q dagger.

Then what I have to do is that I have to use the anti-commutation relation which tells me that it is a delta p q and minus a q dagger p k i p a p and a r a s dagger. So, is this clear that a p a q dagger is nothing, but delta p q which is if p equal to q if this is equal to one. So, if p equal to q, then it is 1 minus a q dagger a p. So, we have changed the ordering of the indices and I have just to remind you that we have a p a q. So, this anti-commutation relation is equal to is equal to delta p q.

So, a p a q dagger plus a q dagger a p equal to delta p q is the anti-commutation relation and so, we have done the first step was the second step second step is simply multiplying it out. So, it is delta p q a r a s dagger we still have to do this and now I have a minus a q dagger a p a r a s dagger. Now let us do this procedure again on the first term and I will have a delta p q and now a delta r s minus a s dagger a r and now I will do it for these terms which are minus a q dagger a p.

Now, I will change the ordering of this such that that is pushed to the right that is that the annihilation operator is pushed to the right. So, it is delta r s minus a s dagger a r. So, these are the two terms that we get. Now, I will simply again multiply it out delta p q and delta r s minus a delta p q a s dagger a r minus delta q s a q dagger a p and a plus a q dagger a p. Now, this a p will be has to be pushed to the right of a s dagger. So, that will do it here. So, a q dagger and there is a delta p s minus a s dagger a p and a r

So, now we have delta p q delta r s minus delta p q a s dagger a r minus delta r s a q dagger a p and plus delta p s a q dagger a r minus a q dagger a s dagger a p a r now that is the complete simplification because in each of the terms wherever there is a creation and an annihilation operator we have been able to push the annihilation operator to the right and that tells me that if I take, now the ground state expectation of this term. So, it is phi 0 and this entire thing that we have written here you see the terms which are the first in the second term the third term the fourth term and the fifth term they all will go to 0.

Because there is all in each of the cases the annihilation operator is standing on the right and the non-interacting ground state may not have a state which is which contains a state which is to annihilation. So, this will annihilation state at r, but the non-interacting ground state may not have a state, but what definitely will not have a state is a vacuum one thing to remember that phi 0 is not the vacuum.

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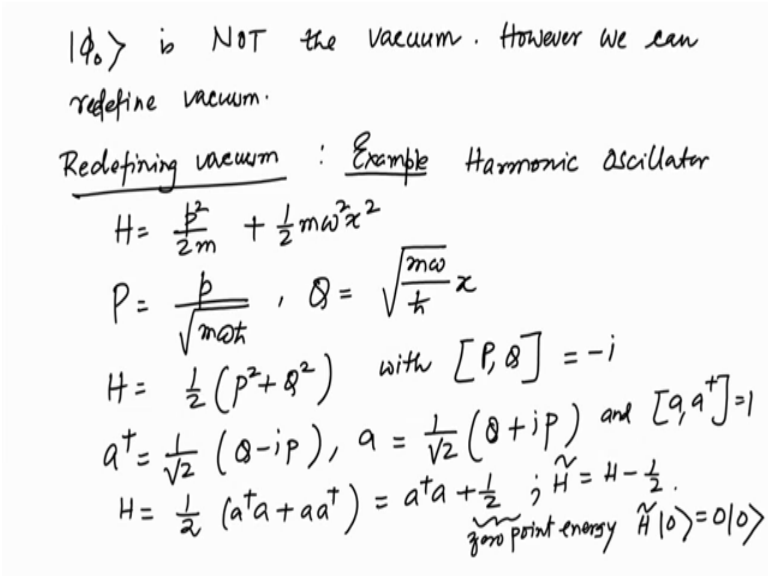

However, we can redefine vacuum redefine vacuum and these 5 0 can be considered as a redefined vacuum which really does not have a state which is occupied which can be annihilated.

So, it seems that. So, how do we redefine a vacuum let us give me an example. So, redefining vacuum I am giving an example of that you have studied the harmonic oscillator in your quantum mechanics course and the harmonic oscillator has Hamiltonian which is given by P square over 2 m plus half m omega square x square.

And you know the full story that goes with it that is if you solve this quantum mechanical Hamiltonian that is the Schrodinger equation with this as the Hamiltonian then you would get an energy spectrum which is n plus half h cross omega and there is a 0 point energy that exists for n equal to 0 and the way functions are going to be Hermite polynomial multiplied by a Gaussian where Hermite polynomials are polynomials with certain properties such as when the indices of these polynomials and even the polynomial is even and when the indices are odd the polynomial is odd you can look up any quantum mechanics book for this purpose, now if in this harmonic oscillator. So, we are talking about simple harmonic oscillator quantum mechanical simple harmonic oscillator.

If you define operators which are like P divided by root over m omega H cross and Q as root over m omega by H cross x and in that case you can write down the Hamiltonian as half of P square plus Q square these are operators that have been made dimensionless.

So, this Hamiltonian is dimensionless you are not seeing any omega etcetera H cross omega which are should have come with the Hamiltonian we have made it dimensionless and there are commutation relations that P and Q satisfied which come from the P and x position and momentum commutation relations in quantum mechanics.

if you further define the raising and the lowering operators by this accuse and piece such that we can write it as Q minus i P and a as one by v 2 Q plus i P with a and a dagger to be commutation of that to be one then my H becomes equal to it is equal to half of a dagger a plus a dagger which come from the P square plus Q square and this if you simplify it becomes a dagger a plus half. Now if I redefine this half comes from the 0 point energy and if we redefine a H tilde which is equal to H minus half.

Now, we do not have a 0 point energy and we have been able to define the ground state without the 0 point energy. So, we have now n starts from one. So, we have so, such that your H acting on 0 gives you a 0 and a 0. So, there is no the 0 point energy has been set to be equal to 0 and this is what. So, the first a non 0 energy is of course, the H cross omega and the 0 point energy is 0. So, this is the way one can redefine vacuum. So, if we redefine vacuum in our case as well then all the annihilation operators acting on the ground state which is now the vacuum should give me 0.

So, the only thing that is nonzero is this part. So, this is the only thing that is nonzero and will only thing that is nonzero here and rest all of them are our 0 ok.

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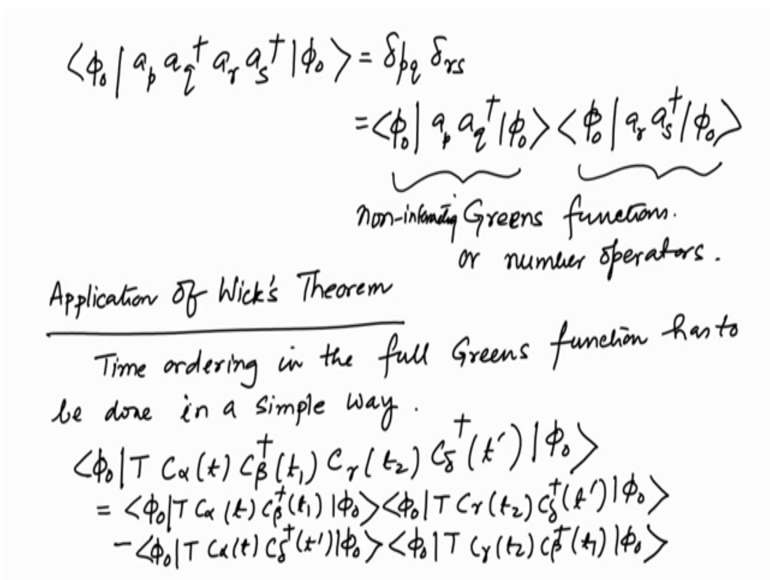

So, this is what it gives and hence we can write this as phi 0 a p a q dagger a r a s dagger phi 0 it is equal to a delta p q and a delta r s which are nothing, but phi 0 a p a q dagger phi 0 and phi 0 a r a s dagger and a phi 0. Now these are the greens functions.

Accepting that we have not written the time indices explicitly, but these will give the greens functions or they will give the or number operators if the time indices are same will come to this. So, these are not only these are greens function, but these are non-interacting greens functions and these one example of this non interacting Green's function we have done why we attended to that example of degenerate electron gas free electron gas.

So, the nutshell is that the total Green's function or the full Green's function will have to be expressed in terms of the non-interacting Green's function and it will be done the normal ordering. Now, the time ordering will be taken care of by the Wick's theorem and let us show how so, now, application of Wick's theorem.

You might wonder that we have not defined Wick's theorem, but we are talking about applications of the Wick's theorem we are just going to come to Wick's theorem, but seeing one application how it works will probably be able to for you to realize better what those words mean when we talk about it. So, the time ordering in the full Green's function has to be done in a simple way.

So, keep in mind that we have equal number of creation and annihilation operators. So, let take an example which is what we have said is T C alpha T C beta t 1 dagger C gamma t 2 and C delta dagger t prime this is really a hypothetical situation because you will never have 2 creation and 2 annihilation operators ever because you will have a h prime which itself will come with 2 creation and 2 annihilation operators; further the Green's function that is that requires one more creation and annihilation operator. So, at least you will have 3 creation or 3 and annihilation operators.

For the first order Green's function to be calculated we are just taking a hypothetical example now what we will do is that we will have to write to terms with the normal ordered product. So, will make them write into non interacting greens function. So, assume the normal ordering is done and we write a C beta dagger t 1 and a phi zero. So, the first 2 terms have been paired and the third and the fourth terms have been paired well will have to write it properly. So, a phi 0 and the time ordered C gamma t 2 C gamma t C gamma t 2 and C delta at t prime and phi 0 remember each of these terms that you see there are they are non-interacting greens functions.

And now there is a minus sign you will see why because you will have to take this C gamma one move and a second move. So, 2 moves 2 swaps of this C delta dagger will create 2 negative signs which will be positive, but; however, I will also take the C beta dagger to the right of C gamma in order to write it as a greens function. So, that is one move that is why we get a minus sign. So, will have a minus sign and this and then a C alpha T C delta dagger t prime and a phi 0 and a phi 0 t C gamma t 2 C beta dagger t 1 and phi 0.

Remember there will be no terms which are consisting of both of them being annihilation operator or both of them being creation operators because that will have 0 expectation value.

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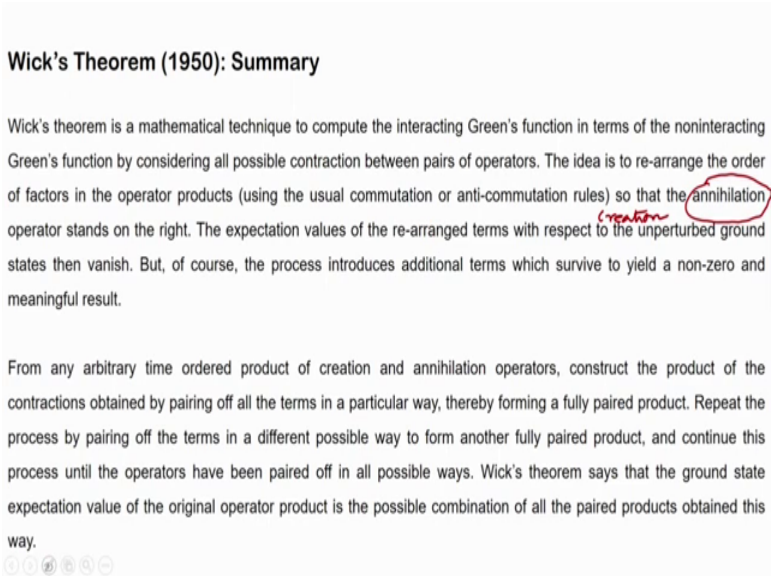

Anyway so, let us come back to this in a while and let me complete this thing.

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$$= \delta_{\alpha\beta}\,\delta_{\gamma\delta}\,\langle\phi_0|T\,c_\alpha(t)\,c_\beta^\dagger(t_1)|\phi_0\rangle\langle\phi_0|T\,c_\gamma(t_2)\,c_\delta^\dagger(t')|\phi_0\rangle$$
$$-\delta_{\alpha\delta}\,\delta_{\gamma\beta}\,\langle\phi_0|\,c_\alpha(t)\,c_\delta^\dagger(t')|\phi_0\rangle\langle\phi_0|T\,c_\gamma(t_2)\,c_\beta^\dagger(t')|\phi_0\rangle$$

$$(-i)^2\langle\phi_0|T\;c_\alpha(t)\;c_\beta^\dagger(t_1)\;c_\gamma(t_2)\;c_\delta^\dagger(t')|\phi_0\rangle$$
$$= \delta_{\alpha\beta}\,\delta_{\gamma\delta}\,G^0(\alpha, t-t_1)\;G^{(0)}(\gamma, t_2-t')$$
$$-\delta_{\alpha\delta}\,\delta_{\gamma\beta}\,G^0(\alpha, t-t')\;G^0(\gamma, t_2-t_1).$$

So, this will be equal to delta alpha beta delta gamma delta which is phi 0 and a T C alpha t C beta dagger t 1 phi 0 and phi 0 T C C gamma t 2 C delta t prime phi naught and a minus delta alpha delta delta gamma beta and phi 0 C alpha T C delta dagger t prime phi 0 and a phi 0 T C gamma t 2 and C beta dagger t prime and phi 0.

Once you get to the habit of writing things will be very smooth and you know the rules of changing science and writing these things. So, I get 2 delta functions coming from 2 of these brackets and so on. So, what happens is that I have to now multiply because there are 2 greens functions if I multiply a the whole term as. So, I have a minus i square because the Green's function if you remember comes with the minus i.

So, minus i square phi naught T C alpha T C beta dagger t 1 C gamma t 2 and C delta dagger t prime and a phi 0 this will be delta alpha beta delta gamma delta which is what we have written alpha t minus t 1 and g 0 gamma t 2 minus t prime and there will be another term which is alpha delta and delta gamma beta g 0 and this is say alpha t minus t prime and g 0 gamma t 2 minus t 1. So, even if it is hypothetical this term is hypothetical.

We still have been able to simplify it and written it in terms of 2 greens functions along with this delta alpha beta and delta gamma delta these delta functions and 2 greens functions and similarly 2 delta functions and the greens functions. So, this is Wick's theorem, let us go back and see what Wick's theorem are and we have included a summary I will go through it slowly and try to explain it. So, that you understand these concepts clear these will be required in computing the Green's function the full Green's function for an interacting system and which is what we plan to do next. So, it is in nineteen hundred and fifty it was put forward by Wick's and some mathematical technique to compute the interacting Green's function which is the full greens function.

In terms of the non-interacting Green's function by considering all possible contraction between pairs of operators so, these are the all possible one possible is C alpha C beta dagger and C gamma C delta dagger the other possible combination is C alpha C delta dagger and C gamma C beta dagger; so, considering all possible contraction between pairs of operators.

Now you see that more number of h primes that you have more will be the number of combinations that you need to take the idea is to rearrange the order of factors in the operator products which are between the ground states using the usual commutation or anti-commutation rail rules in the context of fermions they are anti-commutation and in the context of bosons they are the commutation rules.

So, that the annihilation operator always stands on the right the expectation values this will be. So, when you write these operator products these are the normal ordering of course, required that they have to be the annihilation will have to be on the right, but when you write down greens functions then the creation operators will have to be. So, this has to be replaced by the creation operators the expectation values of the rearrange terms which is between the ground states which are 5 zeros with respect to the unperturbed ground states then vanish ok. So, this is telling you about ok. So, I change this because this talking about the normal ordering once more.

So, let us talk in a sort of systematic manner. So, this talk about the normal ordering, but of course, the process introduce additional terms which survive to yield a nonzero and a meaningful result which is what we have seen here that we have a nonzero result which is meaningful which gives rise to 2 Green's function is what we have done these 2 greens functions. So, this is what the process does.

So, this is that normal ordering now for from any arbitrary time order product of creation and annihilation operators construct the product of the contractions. So, you contract them which means you swap their positions in a physically meaningful and mathematically meaningful way obtained by pairing of all the terms in a particular way thereby forming a fully paired product you see we have formed a fully paired product.

So, there is a C alpha C beta dagger and there is C gamma C delta dagger and similarly the other term repeat the process by pairing of the terms in a different possible way to form another fully pair product and continue this process until the operators have all been paired off in all possible ways to keep matter simple.

We have shown you that how these pairing takes place in for only 4 fermion operators, but as I told for fermion operators is never possible in a full Green's function you should have at least 5 fermion or rather 3 fermion operators and 3 3 annihilation operators and 3 creation operators which means 6 fermion operators is minimum what we need for a Green's function and so, will have to repeat the process of pairing.

So, this is that statement that you repeat the process by pairing of the terms in different possible way to form another fully paid product and continue this process until all the operators have been paired off in all possible ways Wick's theorem says that the ground state expectation value of the original operator is the possible combination of all the product pair products obtained in this way.

So, this Wick's theorem does this time ordering in a simple manner and the normal order product gives only a few possibilities that could survive and by putting all the annihilation operators to the right of the creation operators there by making most of these terms to be equal to 0 and only a few to survive .

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So, to know the rules of applying Wick's theorem is that you form a time ordered product of the operators then go to the normal ordering. So, which means that put all the annihilation operators to the right of the creation operators now you need to take into account a sign change each time a fermion operator changes it is position. So, one should keep the count of the number of interchanges needed to achieve these desired pairing.

So, we are now ready to write down the full Green's function for a given problem and we shall do it; for the simplest case which is coulomb interaction for a foreign electron system so, a system of fermions.