

Dynamics of Classical and Quantum Fields: An Introduction
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Green Functions in Grand Canonical Ensemble
Lecture - 40
Matsubara Green functions - I

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Chapter 10

Green Functions: Matsubara and Nonequilibrium

In this chapter, we discuss the central concept in many-body physics, namely the single-particle Green function. It is shown that many physical observables, such as current and number density, are related to this object. However, this quantity is more important than that since it provides information of the nature of 'quasiparticles'. If we choose to characterize the atomic constituents of the model being studied minus the mutual interactions among the constituents—'particles', then 'quasiparticles' would be the effective description of such particles in the presence of such mutual interaction between the constituents. The single-particle Green function contains information about the energy momentum relation of these quasiparticles and also their lifetime. We consider this concept both for systems in thermodynamic equilibrium and for systems out of equilibrium.

10.1 Matsubara Green Functions

In this section, we define the finite temperature, or Matsubara Green function, of a system of particles for systems that statistical mechanics would classify as grand canonical. This means that we imagine the system exchanging energy and particles with a reservoir where only the average energy and average number of particles are fixed. We imagine the system to be described by a Hamiltonian that may be written in the form $H = H_0 + V$, where H_0 is that part of the Hamiltonian which may be handled exactly. The remaining is denoted by V . Consider the following operator.

Ok. So, in today's class I am going to start a new chapter and that is the topic of Matsubara Green's functions and its non-equilibrium version which goes by various names such as Keldysh formalism and so on and so forth.

So, if you remember that I had already explained to you what a Green's function is in the context of many particle systems. It is all about the overlap of two wave functions, one is suppose you want to talk about the whole, there are two types of Green's function. One is the whole Green's function, the other is particle Green's function.

In the case of whole Green's function, you start with some given state which contains some n number of particles and you remove a particle at a given time, at a given position. And, then you let the state evolve, you let the system evolve naturally and then after a while you reinsert that particle that you have removed at some other point at some

other time. And, then you ask yourself what is the overlap the quantum mechanical overlap between the new state that you obtain immediately after reinserting the particle and the starting state.

So, that is called the whole Green's function. So, you could do a particle Green's function as well where you start with n number of particles, but then you insert a particle rather than remove it. So, you insert a particle from outside and then again you let the system evolve naturally and then you remove that extra particle that you have inserted. So, that would be the particle Green's function.

So, now it so happens that if the system that; so, you see till now we had not discussed anything involving temperature. So, remember that in nature no system is truly isolated. So that means, any system that you are considering, you know a quantum mechanical system is typically you know a solid, a piece of solid or you know or just you know electrons in a solid for example, I mean you whatever system that you are trying to study and none of those entities are truly isolated.

They are always coupled to some surroundings and those surroundings necessarily influence the system that you are studying and that too in a very non-subtle way, it influences it in a very drastic way. So, one of the usual types of coupling to the environment that we are very familiar with is the situation where the system in question exchanges energy with its surroundings freely and comes to a thermal equilibrium.

That means, there is something common between the system that you are considering and the surroundings and that common quantity is called the temperature, the absolute temperature of both the systems and the surroundings, they are both equal. So, that is precisely the situation that I want to study right now, where I have a quantum mechanical system consisting of many particles be their bosons or fermions.

And, I want to study how they behave when you allow them to exchange energy with their surroundings and come to an equilibrium with some common temperature with the surroundings. So, having achieved that equilibrium, now you can ask the same questions that you would ask when the system was isolated. Namely, you can ask the same

question, suppose I remove an electron in such a system which has come to an equilibrium with its surroundings.

And, then I wait for a while and reinsert the particle back into the system, you see what is the quantum mechanical overlap. Now, you see that overlap is going to be is again going to involve summing over states, but then you have to make sure that you associate a Boltzmann weight with respect to each state. So that means, you see that is the idea of canonical statistical mechanics that.

So, if you remember that when I was discussing this idea of a whole Green's function, I kind of alluded to the fact that the system under consideration was in an eigenstate of some Hamiltonian with some eigenvalue. And, then the evolution would then be unitary with precisely that particular energy. But however, when the system is exchanging energy with surroundings, that is no longer the case.

See it does not have a well-defined energy. So, it is going to be in a superposition of states with different energies, but now that superposition now comes with a weight and that is the Boltzmann weight. And so, and you all know what I am talking about and that is basically this. So, this is called the Boltzmann weight. So that means, you see in any I am just refreshing your memory of stat mechanical statistical mechanics; by the way that is supposed to be prerequisite for this course.

Unfortunately, this is an advanced course and many topics are considered prerequisites. So, you see when you do a average in canonical statistical mechanics what you actually mean is that you are summing over all possible eigenstates, but then it is each eigenstate comes with a I mean not all energies are equally probable ok.

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Chapter 10 E_n

Green Functions: Matsubara and Nonequilibrium

$$\langle A \rangle = \frac{\sum_n \langle n | A | n \rangle e^{-E_n / k_B T}}{\sum_n e^{-E_n / k_B T}}$$

In this chapter, we discuss the central concept in many-body physics, namely the single-particle Green function. It is shown that many physical observables, such as current and number density, are related to this object. However, this quantity is more important than that since it provides information of the nature of 'quasiparticles'. If we choose to characterize the atomic constituents of the model being studied minus the mutual interactions among the constituents—'particles', then 'quasiparticles' would be the effective description of such particles in the presence of such mutual interaction between the constituents. The single-particle Green function contains information about the energy-momentum relation of these quasiparticles and also their lifetime. We consider this concept both for systems in thermodynamic equilibrium and for systems out of equilibrium.

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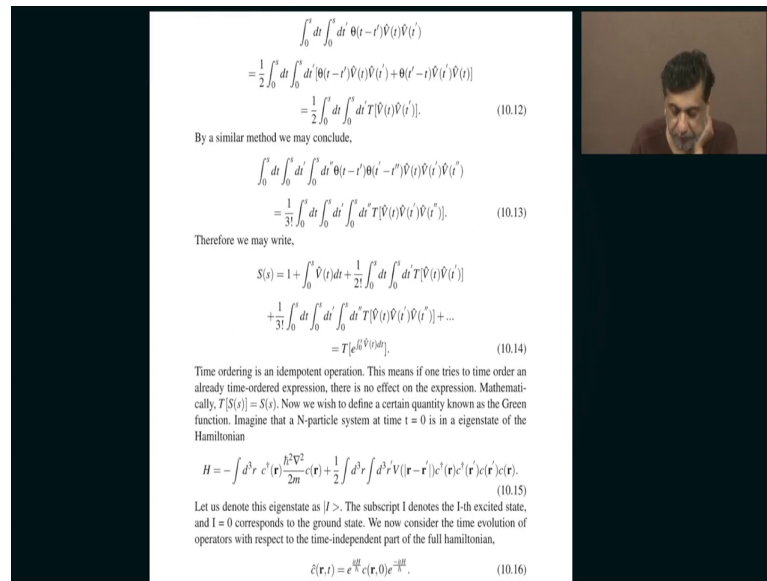
$$U(\beta) = e^{-\beta(H_0 + V)}. \quad (10.1)$$

So, so, it is not just this, this is what I am this is these two would be the same if the system was in a well-defined eigen state like n . And, that n is so; that means, if it is in an eigenstate of n , it also has a well-defined energy called E_n . But that is not possible when the system is exchanging energy with surroundings. So, there is so, in other words there is a probability for that system to be in that eigenstate and that probability is basically proportional to $e^{-E_n / k_B T}$ according to Boltzmann ok.

So, now, this is what I mean by canonical stat mech averaging; that means; so, in canonical statistical mechanics the average of any operator is given by this ok. So, now you see this is what we are going to be doing. So, when I speak of overlap; so, when I speak of time evolution and finding averages, I usually I mean I am going to mean in this chapter average of this kind.

So, where I do a quantum statistical averaging; that means, it is not averaging over eigen states, but averaging over all possible eigenstates. But, each eigenstate comes with a certain weight and that weight is dependent on the absolute temperature ok. So, let us see how that is practically done ok. But, in order for me to do this, I will have to go through some formalism ok and that is basically it will lead us to the Matsubara Green's function.

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$$\int_0^t dt \int_0^t dt' \theta(t-t') \hat{V}(t) \hat{V}(t')$$

$$= \frac{1}{2} \int_0^t dt \int_0^t dt' [\theta(t-t') \hat{V}(t) \hat{V}(t') + \theta(t'-t) \hat{V}(t') \hat{V}(t)]$$

$$= \frac{1}{2} \int_0^t dt \int_0^t dt' T[\hat{V}(t) \hat{V}(t')]. \quad (10.12)$$

By a similar method we may conclude,

$$\int_0^t dt \int_0^t dt' \int_0^t dt'' \theta(t-t') \theta(t'-t'') \hat{V}(t) \hat{V}(t') \hat{V}(t'')$$

$$= \frac{1}{3!} \int_0^t dt \int_0^t dt' \int_0^t dt'' T[\hat{V}(t) \hat{V}(t') \hat{V}(t'')]. \quad (10.13)$$

Therefore we may write,

$$S(t) = 1 + \int_0^t \hat{V}(t) dt + \frac{1}{2!} \int_0^t dt \int_0^t dt' T[\hat{V}(t) \hat{V}(t')] + \frac{1}{3!} \int_0^t dt \int_0^t dt' \int_0^t dt'' T[\hat{V}(t) \hat{V}(t') \hat{V}(t'')] + \dots$$

$$= T[e^{i\int_0^t \hat{V}(t) dt}]. \quad (10.14)$$

Time ordering is an idempotent operation. This means if one tries to time order an already time-ordered expression, there is no effect on the expression. Mathematically, $T[S(t)] = S(t)$. Now we wish to define a certain quantity known as the Green function. Imagine that a N-particle system at time $t = 0$ is in an eigenstate of the Hamiltonian

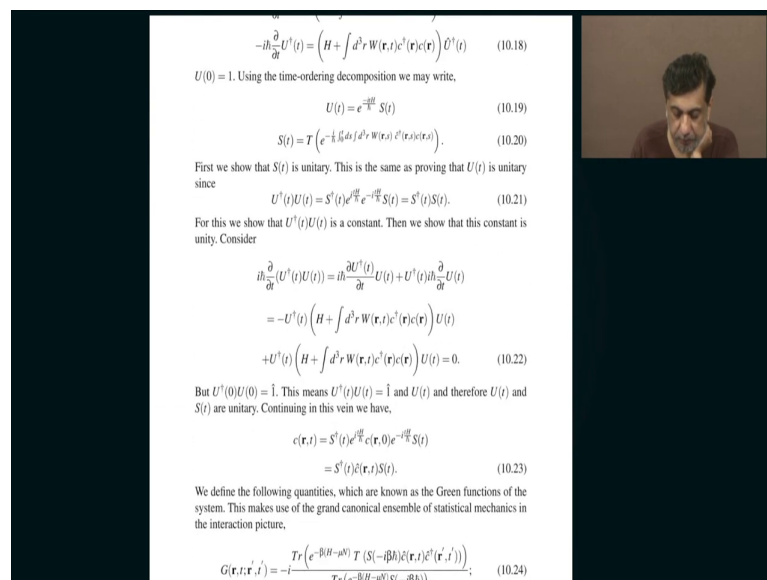
$$H = -\int d^3r c^\dagger(\mathbf{r}) \frac{\hbar^2 \nabla^2}{2m} c(\mathbf{r}) + \frac{1}{2} \int d^3r \int d^3r' V(|\mathbf{r}-\mathbf{r}'|) c^\dagger(\mathbf{r}) c^\dagger(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}). \quad (10.15)$$

Let us denote this eigenstate as $|I\rangle$. The subscript I denotes the I-th excited state, and $I = 0$ corresponds to the ground state. We now consider the time evolution of operators with respect to the time-independent part of the full hamiltonian,

$$\tilde{c}(\mathbf{r}, t) = e^{iH_0 t} c(\mathbf{r}, 0) e^{-iH_0 t}. \quad (10.16)$$

So, Matsubara is the name of Japanese physicist who studied the idea of finite temperature Green's functions quite extensively.

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$$-i\hbar \frac{\partial}{\partial t} U^I(t) = \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U^I(t) \quad (10.18)$$

$U(0) = 1$. Using the time-ordering decomposition we may write,

$$U(t) = e^{-iHt} S(t) \quad (10.19)$$

$$S(t) = T \left(e^{-i \int_0^t dt' \int d^3r W(\mathbf{r}, t') c^\dagger(\mathbf{r}) c(\mathbf{r})} \right). \quad (10.20)$$

First we show that $S(t)$ is unitary. This is the same as proving that $U(t)$ is unitary since

$$U^\dagger(t) U(t) = S^\dagger(t) e^{iHt} e^{-iHt} S(t) = S^\dagger(t) S(t). \quad (10.21)$$

For this we show that $U^\dagger(t) U(t)$ is a constant. Then we show that this constant is unity. Consider

$$i\hbar \frac{\partial}{\partial t} (U^\dagger(t) U(t)) = i\hbar \frac{\partial U^\dagger(t)}{\partial t} U(t) + U^\dagger(t) i\hbar \frac{\partial U(t)}{\partial t}$$

$$= -U^\dagger(t) \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t)$$

$$+ U^\dagger(t) \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t) = 0. \quad (10.22)$$

But $U^\dagger(0) U(0) = 1$. This means $U^\dagger(t) U(t) = 1$ and $U(t)$ and therefore $U(t)$ and $S(t)$ are unitary. Continuing in this vein we have,

$$c(\mathbf{r}, t) = S^\dagger(t) e^{iH_0 t} c(\mathbf{r}, 0) e^{-iH_0 t} S(t)$$

$$= S^\dagger(t) \tilde{c}(\mathbf{r}, t) S(t). \quad (10.23)$$

We define the following quantities, which are known as the Green functions of the system. This makes use of the grand canonical ensemble of statistical mechanics in the interaction picture,

$$G(\mathbf{r}, t; \mathbf{r}', t') = -i \frac{\text{Tr} \left(e^{-\beta(H_0 + \mu N)} T(S(-\beta\hbar) \tilde{c}(\mathbf{r}, t) \tilde{c}^\dagger(\mathbf{r}', t')) \right)}{\text{Tr} \left(e^{-\beta(H_0 + \mu N)} S(-\beta\hbar) \right)}; \quad (10.24)$$

So, you see the idea is that you want to be able to write down, you see remember that I had a I had defined to you what it means to evolve the creation operator or the annihilation operator with respect to time.

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their lifetime. We consider this concept both for systems in thermodynamic equilibrium and for systems out of equilibrium.

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$$U(s) = e^{iH_0 s} e^{-V} \quad (10.1)$$

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If $H_0 V = V H_0$, then we can trivially factorize this as,

$$U(s) = e^{iH_0 s} e^{-V} \quad (10.2)$$

In general, this is not true. However, for practical applications we need such a factorization. Thus we write

$$U(s) = e^{iH_0 s} S(s), \quad (10.3)$$

where

So, if it you see if I had this sort of time evolution, normally in the case of operators that conserve the number of particles, this is very straightforward. It would simply be given by $e^{i t H}$ by H bar $c r 0$ $e^{-i t H}$ by H bar, I mean there is nothing great about this. But, then you see here in this particular case, where c does not conserve the number of particles.

So, I have to reinterpret this H properly, because now this H refers to systems with a different number of particles. So, now, a c of r comma t would then become c of H n minus 1 by H bar c of $r 0$ $e^{-i t H}$ $n 5$. So, you see you have to act this on a state containing n number of particles then you annihilate a particle. So, the first you evolve that state from time t equal to 0 to time t equal to t using the Hamiltonian containing the original number of particles which is n .

And, then you annihilate a particle and then you reduce once you annihilate a particle you reduce the number of particles from n to n minus 1 . Having done that, now whatever operator you act on subsequently is necessarily going to be an operator that is consistent with the new number of particles; that is the new reduced number of particles is now n minus 1 , earlier it was n because I have annihilated its n minus 1 .

So, this is the only caveat you have to keep in mind ok, otherwise it would be the same; it is just that you are you have reduced the number of particles by 1.

So, I want to make practical progress in evaluating these Green's functions. So, to do that I first realized that there will be in most situations of interest the Hamiltonian is not going to be exactly diagonalizable. In other words, I will not know the exact eigenstates and exact eigenvalues. So, if I do a I mean practically you know in principle of course, we can always assume that you can give it some names and proceed.

You can say eigen let the eigenvalues be E_n and we can proceed that way, but practically is speaking it is not possible to know those eigenstates and eigenvalues exactly. So, this particular technique actually enables you to not only define the Green's functions at finite temperature, it also allows you to develop a systematic perturbative technique to explicitly evaluate those Green's functions in situations where your Hamiltonian is not exactly diagonalizable.

So, in order to achieve this what we are going to do is we are going to first start with this assumption that this Hamiltonian even though it is not exactly diagonalizable, we can always split it up into two parts; one part is exactly diagonalizable which is called H_0 and the other part is not. So, that is called a perturbation. So, perturbation does not mean necessarily it is small, I mean the English word perturbation suggests you know a small disturbance.

But, that smallness is not a priori obvious, that we simply separate out a Hamiltonian to two parts. One part we know how to handle, the other part we do not know and we optimistically call that other part perturbation, but whether it deserves that name or not now is determined by subsequent calculations. So, we have to then go ahead and perform certain calculations, estimate its effect, the estimate the effect of the term that we have called perturbation and see if that indeed qualifies to be called that ok.

So, that is the reason why it is very important that we develop a technique which enables us to estimate the effects of this extra term that we are having difficulty in handling ok. So, how do we do that? So, first of all I am going to define an operator which resembles an evolution operator which is called this ok.

So, now, clearly if H_0 and V commute, then it would not be interesting because then H_0 plus V would also be diagonalizable in some sense. So, the interesting situations will be when H_0 and V do not commute, that is the typical situation where H_0 plus V , the eigenstates and eigenvalues of H_0 plus V cannot be determined easily ok.

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If $H_0 V = V H_0$, then we can trivially factorize this as,

$$U(s) = e^{sH_0} e^{sV}, \quad (10.2)$$

In general, this is not true. However, for practical applications we need such a factorization. Thus we write

$$U(s) = e^{sH_0} S(s), \quad (10.3)$$

where

$$S(s) = e^{-sH_0} e^{s(H_0+V)} e^{sH_0} \quad (S(0) = 1) \quad (10.4)$$

We want to express $S(s)$ in some simple way in terms of V . To this end, let us examine some of its properties. In particular let us compute,

$$\begin{aligned} \frac{dS(s)}{ds} &= -H_0 e^{-sH_0} e^{s(H_0+V)} + e^{-sH_0} (H_0+V) e^{s(H_0+V)} \\ &= -H_0 e^{-sH_0} e^{s(H_0+V)} + e^{-sH_0} H_0 e^{s(H_0+V)} + e^{-sH_0} V e^{s(H_0+V)} = e^{-sH_0} V e^{s(H_0+V)}. \end{aligned} \quad (10.5)$$

Define

$$\hat{V}(s) = e^{-sH_0} V e^{sH_0}, \quad (10.6)$$

Therefore,

$$\frac{dS(s)}{ds} = \hat{V}(s) S(s). \quad (10.7)$$

If $[H_0, V] = 0$, then $\hat{V}(s) = V$ and the solution would simply be,

$$S(s) = e^{sV} = e^{\int_0^s V dt}. \quad (10.8)$$

Since trivially, $s = \int_0^s dt$. In general, $S(s)$ is not this simple, hence the solution is symbolically denoted as,

$$S(s) = T \left[e^{\int_0^s \hat{V}(t) dt} \right]. \quad (10.9)$$

The meaning of the symbol $T[\dots]$ will be made clear soon. It may be regarded as a symbolic way of writing the iterative solution to Eq. (10.7). The solution to Eq. (10.7) can be generated as follows,

So, in that case we may still be able to write this U of s in the following way. So, I am going to write U of s as e^{sH_0} times some other unitary operator; well some other at this stage s is can be complex so, I do not know what it is. But, later on we will make s as imaginary and becomes unitary, but whatever it is there should be an s , capital S operator which depends on this parameter small s .

And so, the capital S is trivially equal to this ok. So, now, what I want to do is I want to be able to so, this is a little bit of I mean this is not particularly useful to write it this way. Means, it is not very instructive because you see there is a V in the exponent and it is supposed to be perturbative, it means supposed to be a perturbation. So, what I anticipate is that this s which is a function of this parameter small s should be expressible as a series in powers of this perturbation; because it is only then that this sort of a method has some practical utility.

So, if you very formally symbolically write it this way this is a trivial tautology it is by definition this, but then it is not particularly useful to write it like this. So, the question is how would you now make sense out of this s operator as how would you write S of s in powers of this term, that we are optimistically called a perturbation. So, the way to do that is you first differentiate S with respect to s.

So, when you do that after you perform a series of algebraic maneuvers you will end up with this expression. So, this expression basically tells you that you can always rewrite the rate of change of S with respect to s as a differential equation, where the differential equation is basically involves a pre-factor which is also a function of s ok. So, the idea is that you see S of 0 is clearly what? So, if you s if by definition if you put s is equal to 0, this small s is equal to 0, S of 0 is going to be 1 by definition.

So that means, we should be able to iterate this. So, the idea is that you know if I just solve this integral equation S of s; so, what is this going to be? This is going to be something like 1 plus integral s so, V tau S of tau d tau. So, this is an exact integral form of this taking into account the initial value also. So, the initial value says if you put small s equals 0 its 1 and if I take d by ds on both sides, I get back this.

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$\frac{dS(s)}{ds} = \hat{V}(s)S(s),$ (10.7)

If $[H_0, V] = 0$, then $\hat{V}(s) = V$ and the solution would simply be,

$S(s) = e^{sV} \equiv e^{H_0 \ln s} V.$ (10.8) $S(s) = 1^s$

Since trivially, $s = \int_0^s dt$. In general, $S(s)$ is not this simple, hence the solution is symbolically denoted as,


$S(s) = T[e^{s \int_0^s \hat{V}(t) dt}]$ (10.9) $S(s) \sim 1^s$

The meaning of the symbol $T[\dots]$ will be made clear soon. It may be regarded as a symbolic way of writing the iterative solution to Eq. (10.7). The solution to Eq. (10.7) can be generated as follows,

$$S(s) = 1 + \int_0^s \hat{V}(t) dt + \int_0^s dt \int_0^t \hat{V}(t) \hat{V}(t') dt' + \dots$$

(10.10)

Now we wish to express all of this in a compact form. For this we introduce the notion of time ordering, which involves the use of Heaviside's unit step function.



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But first let us examine the following identity obtained by simply interchanging t and t' .

$$\int_0^s dt \int_0^t dt' \theta(t-t') \hat{V}(t) \hat{V}(t') = \int_0^s dt' \int_0^t dt \theta(t'-t) \hat{V}(t') \hat{V}(t)$$

(10.11)

Here, $\theta(s)$ is Heaviside's step function. If $A = B$, then $A = \frac{1}{2}(A+B)$, hence we may add these two equal quantities and then take half the resultant

Now, all I do is I keep I iterating this I assume that initially the approximate answer is 1. So, then I substitute this back, the next approximate answer would be. So, you just iterate $1 + s \int_0^t \tau \dots$ plus etcetera etcetera. So, now, this so, this is the series that you will get if you iterate ok. So, if you iterate you will get this series and at this series is symbolically written like this ok.

So, if this is called a time ordering symbol ok. So, the time ordering symbol means that what it says is that basically you first pretend that you can go ahead and expand this exponential in powers of this V hat. So that means, you just expand the exponential, you will get all kinds of factorial $1/n$ factorial will appear in the denominator.

But, then notice that that is prominently absent here. So, there is no $1/n$ factorial in the exact answer when you iterate this integral equation. But, then inside this exponential if you expand the exponential that is going to be $1/n$ factorial. So, the idea of this time ordering is that it kind of it forces the. So, basically what time ordering means formally is that if you have $A(t) B(t')$ ok.

So, it basically it is same as $A(t) B(t')$, if t is greater than t' and it is equal to $B(t) A(t')$ if t' is greater than t . So, that is what time ordering means in this context ok. So, the idea is that so, if you use this definition you can actually I mean; so, this makes perfect sense. You can convince yourself that so, this you see this sort of resembles the expansion of an exponential. So, what is missing is basically; firstly, it is exactly it is not exactly that because you see in if it were truly expansion in exponent, then all the upper limits should be s , but in this case it is not s .

So, the it goes from 0 to t' , then there is an it is an there is some nesting here, it is not all s . So, that is one difference. The other difference is the n factorial is missing. So, you will see that you can actually represent this summation, where the upper limits are all nested in this way and n factorial is missing by pretending its first and exponential and then you insert this time ordering symbol ok.

So, the point is that I mean it makes the time ordering symbol is very convenient because, it prevents you from dragging this series all over the place all the time. So that means, it is like an enormous baggage that you have to keep dragging all over the place.

So, when you do calculations, you are typically have this is called by the way it is called S matrix.

Firstly, it is an operator so, it is every operators though can be thought of as a matrix. So, it is called the S matrix. So, this S matrix is said by definition this series, but then you know lugging this series around all the time is not convenient. So, it is nice to represent this in terms of some compact expression like this. So, if you express it in terms of something more compact like this, then you can carry this along everywhere without much trouble.

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$$= \frac{1}{2} \int_0^t dt \int_0^t dt' [\theta(t-t') \hat{V}(t) \hat{V}(t') + \theta(t'-t) \hat{V}(t') \hat{V}(t)]$$

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Time ordering is an idempotent operation. This means if one tries to time order an already time-ordered expression, there is no effect on the expression. Mathematically, $T[S(t)] = S(t)$. Now we wish to define a certain quantity known as the Green function. Imagine that a N-particle system at time $t = 0$ is in an eigenstate of the Hamiltonian

$$H = -\int d^3r c^\dagger(\mathbf{r}) \frac{\hbar^2 \nabla^2}{2m} c(\mathbf{r}) + \frac{1}{2} \int d^3r \int d^3r' V(|\mathbf{r}-\mathbf{r}'|) c^\dagger(\mathbf{r}) c^\dagger(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}). \quad (10.15)$$

Let us denote this eigenstate as $|l\rangle$. The subscript l denotes the l -th excited state, and $l = 0$ corresponds to the ground state. We now consider the time evolution of operators with respect to the time-independent part of the full Hamiltonian,

$$\tilde{c}(\mathbf{r}, t) = e^{iH_0 t} c(\mathbf{r}, 0) e^{-iH_0 t}. \quad (10.16)$$

So, that is the reason why we write it in this compact way ok. So, that gives you an introduction a flavor to something called the S matrix. So, now, let us go ahead and see how the S matrix looks like if the perturbation in question is something that we know exists, but we have been scared of dealing with till now. And, that perturbation is basically the interaction between particles. So, remember that till now we are not given too much importance to this important concept.

I mean well, it is likely to be important because you see after all electrons are charged particles and you know that electromagnetic force is long ranged. So, there is every reason to believe that it is a bad idea to ignore the inter interaction between electrically

charged particles like an electrons. But, because of the difficulty in handling that till now we have been conveniently ignoring that.

But, now the question is we are now that we have we seem to have a handle on this S matrix, we should be able to we should not hesitate in introducing this as a perturbation and see if it leads us to some something interesting ok.

So, now, let me get back to this original issue, namely you see if I have this time evolution of the annihilation operator. So, remember that if you write H also in the second quantized representation second quantized form is not necessary to constantly remind yourself that there are the n particles the n minus the.

So, this thing already keeps track of that. So, that is the reason why I have not put a subscript in n minus 1 and all that. So, so it leads you to familiar territory. So, this is a familiar way of defining a time evolution of operators in the Eisenberg picture. So, now, the question is see the point is that because I remember that I was able to write. So, this is what I wanted to write in terms of the S matrix.

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10.1 Matsubara Green Functions

In this section, we define the finite temperature, or Matsubara Green function, of a system of particles for systems that statistical mechanics would classify as grand canonical. This means that we imagine the system exchanging energy and particles with a reservoir where only the average energy and average number of particles are fixed. We imagine the system to be described by a Hamiltonian that may be written in the form $H = H_0 + V$, where H_0 is that part of the Hamiltonian which may be handled exactly. The remaining is denoted by V . Consider the following operator,

$$U(s) = e^{s(H_0 + V)} \quad (10.1)$$

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If $H_0 V = V H_0$, then we can trivially factorize this as,

$$U(s) = e^{sH_0} e^{sV} \quad (10.2)$$

In general, this is not true. However, for practical applications we need such a factorization. Thus we write

$$U(s) = e^{sH_0} S(s), \quad (10.3)$$

where

$$S(s) = e^{-sH_0} e^{s(H_0 + V)} \quad (10.4)$$

We want to express $S(s)$ in some simple way in terms of V . To this end, let us examine some of its properties. In particular let us compute,

So, we see so, this has some so, if I choose S as i T by h bar, this is my you know inverse of the evolution operator as it were. So, that has this form in terms of the S matrix.

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ally, $T[S(t)] = S(t)$. Now we wish to define a certain quantity known as the Green function. Imagine that a N -particle system at time $t = 0$ is in an eigenstate of the Hamiltonian

$$H = - \int d^3r \, c^\dagger(\mathbf{r}) \frac{\hbar^2 \nabla^2}{2m} c(\mathbf{r}) + \frac{1}{2} \int d^3r \int d^3r' V(|\mathbf{r} - \mathbf{r}'|) c^\dagger(\mathbf{r}) c^\dagger(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}). \quad (10.15)$$

Let us denote this eigenstate as $|I\rangle$. The subscript I denotes the I -th excited state, and $I = 0$ corresponds to the ground state. We now consider the time evolution of operators with respect to the time-independent part of the full Hamiltonian,

$$\tilde{c}(\mathbf{r}, t) = e^{iH_0 t} c(\mathbf{r}, 0) e^{-iH_0 t}. \quad (10.16)$$

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In the presence of the external time-dependent potential, we have to define the time evolution differently. We formally introduce a time-dependent external potential that is also defined in imaginary time.

$$c(\mathbf{r}, t) = U^\dagger(t) c(\mathbf{r}, 0) U(t) \quad (10.17)$$

$$i\hbar \frac{\partial}{\partial t} U(t) = \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t) \quad (10.18)$$

$$-i\hbar \frac{\partial}{\partial t} U^\dagger(t) = \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U^\dagger(t) \quad (10.18)$$

$U(0) = 1$. Using the time-ordering decomposition we may write,

$$U(t) = e^{-i\int_0^t U(t') dt'} \quad (10.19)$$

$$S(t) = T \left(e^{-i \int_0^t \int d^3x W(x, t') c^\dagger(x, t') c(x, t')} \right). \quad (10.20)$$

So, now, I want to be able to write this and this in terms of the S matrix ok. So, now, question is how would you do that? So, the first of all you write down the time evolution of the S matrix ok. So, first of all you write it in this way and also I am going to assume that I introduce some sources. So, for reasons I will tell you later, it is not part of this Hamiltonian, but the effective Hamiltonian is going to be this plus this source ok.

So, I am going to assume that it has a one more term which I did not initially tell you ok. So, there is this term also part of the so, there was this H. So, what does H consists of? H consists of something I can very easily manage just the kinetic energy of fermions which is already diagonal. But, also it includes something very nasty which is the Coulomb interaction between fermions.

So, that is what makes this problem very hard, but then there is also another term which is basically the source term. So, which is something like a you know maybe an electric field applied at some point. So, or basically this is some electric potential. So, that gives you some extra energy because of that, but this is going to be necessary because later on now is it is also used as a mathematical device.

So, later on I will be able to differentiate with respect to W and obtain some interesting results. So, even though later on maybe o W can actually be set to 0, if there is no such

field involved. Just for the purposes of being able to do some clever mathematical manipulation, I am entitled to introduce this W and later on get rid of it, if indeed there is no such external field. So, now, the question is suppose there is such an external field and clearly I should be able to write down the evolution of my unitary operator in this way ok.

So, now this unitary operator from my S matrix idea is clearly this and this is my S matrix ok. So, ok at this stage this S matrix is only with respect to W , because I have I have introduced I have not split this H into H_0 and V yet. So, this H includes the H_0 and it includes this is H_0 and this is V , it includes both.

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$-i\hbar \frac{\partial}{\partial t} U(t) = \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t)$ (10.18)

$U(0) = 1$. Using the time-ordering decomposition we may write,

$$U(t) = e^{-iHt} S(t)$$
 (10.19)

$S(t) = T \left(e^{-i \int_0^t d^3r W(\mathbf{r}, \tau) c^\dagger(\mathbf{r}, \tau) c(\mathbf{r}, \tau)} \right)$ (10.20)

First we show that $S(t)$ is unitary. This is the same as proving that $U(t)$ is unitary since

$$U^\dagger(t) U(t) = S^\dagger(t) e^{iHt} e^{-iHt} S(t) = S^\dagger(t) S(t)$$
 (10.21)

For this we show that $U^\dagger(t) U(t)$ is a constant. Then we show that this constant is unity. Consider

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} (U^\dagger(t) U(t)) &= i\hbar \frac{\partial U^\dagger(t)}{\partial t} U(t) + U^\dagger(t) i\hbar \frac{\partial U(t)}{\partial t} \\ &= -U^\dagger(t) \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t) \\ &\quad + U^\dagger(t) \left(H + \int d^3r W(\mathbf{r}, t) c^\dagger(\mathbf{r}) c(\mathbf{r}) \right) U(t) = 0. \end{aligned}$$
 (10.22)

But $U^\dagger(0) U(0) = 1$. This means $U^\dagger(t) U(t) = 1$ and $U(t)$ and therefore $U(t)$ and $S(t)$ are unitary. Continuing in this vein we have,

$$\begin{aligned} c(\mathbf{r}, t) &= S^\dagger(t) e^{iHt} c(\mathbf{r}, 0) e^{-iHt} S(t) \\ &= S^\dagger(t) c(\mathbf{r}, t) S(t). \end{aligned}$$
 (10.23)

We define the following quantities, which are known as the Green functions of the system. This makes use of the grand canonical ensemble of statistical mechanics in the interaction picture,

$$G(\mathbf{r}, t; \mathbf{r}', t') = -i \frac{\text{Tr} \left(e^{-\beta(H - \mu N)} T(S(-\beta\hbar) c(\mathbf{r}, t) c^\dagger(\mathbf{r}', t')) \right)}{\text{Tr} \left(e^{-\beta(H - \mu N)} S(-\beta\hbar) \right)}$$
 (10.24)

So, at this stage I have not split it up, but you will see why I have not split it up at this stage because, I am going to do something very clever. So, this S matrix is with respect to it is like it is as if I am treating this external source as a perturbation ok. So, the point is that well this is its clearly unitary, I mean I am making a big fuss out of something very simple. So, U and S are clearly unitary.

So, the point is that the time evolution of the annihilation operator is now going to be expressible in terms of the time evolution without the source. So, this is without the source. So, the source is W and this is the S matrix of the source of the source.

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$$c(\mathbf{r},t) = S^\dagger(t) e^{i\mathcal{H}_0 t} c(\mathbf{r},0) e^{-i\mathcal{H}_0 t} S(t) = S^\dagger(t) \tilde{c}(\mathbf{r},t) S(t) \quad (10.23)$$

We define the following quantities, which are known as the Green functions of the system. This makes use of the grand canonical ensemble of statistical mechanics in the interaction picture,

$$G(\mathbf{r},t; \mathbf{r}',t') = -i \frac{\text{Tr} \left(e^{-\beta(H-\mu N)} T \left(S(-\beta\hbar) \tilde{c}(\mathbf{r},t) \tilde{c}^\dagger(\mathbf{r}',t') \right) \right)}{\text{Tr} \left(e^{-\beta(H-\mu N)} S(-\beta\hbar) \right)} \quad (10.24)$$

$$G(\mathbf{r},t; \mathbf{r}',t') = -i \frac{\sum_{N=0}^{\infty} \langle I, N | e^{-\beta(H-\mu N)} T \left(S(-\beta\hbar) \tilde{c}(\mathbf{r},t) \tilde{c}^\dagger(\mathbf{r}',t') \right) | I, N \rangle}{\sum_{N=0}^{\infty} e^{-\beta(E_{I,N} - \mu N)} \langle I, N | S(-\beta\hbar) | I, N \rangle} \quad (10.25)$$

Here $\epsilon_{I,N}$ is the energy of the I-th eigenstate of an N-particle system. That is, $H|I,N\rangle = \epsilon_{I,N}|I,N\rangle$ and N is the total number of particles. We show in the next section that the complicated-looking expression in Eq. (10.24) that at present is not properly motivated is actually a simple and intuitive concept. The time-ordering notion in the expression required clarification. We imagine that all times t, t' lie in the interval $[0, -\beta\hbar]$. This means we consider the times to be imaginary. This purely mathematical device enables us to exploit a certain kind of periodicity that occurs only in imaginary time. In order to define time ordering we have to determine that some point in this interval is 'greater' or 'less' than other points. We postulate $-\beta\hbar \geq t, t' \geq 0$. That is, the times t, t' etc, go from the 'smallest' possible value 0 to the largest possible value $-\beta\hbar$ along the vertical imaginary axis. For

So, you have two things. So, now, I am going to convince you that the appropriate way of defining a Green's function of this system. So, what is the system? You have a system of fermions with kinetic energy with mutual Coulomb interactions and a couple to an external source called W.

So, if that is the case then the Green's function of this system so, this ok. So, I am I am jumping many steps here ok. So, I think this is not the logical way of doing this. So, let me let me some spend time explaining this so, it is kind of very abrupt. So, let me explain why I did this. So, the idea is that I want to be able to define something called the whole Green's function and the particle Green's function ok.

So, in order to do that, I have to make sense out of this sort of an average. But, remember what I told you about averages when the system is in contact with an external surroundings where it is exchanging energy with that surroundings. So, in that case, this is not going to be the simple averaging that you are normally familiar with. It is going to involve you know multiplying by the Boltzmann weight and summing over all the eigenstates.

But, then there is another issue here that which also something I should have mentioned earlier. So, you see in addition to exchanging energy with surroundings, you can also

have a situation where particles can actually come in and out of the system. So, you might be thinking is not that an unusual occurrence, that may very well be, but you see what happens in many cases that we usually use this grand canonical ensemble approach as a convenient way of studying a statistical mechanical systems; even when the number of particles is fixed.

See, usually it is the energy of the system is anyway usually not fixed. So, that is the reason why most of the time the system that you consider is of the canonical variety. Remember, the three types of ensembles, the there is the micro canonical ensemble where the energy of the system is fixed, the number of particles is fixed, volume is fixed. So, that is the micro canonical ensemble and that is very rarely encountered in practice.

Because, in practice the system that you are considering usually exchanges energy with surroundings, but then a number of particles can still be fixed. But, what happens is that you see the reason why we study grand canonical ensemble is that if you allow for the possibility that the number of particles can also fluctuate and then there is it can exchange in a particles with the surroundings and energy also with the surroundings and then come to an equilibrium.

Then, you see not only is the temperature of the system and surroundings the same, there is something else that becomes the same between the system and the surrounding and that is called the chemical potential. And, you might be wondering why am I allowing the number of particles in the system to fluctuate, is not that very unusual. So firstly, it need not be unusual for example, in some situations you will find that the system that you are actually interested in is part of a larger system.

And, there is that that boundary between the system that you are considering and the surroundings may actually be an imaginary one. The one that you have imagined to be, there may be no actual physical boundary at all that you have decided that you have arbitrarily in your mind drawn some boundary and said this is my system and that is my surroundings. So, in which case clearly there is going to be exchange of both particles and energy.

So, the second reason is that even if you assume that there is a physical boundary that prevents particles from entering or exiting, it is still convenient to first study a situation where you allow particles to get exchange with the surroundings and come to an equilibrium. Because, see in the thermodynamic limit the problem of studying a system with fixed number of particles is made simpler by studying the grand canonical version. That means, you first study a system where not only energy, but the number of particles also fluctuates.

So, that actually is mathematically much simpler and when you study that the results that you get are in fact, in the thermodynamic limit are equivalent to the research that you would have gotten, had you studied the canonical system where the number of particles strictly conserved. So, you see the difference between strictly conserved and conserved on an average, as it is in the grand canonical ensemble; these two approaches are nearly the same in the thermodynamic limits.

So, because the fluctuations in the number of particles is in goes inversely at the square root of the size of the system. So, in situations where the size of the system is very large, you can sort of safely ignore these differences. So, that is the reason why we actually allow for fluctuation in the number of particles. So, when you do that, you see you have to now force yourself to introduce a chemical potential. So, not only your interest so, remember that beta is $1/kT$ and I also told you that I do not like k there.

So, I put $1/T$; so, in my notes it is all $1/T$, I am just putting kT because you know psychologically it is nice to think of kT as your T I mean, it is nice to remind yourself what I am talking about; T is temperature in energy units whereas, here T is temperature in kelvin. So, here T is temperature in energy units. But, whatever it is beta is $1/T$ temperature in energy units and μ is your chemical potential ok.

And, chemical potential is basically the energy required to remove one particle from the system or add or remove one particles in the system. So, bottom line is that if you want to find the average of a system or average of any property of the system where that system is not only exchanging energy with surroundings, but it is also exchanging the

number of particles. So, what Boltzmann would have you do is that you are now compelled to multiply by this weight, namely it is.

So, the trace remember is just the diagonal expectation value. So, if you take diagonal expectation value formally, it is just going to be this. So, these are the eigenvalues. So, I have just taken the diagonal expectation values and then I have multiplied it this way. So, now, you might be wondering what is all this, you see this you will see is that because yeah; so, this requires some effort to explain. The point is that the Hamiltonian, it commutes with the number of particles.

So, you see that Hamiltonian commutes with a number of particles, the density commutes with the number of particles, but the annihilation operator clearly does not. So in fact, and not only that what is even more important is the annihilation operator does not even commute with the total number of particles, let alone the Hamiltonian ok. I invite you to actually insert this remember what this S was, what was S ? S was this. So, if you insert this back into this formula and you work this out, you will see that you get back.

So, this in effect is only this ok. So, you might be thinking why have I written it like this. In fact, this whole thing is nothing, but c of r , t c dagger of r dash t dash, that is what it is. But, then if I split this up into c hat and S and S dagger, you will find that because of the unitary nature of this operator, most parts of this will cancel out except this part which will survive ok, because this part of the S operator will not commute with the annihilation operator.

So, I understand that the motivation for this is actually not very well given in these notes ok, because you know it is kind of very tedious to write all this very explicitly. So, perhaps what we can do is that we can have some kind of you know worked out assignment where I explain how to go from my original definition of Green's function and reach here. So, that this has to be well motivated. So, if you accept that that is a reasonable way of defining the Green's function of the system.

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tion in the expression required clarification. We imagine that all times t, t' lie in the interval $[0, -i\beta\hbar]$. This means we consider the times to be imaginary. This purely mathematical device enables us to exploit a certain kind of periodicity that occurs only in imaginary time. In order to define time ordering we have to determine that some point in this interval is 'greater' or 'less' than other points. We postulate $-i\beta\hbar \geq t \geq t' \geq 0$. That is, the times t, t' etc. go from the 'smallest' possible value 0 to the largest possible value $-i\beta\hbar$ along the vertical imaginary axis. For particles with statistics ' σ ' ($\sigma = +1$ for bosons and $\sigma = -1$ for fermions), we may define the following time-ordering prescriptions:

$$T[c(\mathbf{r}, t)c^\dagger(\mathbf{r}', t')] = c(\mathbf{r}, t)c^\dagger(\mathbf{r}', t'); t > t' \quad (10.26)$$

$$T[c(\mathbf{r}, t)c^\dagger(\mathbf{r}', t')] = \sigma c^\dagger(\mathbf{r}', t')c(\mathbf{r}, t); t < t' \quad (10.27)$$

Here $t > t'$ means t is closer to $-i\beta\hbar$ than t' and both lie on the imaginary axis between the points 0 and $-i\beta\hbar$.

Some Simple Cases. Before studying the difficult problem of mutually interacting particles in an external field, which is what evaluation of the Green function in Eq. (10.24) is meant to do, we first focus on the simple case of non-interacting particles ($V = 0$) with no external field ($W = 0$). In this case the Green function is simply,


$$G_0(\mathbf{r}, t; \mathbf{r}', t') = -i \frac{[T e^{-\beta(H_0 - \mu N)} T c(\mathbf{r}, t) c^\dagger(\mathbf{r}', t')]}{T e^{-\beta(H_0 - \mu N)}} \quad (10.28)$$

$$c(\mathbf{r}, t) = e^{iH_0 t} c(\mathbf{r}, 0) e^{-iH_0 t} \quad (10.29)$$

$$H_0 = -\int d^3r c^\dagger(\mathbf{r}) \frac{\hbar^2 \nabla^2}{2m} c(\mathbf{r}). \quad (10.30)$$

In order to facilitate progress, we use the momentum state representation (the spatial Fourier transform)

$$c(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}} \quad (10.31)$$



Then, you can go ahead and ask yourself what this Green's function looks like in the case of some you know when you specialize to where some very simple cases, some simple situations. So, one of the simplest situation is when you turn off everything, when you turn off the Coulomb interaction between particles you turn off the source. So, in that case you see it is very clear what; that means, so it is basically just this.

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We make a distinction between real space objects, where the position variable is in the parenthesis, and momentum space objects, where the momentum labels are in the subscripts. In three dimensions,

$$\sum_{\mathbf{k}} [\dots] = \frac{V}{(2\pi)^3} \int d^3k [\dots] \quad (10.32)$$

where V is the volume of the system. Firstly, since $[c(\mathbf{r}), c^\dagger(\mathbf{r}')]_{\sigma} = 0$ and $[c(\mathbf{r}), c^\dagger(\mathbf{r}')]_{\sigma} = \delta(\mathbf{r} - \mathbf{r}')$, we must have $[c_{\mathbf{k}}, c_{\mathbf{k}'}]_{\sigma} = 0$ and $[c_{\mathbf{k}}, c_{\mathbf{k}'}]_{\sigma} = \delta_{\mathbf{k}, \mathbf{k}'}$. If we substitute Eq. (10.31) into Eq. (10.30) we get

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger(\mathbf{k}) c(\mathbf{k}), \quad (10.33)$$

where $\epsilon_{\mathbf{k}} \equiv \frac{\hbar^2 k^2}{2m}$. Also, the time-evolved annihilation operators are


$$c(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\epsilon_{\mathbf{k}} t} c_{\mathbf{k}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}} e^{-i\epsilon_{\mathbf{k}} t}. \quad (10.34)$$

Let us first assume that in Eq. (10.28) $t > t'$, this means t' is closer to $-i\beta\hbar$ than t and both lie between 0 and $-i\beta\hbar$ on the negative imaginary axis. Further, we set $Z = T e^{-\beta(H_0 - \mu N)}$.

$$G_0^>(\mathbf{r}, t; \mathbf{r}', t') = -\sigma \frac{1}{Z} T e^{-\beta(H_0 - \mu N)} c^\dagger(\mathbf{r}', t') c(\mathbf{r}, t) \quad (10.35)$$

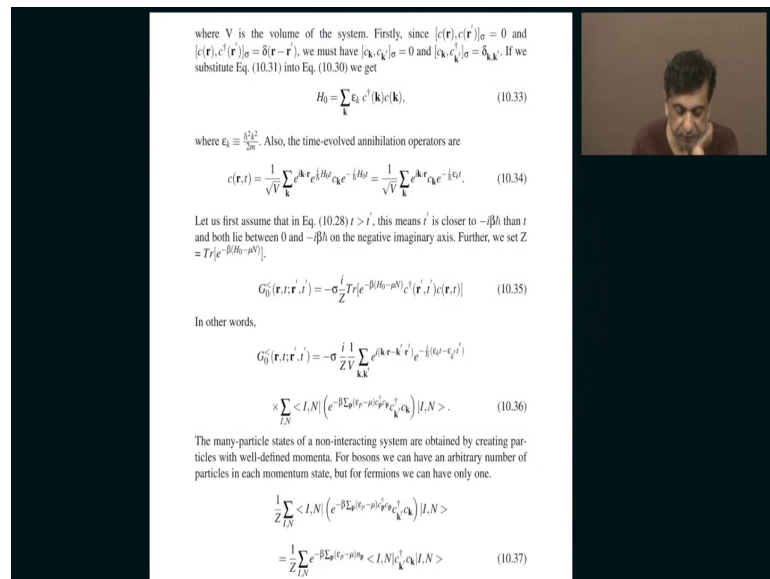
In other words,

$$G_0^>(\mathbf{r}, t; \mathbf{r}', t') = -\sigma \frac{1}{ZV} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{r} - \mathbf{k}'\cdot\mathbf{r}') - i(\epsilon_{\mathbf{k}} t - \epsilon_{\mathbf{k}'} t')} \times \sum_{\{N\}} \langle N | (e^{-\beta(H_0 - \mu N)} c_{\mathbf{k}'}^\dagger c_{\mathbf{k}}) | N \rangle. \quad (10.36)$$



So, you can now explicitly work this out. So, the idea is that you want to be able to work this out in practice. So, so, to work this out explicitly so, what I have done is that I have decided to because, you see if there is no Coulomb interaction, there is no so that means, just free particles. So, free particles means momentum is a good quantum number. So, I might as well go and do the momentum representation, where $\hbar k$ is the momentum.

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where V is the volume of the system. Firstly, since $[c(\mathbf{r}), c(\mathbf{r}')^\dagger]_0 = 0$ and $[c(\mathbf{r}), c^\dagger(\mathbf{r}')]_0 = \delta(\mathbf{r} - \mathbf{r}')$, we must have $\langle c_{\mathbf{k}}, c_{\mathbf{k}'} \rangle_0 = 0$ and $\langle c_{\mathbf{k}}, c_{\mathbf{k}'}^\dagger \rangle_0 = \delta_{\mathbf{k}, \mathbf{k}'}$. If we substitute Eq. (10.31) into Eq. (10.30) we get

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \quad (10.33)$$

where $\epsilon_{\mathbf{k}} \equiv \frac{\hbar^2 k^2}{2m}$. Also, the time-evolved annihilation operators are

$$c(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\epsilon_{\mathbf{k}} t} c_{\mathbf{k}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}} e^{-i\epsilon_{\mathbf{k}} t} \quad (10.34)$$

Let us first assume that in Eq. (10.28) $t > t'$, this means t' is closer to $-\beta\hbar$ than t and both lie between 0 and $-\beta\hbar$ on the negative imaginary axis. Further, we set $Z = \text{Tr} [e^{-\beta(\hat{H}_0 - \mu N)}]$.

$$G_0^$\langle \mathbf{r}, t; \mathbf{r}', t' \rangle = -\sigma \frac{1}{Z} \text{Tr} [e^{-\beta(\hat{H}_0 - \mu N)} c^\dagger(\mathbf{r}', t') c(\mathbf{r}, t)] \quad (10.35)$$$

In other words,

$$G_0^$\langle \mathbf{r}, t; \mathbf{r}', t' \rangle = -\sigma \frac{1}{ZV} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{r} - \mathbf{k}'\cdot\mathbf{r}')} e^{-i(\epsilon_{\mathbf{k}} t - \epsilon_{\mathbf{k}'} t')} \quad (10.36)$$$

$$\times \sum_{I, N} \langle I, N | (e^{-\beta \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}}}) | I, N \rangle$$

The many-particle states of a non-interacting system are obtained by creating particles with well-defined momenta. For bosons we can have an arbitrary number of particles in each momentum state, but for fermions we can have only one.

$$\frac{1}{Z} \sum_{I, N} \langle I, N | (e^{-\beta \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}}}) | I, N \rangle = \frac{1}{Z} \sum_{I, N} e^{-\beta \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}}} \langle I, N | c_{\mathbf{k}}^\dagger c_{\mathbf{k}} | I, N \rangle \quad (10.37)$$

So, in that case I can very simply rewrite all these Green's functions in terms of the averages of this sort ok. So, I am going to be able to write it this way ok, it is I mean I have to admit that it can be very intimidating for somebody who is been doing this for the first time; because there is a lot of unfamiliar algebra in more. But, that is the reason why these lectures are merely meant as a kind of you know, it is meant to show you the path. Basically, it is meant to indicate in which direction you should proceed in order to learn this subject.

So, it is not a substitute for self-learning, it is not also a substitute for actually doing the assignment. So, and I have to also make sure that I you know assign enough problems to fill all the gaps that are there in these notes ok, that is something I intend doing in the next couple of classes.

So, I am going to actually fill these gaps in the form of assignments. So, which we can then solve explicitly. But, bottom line is that you see because it is a translationally this situation corresponds to a free particle, it is clear that it is going to be extremely convenient to work in momentum space. And, when you do that, you end up with this sort of a Green's function ok.

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The states $c_{\mathbf{k}}|I, N\rangle$ and $c_{\mathbf{k}}^{\dagger}|I, N\rangle$ are orthogonal for $\mathbf{k} \neq \mathbf{k}$ and $n_{\mathbf{k}}|I, N\rangle = N_{\mathbf{k}}|I, N\rangle$. If $\sigma = -1$ (fermions) the above expression becomes

$$\frac{1}{Z} \sum_{I, N} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \langle I, N | c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} | I, N \rangle =$$

$$\delta_{\mathbf{k}, \mathbf{k}'} \frac{\sum_{\{n_{\mathbf{k}}\}=0,1} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \sum_{\{N_{\mathbf{k}}\}=0,1} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} N_{\mathbf{k}}}}{\sum_{\{n_{\mathbf{k}}\}=0,1} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \sum_{\{N_{\mathbf{k}}\}=0,1} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} N_{\mathbf{k}}}} \quad (10.38)$$

If $\sigma = +1$ (bosons) the above expression becomes

$$\frac{1}{Z} \sum_{I, N} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \langle I, N | (c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}) | I, N \rangle =$$

$$\delta_{\mathbf{k}, \mathbf{k}'} \frac{\sum_{\{n_{\mathbf{k}}\}=0,1,2,3,\dots} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \sum_{\{N_{\mathbf{k}}\}=0,1,2,3,\dots} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} N_{\mathbf{k}}}}{\sum_{\{n_{\mathbf{k}}\}=0,1,2,3,\dots} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}} \sum_{\{N_{\mathbf{k}}\}=0,1,2,3,\dots} e^{-\beta \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} N_{\mathbf{k}}}} \quad (10.39)$$

Define the following quantities

$$f_{\mathbf{k}}(\lambda) = \sum_{N=0,1,2,3,\dots} e^{-\lambda N} = \frac{1}{1 - e^{-\lambda}} \quad (10.40)$$


$$f_{\mathbf{k}}(\lambda) = \sum_{N=0,1} e^{-\lambda N} = 1 + e^{-\lambda} \quad (10.41)$$

Then,

$$\frac{d}{d\lambda} \ln[f_{\mathbf{k}}(\lambda)] = \frac{\sum_{N=0,1,2,3,\dots} N e^{-\lambda N}}{\sum_{N=0,1,2,3,\dots} e^{-\lambda N}} = \frac{1}{e^{\lambda} - 1}$$

$$\frac{d}{d\lambda} \ln[f_{\mathbf{k}}(\lambda)] = \frac{\sum_{N=0,1} N e^{-\lambda N}}{\sum_{N=0,1} e^{-\lambda N}} = \frac{1}{e^{\lambda} + 1} \quad (10.42)$$

If we set $\lambda = \beta(\epsilon_{\mathbf{k}} - \mu)$, then we can say



So, the Green's function that you will consider basically inverse the Fermi Dirac and the Bose Einstein sort of distributions.

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Then,

$$\frac{d}{d\lambda} \text{Ln}[f_B(\lambda)] = \frac{\sum_{N=0,1,2,3} N e^{-\lambda N}}{\sum_{N=0,1,2,3} e^{-\lambda N}} = \frac{1}{e^\lambda - 1}$$

$$\frac{d}{d\lambda} \text{Ln}[f_F(\lambda)] = \frac{\sum_{N=0,1,2,3} N e^{-\lambda N}}{\sum_{N=0,1,2,3} e^{-\lambda N}} = \frac{1}{e^\lambda + 1} \quad (10.42)$$

If we set $\lambda = \beta(\epsilon_k - \mu)$, then we can say


$$G_0^<(r, t; r', t') = -\sigma \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\epsilon_k(t-t')} n_{\sigma}(\mathbf{k}), \quad (10.43)$$

where

$$n_{\sigma}(\mathbf{k}) = \frac{1}{e^{\beta(\epsilon_k - \mu)} - \sigma} \quad \begin{matrix} \sigma = -1 \text{ for } \downarrow \\ \sigma = +1 \text{ for } \uparrow \end{matrix} \quad (10.44)$$

Similarly, we can show that when $t > t'$,

$$G_0^>(r, t; r', t') = -\frac{i}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\epsilon_k(t-t')} (1 + \sigma n_{\sigma}(\mathbf{k})). \quad (10.45)$$



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We may now relate these two quantities using a clever observation.

$$G_0^<(r, t; r', t') = -\frac{i}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\epsilon_k t'} e^{-i\epsilon_k t} (1 + \sigma n_{\sigma}(\mathbf{k})) \quad (10.46)$$

Now consider,

$$e^{-\beta\epsilon_k} (1 + \sigma n_{\sigma}(\mathbf{k})) = e^{-\beta\mu} n_{\sigma}(\mathbf{k}). \quad (10.47)$$

Therefore

So, clearly that is what that is. So, if I am talking about the Fermi Dirac distribution and sigma will be minus 1, if its Bose Einstein sigma is plus 1. So, just like your whole end particle Green's function, here also you have whole particle Green's functions and so on so forth.

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We may now relate these two quantities using a clever observation.

$$G_0^<(r, t; r', t') = -\frac{i}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\epsilon_k t'} e^{-i\epsilon_k t} (1 + \sigma n_{\sigma}(\mathbf{k})) \quad (10.46)$$

Now consider,

$$e^{-\beta\epsilon_k} (1 + \sigma n_{\sigma}(\mathbf{k})) = e^{-\beta\mu} n_{\sigma}(\mathbf{k}). \quad (10.47)$$

Therefore,

$$G_0^<(r, t; r', t') = -\frac{i}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\epsilon_k t'} e^{-\beta\mu} n_{\sigma}(\mathbf{k})$$

$$= \sigma e^{-\beta\mu} G_0^<(r, t; 0; r', t'). \quad (10.48)$$

Therefore we have

$$G_0(r, t; r', t') = \sigma e^{-\beta\mu} G_0(r, t; 0; r', t'). \quad (10.49)$$

Here, G_0 is the time-ordered Green function. The above equation is known as the Kubo-Martin-Schwinger (KMS) boundary condition. We may now rewrite the Green function of the noninteracting system as $G_0(r - r', t - t'; 0, 0)$ since we know that it depends only on the differences between the time and position coordinates. A quantity that obeys such a periodicity property may be discrete Fourier transformed. These discrete frequencies are known as Matsubara frequencies. We may write


$$G_0(r - r', t - t'; 0, 0) = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{-\beta\hbar} \sum_{\tau_n} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\mu(t-t')} e^{i\epsilon_k(t-t')} G_0(\mathbf{k}, \tau_n) \quad (10.50)$$

Since G_0 has to obey the KMS boundary condition we must have,

$$e^{i(-\beta\hbar - t')} = \sigma e^{i(0 - t')} \quad (10.51)$$

$$e^{-i\tau_n \beta \hbar} = \sigma. \quad (10.52)$$

Thus $\tau_n = \frac{(2n+1)\pi}{\beta\hbar}$ if $\sigma = -1$ and $\tau_n = \frac{2n\pi}{\beta\hbar}$ if $\sigma = 1$. We make some observations about these Matsubara frequencies,



So, these are these are the traditional whole and particle Green's function. But, the interesting point is that you see one very important feature; so, these are by the way

called Matsubara Green's function. Because, they are Green's functions of a system that is coupled to the environment and its exchanging energy with environment and coming to an equilibrium. So, that is the reason why it is called a Matsubara Green's function.

And, these Matsubara Green's functions have some very interesting and important property and that is that they obey a kind of periodicity in imaginary times; that means, if you assume that the times that you are considering; so, if you analytically continue to a situation where the times are on the imaginary axis ok. In fact, this time ordering that we can see remember that I use this symbol time ordering. So in fact, in this particular example this time ordering as a specific meaning, it is only within in imaginary time.

So, I have to assume that the times are all between 0 and minus $i\beta\hbar$; so, then only this time ordering makes sense. So, $t > t'$ means t is closer to minus $i\beta\hbar$ than t' . So, in other words all my times are here, this is minus $i\beta\hbar$ and 0. So, these are my times. So, if I assume that all my times are imaginary so, you might be thinking why are we doing that, that seems completely bizarre; you might think I have gone crazy.

But, actually it is not because you will see that this mathematical device of working in imaginary time allows for very elegant solutions for these Green's functions which you can then continue back to real time later on. So, in imaginary time the Green's function, the time ordered Green's function along the imaginary axis actually of base this sort of a boundary condition. And, this is called the Kubo Martin Schwinger boundary condition.

So, the idea is that because of this, you can actually show that these Green's functions are expressible in terms of these discrete frequencies. So, because there is periodicity in the time domain, you can see the corresponding frequencies become discrete.

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Since G_0 has to obey the KMS boundary condition we must have,

$$e^{z_0(-\beta\hbar - t')} = \alpha e^{z_0(0 - t')} \quad (10.51)$$


$$e^{-z_0\beta\hbar} = \sigma. \quad (10.52)$$

Thus $z_0 = \frac{i2\pi n}{\beta\hbar}$ if $\sigma = -1$ and $z_0 = \frac{i2\pi n}{\beta\hbar}$ if $\sigma = 1$. We make some observations about these Matsubara frequencies,

$$\frac{1}{-\beta\hbar} \sum_n e^{z_n(t-t')} = \delta_p(t-t'). \quad (10.53)$$

Here $\delta_p(t-t')$ is the periodic delta function. It has the property $\delta_p(-\beta\hbar - t') = \sigma \delta_p(0 - t')$. For any function $f(t)$ defined in the interval $[0, -\beta\hbar]$ and obeying the property, $f(-\beta\hbar) = \sigma f(0)$, we have,

$$\int_0^{-\beta\hbar} \delta_p(t-t') f(t') dt' = f(t). \quad (10.54)$$



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We can similarly define a periodic step function

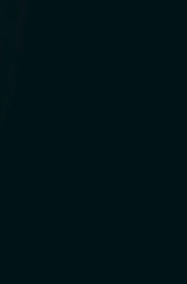
$$\frac{\partial}{\partial t} \theta_p(t-t') = \delta_p(t-t') \quad (10.55)$$

or

$$\theta_p(t-t') = \frac{1}{-\beta\hbar} \sum_n \frac{e^{z_n(t-t')}}{z_n + i\delta} \quad (10.56)$$

From Eq. (10.11) and Eq. (10.12) we find,

$$i\hbar \frac{\partial}{\partial t} G_0^{<|>}(\mathbf{r}, t; \mathbf{r}', t') = -\frac{\hbar^2 \nabla^2}{2m} G_0^{<|>}(\mathbf{r}, t; \mathbf{r}', t'). \quad (10.57)$$



And, the discrete frequencies depend on whether its bosons or fermions. For boson stuff discrete frequency are $2\pi n$ divided by $\beta\hbar$ and; that means, even integer into π by $\beta\hbar$ or if its fermion is odd integer into π by \hbar ok. So, that is the reason why these are basically called bosonic and fermionic Matsubara frequencies alright.

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But we know that

$$G_0(\mathbf{r}, t; \mathbf{r}', t') = \theta_p(t-t') G_0^>(\mathbf{r}, t; \mathbf{r}', t') + \theta_p(t-t') G_0^<(\mathbf{r}, t; \mathbf{r}', t'). \quad (10.58)$$

Therefore,

$$i\hbar \frac{\partial}{\partial t} G_0(\mathbf{r}, t; \mathbf{r}', t') = i\hbar \frac{\partial \theta_p(t-t')}{\partial t} G_0^>(\mathbf{r}, t; \mathbf{r}', t') + i\hbar \theta_p(t-t') \frac{\partial G_0^>(\mathbf{r}, t; \mathbf{r}', t')}{\partial t} + i\hbar \theta_p(t-t') \frac{\partial G_0^<(\mathbf{r}, t; \mathbf{r}', t')}{\partial t} + i\hbar \theta_p(t-t') \frac{\partial G_0^<(\mathbf{r}, t; \mathbf{r}', t')}{\partial t} - \frac{\hbar^2 \nabla^2}{2m} G_0(\mathbf{r}, t; \mathbf{r}', t'). \quad (10.59)$$

From Eq.(10.11) and Eq.(10.12) we have

$$[G_0^>(\mathbf{r}, t; \mathbf{r}', t') - G_0^<(\mathbf{r}, t; \mathbf{r}', t')]$$

$$= -i \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} (1 + \sigma n_{\mathbf{k}}) + \sigma i \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} n_{\mathbf{k}}$$


$$= -i \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} = -\delta(\mathbf{r}-\mathbf{r}'), \quad (10.60)$$

and

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \nabla^2}{2m} \right) G_0(\mathbf{r}-\mathbf{r}', t-t'; \mathbf{0}, 0) = \hbar \delta_p(t-t') \delta(\mathbf{r}-\mathbf{r}'). \quad (10.61)$$

Eq. (10.16) into Eq. (10.17), we get a formula for $G(\mathbf{k}, z_0)$.

$$\frac{1}{V} \sum_{\mathbf{k}} \frac{1}{-\beta\hbar} \sum_n e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} e^{-i\mu(t-t')} e^{z_n(t-t')} (i\hbar z_n - \epsilon_{\mathbf{k}} + \mu) G_0(\mathbf{k}, z_0)$$



So, the point is that these Green's functions also obey this sort of an equation which then means that the definition that we introduced using many body physics consideration

which involves the time monitoring and you know grand canonical, statistical mechanical averaging and so on. It also obeys an equation which a mathematician would also recognize as that of a Green's function.

So, remember that Green was a mathematician and he had no knowledge of this sort of physics and he studied Green's functions for his own reasons. And, mathematicians have been studying Green's functions for ages for their own reasons. And, it is nice to know that the Green's functions, see we had no business of calling some bizarre definition like this like Green's function; because already Green's function has a well-defined meaning in mathematics.

So, at the outset you should have objected. So, I cannot randomly call some crazy definition like this like Green's function. So, the reason why in hindsight it was not a bad idea is because, see if you write down the equation obeyed by that function; it indeed is the equation obeyed by a Green's function as mathematicians would recognize it. So that means, it deserves to be called a Green's function, because in some sense it is a Green's function alright.

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Eq. (10.16) into Eq. (10.17), we get a formula for $G(\mathbf{k}, z_0)$.

$$\frac{1}{V} \sum_{\mathbf{k}} \frac{1}{-\beta \hbar} \sum_n e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}') - i\beta \hbar \epsilon_n} e^{i\beta \hbar \epsilon_n} (i\hbar z_0 - \epsilon_n + \mu) G_0(\mathbf{k}, z_0)$$

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$$= \hbar \delta_{\mathbf{r}(\mathbf{r}-\mathbf{r}')} \delta_{\mathbf{p}(\mathbf{r}-\mathbf{r}')} \quad (10.62)$$

If we choose $(i\hbar z_0 - \epsilon_n + \mu) G_0(\mathbf{k}, z_0) = \hbar$, then the left-hand side becomes,

$$LHS = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{-\beta \hbar} \sum_n e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}') - i\beta \hbar \epsilon_n} e^{i\beta \hbar \epsilon_n} \hbar$$

$$= \hbar \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \frac{1}{-\beta \hbar} \sum_n e^{i\beta \hbar \epsilon_n} e^{-i\beta \hbar \epsilon_n}$$

$$= \hbar \delta_{\mathbf{r}(\mathbf{r}-\mathbf{r}')} \delta_{\mathbf{p}(\mathbf{r}-\mathbf{r}')} = RHS. \quad (10.63)$$

Therefore, the Green function in Fourier space has a particularly simple form,

$$G_0(\mathbf{k}, z_0) = \frac{1}{(i\hbar z_0 - \epsilon_{\mathbf{k}} + \mu)}. \quad (10.64)$$

In the literature it is customary to work in natural units where $\hbar = 1$, which makes the above Green function take the familiar form

$$G_0(\mathbf{k}, z_0) = \frac{1}{(iz_0 - \epsilon_{\mathbf{k}} + \mu)} \quad (10.65)$$

where $z_0 = \frac{i2\pi + \mu}{\beta}$ for fermions and $z_0 = \frac{2\pi i}{\beta}$ for bosons. When mutual interactions

So, what I am going to do is that given the fact that it is going to be very hard for you to swallow what I am saying without going through all these steps on your own, I think I

should allow you to spend some time working through all the steps. And, if you cannot understand anything in between and I am sure there are many points in my notes where you would probably have trouble understanding.

Because, this is a kind of a difficult subject and its impossible for any author to put everything down explicitly. Well, that would make the book almost unreadable as it is pretty hard to read. So, so, this it is the nature of the subject itself. So, it is not anybody's fault, it is how the subject is. So, you have to put in effort and try to understand all these ideas and I will try my best to remedy the situation through assignments.

So, I will work out many intermediate steps and post videos, just like I posted that video on the rubber band solution of the rubber band problem. Similarly, I can start posting videos about solving some you know some intermediate, some theorem proving of this Matsubara of Green's function and so on. So, that might fix some issues, but the remaining issues you have to fix on your own ok.

So, I am sorry, this is the three-dimensional Dirac delta ok. So, the remaining you have to fix on your own. So, I am going to stop here now and before the next class, I will see if I can provide some of those missing steps in all these proofs. So, but in the meanwhile please make an effort to seriously work out all these steps and see if your understanding. But, even if you do not understand something, you just assume that is true and proceed and see if you can understand the remaining things.

So, you just make a note in the margin, that you have not understood that step. But, then provisionally you assume you have understood it and proceed further and see if you can then come back and you know understand why that has to be also correct. But, if you do not follow certain things which you know those margin question marks still remain at the end you can of course, you should of course, always ask me through email and all that ok.

So, I am going to stop here now. And, in the next class, we will continue this discussion, but perhaps you know after taking the appropriate steps to ensure that the derivations are all clarified.

Thank you.