**Formal Properties of Green’s Functions**

So we want to calculate the thermodynamic expectation of correlation functions/green’s function – or basically, we want to thermodynamically average time-dependent perturbation theory that we covered in quantum mechanics. Now we can of course manually TD average the perturbation theory, but doing so would be rather cumbersome. Doing a TD average of Green’s functions is more readily accomplished. And it can be instructive since it will tell us in what different temperature windows different excitations of the system are turned on.

**Various Quantum Green’s Functions introduced**

So we have the usual GF’s as before. We will presume that our operators evolve according to some *time-independent* H:



But this time we are not taking their expectation against a single state, but thermally averaging over all states of the system, in the Grand Canonical Ensemble. Meaning:



where,



and we define K = H – μN. If we’re dealing with distinct particles, rather, like a lattice, then we can carry over the same formalism with a simple change. In the excitation space of the lattice, the ‘particles’ are excitations rather, and summing over all states is the same as summing over all excitations. So the thermal trace would be using:



which is the same as above, but with μ = 0. The same reasoning would hold true for taking thermal averages of quantum field operators I think, since ‘particles’ in that context are just excitations of a quantum field.

A and B are just general quantum mechanical operators – they don’t have to be Hermitian or anything but we are presuming that A(t), etc., *evolve according to the same time-independent H, against which we are doing the thermal averaging*. For the Heisenberg picture operators, I think we must use the typical U(t,t0) = U0(t,t0)S(t,t0), as I don’t think the mixed phase convention time-development operator (see QM/Time-Dependent/RSPT files) is equivalent with the usual one because of the thermal averaging procedure. Anyway, now we have:



And we’ll introduce another, that we’ll find useful, the complex time-ordered GF, where τ = it.



where τ, τ´ is a real number τ є (0, β). The usefulness here is that the complex time GF has the same pole structure, and it is easier to calculate. And when we jump to time-dependent evolution, we can calculate GR by analytic continuation much more easily with GC\* than with any of the others.

These GF’s also implicitly carry with them exponential convergence factors that come in with the θ functions: θ(t) → θ(t)e-ηt, θ(-t) → θ(-t)eηt, where η = 0+ is an infinitesimal positive number, eventually taken to zero. Also, I think even the >,< GF’s carry these factors, and should be technically defined as, for instance,

G>(t,t´) = -iθ(t-t´)<AH(t)BH(t´)> - iθ(t´-t)<AH(t)BH(t´)>

→

G>(t,t´) = -iθ(t-t´)e-η(t-t´)<AH(t)BH(t´)> - iθ(t´-t)eη(t-t´)<AH(t)BH(t´)>.

Anyway, since this limit gives us 1 (unless t = ∞, or t´ = -∞), we will just leave it off, to save space, unless necessary. The exponential convergence factors are there, I think, because of the eventual use of the non-equilibrium distribution function f(Ω), which includes an ‘ad-hoc’ exponential factor within it to approximately model coupling to a thermal bath, and to that end, to prevent quantum recurrences. This is where the eηt factors would show up in calculations. And I believe this convergence factor, initially in f (see Stat Mech/Kubo Formula), gets transferred to the GF’s and so effectively becomes part of their definition for any calculation involving times in infinite past or future. For finite times, the exponential factors are superfluous, as their limit will always gives us 1.

Another thing: there doesn’t seem to be any reason to restrict our interpretation of these GF’s as being strictly many-body. They could pertain to single particles or fields too.

**Algebraic relationships between the various Green’s functions**

The green’s functions aren’t independent. And we have the usual algebraic relations between them [note G> = G+-, G< = G-+, GC = G--, GAC = G++], covered in previous files, because they didn’t depend on how we were evaluating any expectations.



**Symmetries of GF’s**

Consider a GF developed against some time-independent H (implying energy conservation), and a thermal expectation taken against the same. Then for instance our GF should depend only on t-t´, i.e., be time-translationally invariant.



So there we have it. But note that this wouldn’t work if we were thermally averaging against states that weren’t eigenstates of the time-development operator. Now suppose that momentum were a conserved quantity, and we were working with a single-particle GF of form,



First, we know that the momentum operator would commute with the Hamiltonian if we have momentum conservation (which requires the absence of a single particle potential, basically). And so this means H would commute with the translation operator. So we can say:



From the *QM/Identical Particles/2nd quantization in position space* file, we know the result of this operation on the ψ’s,



If we said d = r´, then we’d have:



So that tells us our GF is translationally invariant. Well now say we look at the spin-rotation operator. Say we rotate spins 180o with D(π**j**) = e-iπS\_y operator. Usually, the Hamiltonian will commute with such operators, again unless we have a magnetic field present. Recalling the effect of the rotation operator on the creation/annihilation operators, and going through the same process as above, we will find:



So we have:



Now let’s presume we also have symmetry for rotations of π rad about the x-axis. Again refering to that QM/Identical Particles/2nd quantization in position space file, we know how that operator acts on the creation/annihilation operators, and so we have:



So we have:



This, in conjunction with the other rotation symmetry means that opposite-spin GF’s must be zero, and of course up-spin GF’s are the same as down-spin GF’s. Now let’s consider time-reversal symmetry. We’ll suppose our Hamiltonian is TR symmetric, meaning it commutes with the TR operator Θ. This should be the case unless we have magnetic fields present. We’ll recall the properties of Θ from the Quantum Mechanics/Foundations/TRS file, and what it does to creation/annihilation operators from the Quantum Mechanics/Multiple Particles/Identical Particles/2nd quantization position space file.



So we have:



Now suppose we did the same analysis on the complex time GF. Then we would’ve obtained,



This reproduces previous results.

**Analytic properties: GF’s in terms of the Spectral Function**

The following discussion will assume that we’re using the exact energy eigenbasis |n> for the full Hamiltonian, H = H0 + V1 + V2. As mentioned, we must assume H’s time-independence here for the following spectral properties to hold.

**Retarded Green’s Function**

Consider that we have the retarded Green’s function GR(t-t´). We can take the Fourier transform with the aid of the aforementioned implicit convergence factor…



It seems that here we agree to redefine the time-development of the operators from A(t) = eiHtA(0)e-iHt to eiKtA(0)e-iKt, where again, K = H – μN. I’m not sure of the legality of doing this. In a sense it should be kosher because this would be merely redefining the single particle zero point energy from 0 to μ. And since energy is only defined up to a constant, this should be okay in a physical sense. Well in this case, we now have:



and let’s say the |m> are eigenstates of K with eigenvalues E´m = Em – μNm. Then we have:



and,



And finally this can be written as



where,



**Advanced Green’s Function**

If we carry out the same procedure on the advanced Green’s function, we would evaluate the Fourier transform, as a function of ω in the lower half plane. So considered as a function of complex ω, GA(ω) is analytic in the l.h.p. And we’d get



**Greater Green’s Function**

Now let’s consider,



We have,



recalling that (see below) the spectral function can be written as (unfortunately A means two different things now),



We see that this can be written as,



So we have,



which conforms to the expectation set by our considerations in the Quantum folder.

**Lesser Green’s Function**

And we also have for the lesser GF.



We can put this in terms of the spectral function as well (see below for more spectral function forms).



which also conforms to expectations, with nF/B(ω) being this case’s f(ω). And we also have,



**Causal Green’s Function**

And we also have for the causal GF.



We can put this in terms of the spectral function as well, and we’ll find, most simply from the algebraic relations at the top of the page



**Anti-causal Green’s Function**

And we also have for the causal GF.



We can put this in terms of the spectral function as well, and we’ll find, most simply from the algebraic relations at the top of the page



**Complex time Green’s Function**

So consider the complex time GF:



If we were to let τ range over the whole real line, I don’t think it would have a Fourier transform. So we initially restrict τ – τ´ to the interval (-β, β). It turns out that G obeys a periodicity condition that will allow us to analytically continue the GF to technically range over the whole real line. Recognizing that the Green’s function is a function only of the time difference τ – τ´, we can consider GC\*(τ) only. Suppose τ ∈ [0,β]. Then τ – β ∈ [-β,0]. Now we will relate the Green’s function at τ – β to the one at τ. Guess I’m going to notate A(-iτ) as just A(τ) from now on.



on the other hand,



So we can say that:



So in any event, it’s a function of τ – τ´. Now let’s demonstrate a periodicity property – namely that if we restrict τ to the interval (0, β), then GC\*(τ-β) = -εGC\*(τ).



where ε = ± for Fermions/Bosons. Or could just say,



So either way, we see that for τ ∈ [-β, β], GC\*(τ) is antiperiodic/periodic over an interval β if A and B are Fermionic/Bosonic operators. Seems that wouldn’t be the case if τ were not restricted to that interval. But also seems we’re just going to ‘analtyically continue’ the function to make it so. We’ll deal first with the case of Fermionic operators. Since it is anti – periodic, we can expand it in a Fourier series of anti – periodic functions, which are:



So we can say,



where,



and for the bosonic case, it is periodic so we can expand it in a Fourier series of periodic functions



where,



We can again construct the exact representation of the Fourier transformed temporal Green’s function using the energy eigenstates, and hence find the spectral function. Note below that we’re integrating between τ ∈ [0, β] > 0. Therefore, our time ordering has been decided for us. A comes first, and B after it. Gonna leave the tilde off the Fourier transform.



(unfortunate that iωn has n subscript; it is not intended to be summed over) So we will find that in both the fermionic and bosonic cases, the Fourier transformed temporal Green’s function will reduce to



Let’s now discuss a few salient properties, consequences of the spectral representation of the green’s functions.

**Further properties of complex time GF**

There are more properties which follow from the periodicity of the complex time GF. From the spectral decomposition, we have:



What’s the Fourier transform of the GF where we switch the order of the operators?



So in real time, we’d have:



Now let’s look at the Fourier transform of the transposed dagger GF,



And so in real time we’d have:



**Properties of the Spectral Function**

We can see that the spectral function can be inferred by:



We can write it out explicitly in more convenient ways. Recall the basic definition is:



And consider these manipulations:



So,



or another way to do the same thing is:



From this, it is immediately apparent that A(x) is real if A† = A, B† = B, in other words, if A and B are either Hermitian or Hermitian conjugates of one another. In that case,



and further we have:



**Analytic Continuation**

Analytic continuation of the complex time green’s function from a discrete set of complex frequencies iωn to all complex frequencies, ω, is usually desirable because calculating frequency sums, which could be done by contour integration techniques, would require it. So usually, we can just take the complex time GC\*(iωn) and make the replacement iωn → ω.



where A(x) is of course the spectral function determined above, and ω is now complex. This doesn’t always work because there are many functions that are analytic in the complex plane and yet agree with GC\*AB(iωn) at the points iωn. This is evidenced by just making the replacement iωn → ω and then adding to it a function, f(ω), that is zero at all ω = iωn. So we must make sure that we have the correct continuation. This is ensured if the analytically continued function goes as:



where const. is some constant. So if just blindly making the replacement G(ω) = GC\*(iωn → ω)gives you a function that possesses this limit, then you’ve got it. If not, then you need to add to it an analytic function that is 0 at all points *iωn*, so that G(ω) = GC\*(iωn → ω) + f(ω) satisfies that limit. The other nice thing about having this analytically continued GF, G(ω) is that then we can get the retarded and advanced GF’s via GR,A(ω) = G(ω → ω±i0+). And in practice, we can usually say, accordingly, GR,A(ω) = GC\*(iωn → ω±i0+).

**Kramers - Kronig relations obeyed by GF’s and A(ω)**

Repeating the arguments from the single particle file, we have, *presuming* A(ω) is real:



where the Hilbert transform is:



and for the spectral function, we have:



and concommitantly:



**Expectations from Green’s Functions**

I suppose it is here where Green’s functions demonstrate their utility. The expectation of any single particle operator



can be calculated from its causal Green’s function like before. It can also be calculated from the complex time causal GF. We’ll pursue the latter option since we’ve done the other before already. So the consider we start in a thermal averaged ensemble. Then we develop all of our thermally averaged states in (complex) time and see how the expectation of A changes. This is:



(remember there is -ε cost for any transposition) where we recall:



For example, we can calculate the particle density (as a function of time):



We can get the spin density:



Now let’s say we have a general spin-independent Hamiltonian,



We can calculate the Kinetic Energy



So we have,



where the gradient acts on r alone. The single particle potential energy would be similarly,



(though the r+ is unnecessary) And we can calculate the interaction potential energy as well. We need the equation of motion for ψ evolving (in complex time) w/r to the Kamiltonian K (so really should probably make K the subscript down there but whatever…). Can verify that this is simply, based off of analogy from the real time differential equation obeyed by ψ (see Quantum Mechanics/Identical Particles/2nd quantization):



where,



And then we have:



so our two results are:



and the total energy would be the average of these two:



We could get the total energy by itself by calculating <N> as we do any single particle potential and adding μ<N> to this. With the total energy and particle number available from calculation of the green’s function we can obtain the thermodynamic potentials, and hence calculate all quantities of interest.

**Expectations from the spectral function**

From the definition of G<, we have:



And we can verify this directly from the Lehman representation of the spectral function. Consider:



So there we go. We also have,



This property actually follows from the definition of A in terms of GR and GA. So it is completely general. Let’s also verify this from the Lehman representation.



So there. Now let’s consider calculating <AB>. We already know.



We can clearly find the appropriate linear combination of the two above. And then we’ll have,



Can also write this as:



which, for Fermions anyway, can be written,



Another way to write it is:



We can explicitly confirm this equality by using the Lehman representation of the spectral function. Consider…



So there we go. Going back to this guy,



Since we usually expect this last equation to be finite (since the commutator ought to be), this implies that



Thus GAB(ω) approaches zero as fast as 1/ω for large ω if A and B aren’t singular operators, and even faster if the commutator expectation is 0.