**Quantum Model**

Now we’ll analyze transport from a quantum perspective. We’ll need to calculate the thermal average of the current operator. And to do that we have to first define it of course. And we also need to work out the Hamiltonian in the presence of an EM field. Then we can use the Kubo formula derived in the Stat Mech file to extract the conductivity. So first,

**Current operator**

First remember the velocity operator is disconnected a bit from the canonical momentum operator when B fields are present. Recall an H with an EM field is given by:



where **A** is the vector (magnetic) potential, Φ is the electric potential, and p is the canonical momentum operator, which obeys [x,p] = i, and figures into the translation operator T(d) = e-ip·d, and given by position space representation p = -i∇, etc. But it isn’t the physical momentum in this case. The physical momentum, m, is defined via:



and it follows that:



where (see CM folder/Hamilton’s Equations of Motion or EM folder):



With that said, to keep the narration smooth, I’m going to introduce the definition of the charge density and the definitions of the various current densities and some other preliminary results. Charge density is:



and complex current density is:



where by and I mean the position space operators -i∇/m and -i∇. So,



where ρ(r) is the charge density, **j**p(r) is the 'paramagnetic' current density, so named because its response is in the direction of the electric field. One might call this the ‘canonical’ current density, and **j**d(r,t) is the 'diamagnetic current density'. Presumably its response is in the opposite direction to the magnetic field (a result of the minus sign I suppose). For a normal non-superconducting metal (because if it superconducts, then there is no proportionality between **j** and **E** per se´; **j** is independent of **E**), the current density is related to the electric field via a **non-local** conductivity tensor:



Provided that **E**(r,t) varies slowly on the length scale of spatial inhomogeneity (e.g., atomic length scales for microscopically homogeneous systems) then it is possible to presume σ(r-rʹ,t-tʹ), and then we can profitably take the spatio-temporal Fourier transform, to say:



The electric field entering here is the total electric field, which can be split into an induced part and an external part.



**Hamiltonian of Particle in EM field**

The Hamiltonian of all electrons (and protons) together is (see EM folder/Least Action, say):



**A** = **A**ind + **A**ext is the total vector potential combining external sources of field, and internal sources due to motions of the particles themselves in our conductor. And φext is the electric potential coming from external fields. And of course the total fields are given by: **E** = ∂**A**/∂t - ∇φ, **B** = ∇×**A**. Maybe see the EM folder/Least Action or Quantum Mechanics/Identical Particles/Stark-Zeeman Interaction. Like before, we’re going to presume the e-e (and p-p) interaction terms just give us a constant. We can do this as long as the external field frequency, ω, isn’t too small or too large compared to its spatial variation, **q**, to have caused significant induced charge densities or currents. As a rule of thumb, these conditions are met if either the external electric field is transverse, i.e. **q**·**E** = 0 and/or the limit q → 0, is taken before the limit ω → 0, which I suppose means that the spatial variation of the field is ‘much less’ than the temporal variation and are both close to 0 [can verify – see Interacting Electrons/Nearly Free/Collective Excitations – that ΠC”irr(q,iνn) → 0 when set q = 0, and this makes ε(q,ω) → 1, which means φ = φext and so we have no induced charge density]. We’ll presume this to be so. And we will accordingly replace φext with φ itself, and say:



Furthermore, like before we’ll presume the crystal potential enters in only to renormalize the mass m → m\* (but I’m still going to call it m) so:



Now let’s do some work on our H. We only need it to first order in A, φ (‘cause Kubo formula is only good to first order anyway), but we’ll keep all terms for now. So our 2nd quantized H is:



where is the position space operator. Note the p behind A is acting on *both* A and ψσ. The perturbation, VEM, is:



We can straight away use the Kubo formula to evaluate the expected current density to first order in the electric field, but the resulting GF will be nasty, as it will involve the commutator of j and all those terms. So first we’ll take advantage of gauge freedom in A and φ to try to simplify the perturbation. One option, especially if dealing with a constant E field, is to just set A = 0. Maybe should pursue this sometime. But if we want to allow electric and magnetic fields we need A too. On the other hand, we can just get rid of φ instead by using the temporal gauge [see EM folder]. The equations for the vector potential are, in this gauge (and in faux-Gaussian units which set ε0 = 1/4π, and μ0 = 4π):



Now what about the –(∂/∂t)∇·A = ρ/ε0 term? As mentioned above, we expect no appreciable charge density accumulation here because we’re restricted ω to the requisite range for this to be so. So we should have the net ρ = 0 → ∇·A = 0 (or at least we *can* set divergence to zero). But what if this condition were not met? This would be the case if we had, say, collective oscillations, i.e., charge density fluctuations/oscillations in our metal. And I’m guessing this would give rise to a term involving the electric susceptibility, χ(q,ω), or concomittantly, the diffusivity D(q,ω)? Or maybe it’s the φψ†ψ term which would give rise to that. But I’ll look into that, or not, some other time. So presuming ρ → 0, we can now say:



Now let’s IBP on the middle term,



where we used the ∇·A = 0 property again. Now we’ll recognize the paramagnetic current:



to write,



and therefore our total H is:



where again,



(for momentum space representations of these operators see Quantum Mechanics/Identical Particles/2nd quantization) But of course, we only need to first order. So we can just say:



and as aforementioned, the local conductivity tensor is the proportionality between the induced local current and the *total* field at that position.

**Current density to O(A) & Extraction of Linear Response Coefficient**

Now we can go on to calculate the current density to first order, and hence the linear response – the conductivity. Using the fact that <**j**>eq = 0, and <ρ>eq. = ne, we have that **j** to first order in A is equal to [f = feq + f1 is the statistical evolution operator, out to first order]. I’m denoting Heq the one without the EM field – i.e. has just kinetic energy, crystal potential, and disorder potential. And Ueq would be the corresponding time-development operator. I’m going to use the f1 from the Stat Mech file.



where n is the overall electron density. The exponential infinitesimal convergence factor in f1, designed to prevent recurrences, limits the applicability of our results to the thermodynamic limit, because only here would energy spacings be infinitesimally small. Imry says one \*can\* apply it to finite systems if can argue that it is coupled to say, a phonon bath, which would narrow the levels into a continuum. So – how are diagrammatic WL corrections justified? Also used the cyclic property of traces. Oh and j, V, are in the interaction picture now of course. Now we’ll plug in our expression for V(t)…



Of course we can recognize a GF here – the current, current correlation function.



so we’ll say:



The steady state result would be obtained by taking t0 → -∞. So we’ll do this. After disorder averaging, we should have homogeneity, and so then a Fourier transform on time/space would give us,



Now we can extract the conductivity tensor. In our gauge, if we have an electric field then it would be given by:



So now we have:



So we can identify the complex conductivity tensor as:



With reference to the restrictions that we placed on the E and B fields to approximately equate the total and external components, to obtain the DC conductivity we would perform:



I believe we take the q → 0 limit first so as to eliminate the contribution to σ(q,ω) coming from charge density gradients, i.e., diffusion (see EM folder/Metals, and Stat Mech folder/Diffusivity, etc.) Note that we expect this limit to be real, as in not complex, since the current should be in phase with the voltage. Therefore we must have that:



and so we should have both (this relation however is violated in SC materials):



and,



If we have a homogeneous medium, then σ should be proportional to the identity tensor, and so we can say:



I’m going to define:



So then I can say,



For what it’s worth, there are other expressions for σ, at least in the 0 = q limit:



**Diagrammatic Expansion of ΠRαβ(r,r´; t,t´)**

So get the conductivity tensor, we need to calculate the Green’s function: . One way is by direct calculation of the time-dependent ΠR:



But this is complicated, requiring the coupled contour ordering diagrammatic approach, so we’ll bypass this direct route in favor of calculating,



So the complex time ordered GF is:



Question is how do we get it?

**Approach 1**

We could straight away try to evaluate the product and the disorder averaging (see 2nd quantization stuff in QM folder for j expression),



now this should be a function of r1 – r2, upon disorder averaging, which would require the disorder averaged correlation function to be proportional to δq1,-q2,



Then taking the Fourier transform,



So now filling in jαp(q) (see QM/ManyParticles/2nd Quant), we have:



We can use Wick’s theorem because the Hamiltonian is bilinear in creation/annihilation operators. So,



Each individual GF doesn’t conserve momentum, thanks to the disorder averaging happening over the product, instead of the individual GF’s themselves. Now to put in form we’ll see below, let’s subtract q from k´,



Okay I think what I did below should be like this, but I’m going to hope that Π is symmetric in q, which would make it spatially real. Seems reasonable. So then, also transposing the two GF’s



where I call those two GF’s to be GC\*σσ´(k,k´;τ1 – τ2) and GC\*σ´σ(k´+q,k+q;τ2-τ1). Now let’s take the temporal Fourier transform.



and so we have:



Now we’re off by a factor of 1/V from what we have below. Hmmmmm. Well this is correct, but it looks like I defined this G a little differently than I did the ones below. Those were Fourier transformed in both coordinates? And this just one. Well either way. General rule is, we will ultimately (1/V)Σk = ∫d3k/(2π)3 over each free momentum variable.

**Approach 2**

But the typical approach is to start in real space first. Expanding the current operator, we have (with an implicit summation over spins).



(the time-ordering operator obviously acts on both lines) Now we do a sort of useful trick. We prime the second in each pair of 1′s and 2′s. Later we will take the limit as 1′1, 2′2 from below (since we want the unprimed is later than the primed since the unprimed dagger operators come first). But doing it this way allows us to switch terms around with impunity.



We’ll ignore the prefactor for the time being, and expanding the product gives us:



Now we factor out the differential operators – this is why using the primes is beneficial.



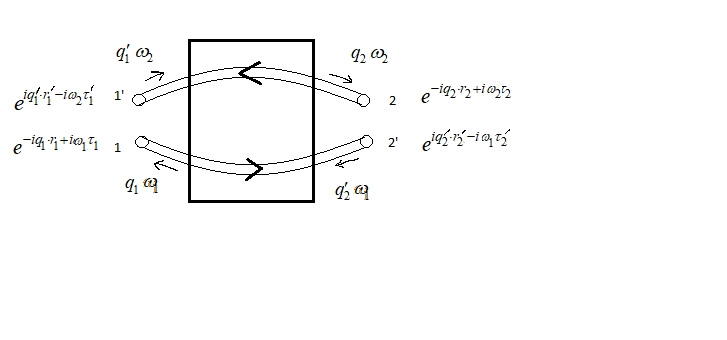
If you’re concerned that taking the limit ought to give zero, then note how lim[O(f)] ≠ [limO](f). For example consider: O = d/dx – d/dy, and f(x,y) = x - y. Then lim(O(f)) ≠ 0. Now we’ll use Wick’s theorem (this is justified because the ψ’s are developing in time according to Heq which is exp{-i(H0 + Vdis – μ)τ}, and H0, Vdis are both bilinear in ψ)



Where we have noted that the first term is just the expectation of the current in equilibrium at position 1 times the same for position 2 (once we take the limit that primed goes to unprimed. And now we’ll express the Green’s functions in terms of their ‘Fourier transforms’. Each coordinate in the two G’s will be Fourier transformed, so that’s why we have 1/V4 factor. We would do same for time coordinate, but we’ll note that the frequency will be the same on both ends of the same Green’s function because we must have frequency conservation at every vertex since the perturbation V, doesn’t depend on time. Thus there can be no net ‘energy’ flowing down any of the interaction legs into either of the Green’s functions. So two of the frequency sums would collapse, leaving us with just 1/β2 factor (the tilde on the GF’s means ‘Fourier Transform’).



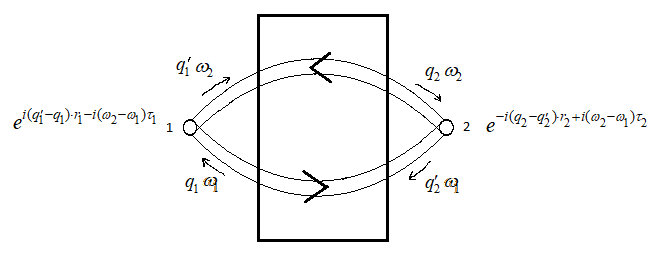
Diagrammatically, it looks like this:



Note that the box stands for all the impurity line vertices, etc., not shown. Now apply the gradients, and take the limit of primed coordinates going to unprimed coordinates:



which will look like this:



Now we disorder average our expression. Thus we must have momentum conservation at all the points integrated over inside the box. This enforces that the momentum going into the box equals the momentum coming out of the box. So we can say:



and this will imply,



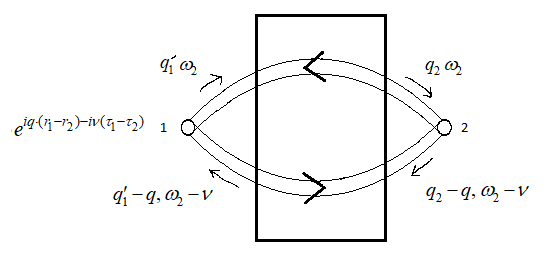
We might as well also note the two fermionic frequencies subtract to give a bosonic frequency:



And now we’ll have:



which we could picture as:



which is:



So now one of the momentum sums collapses, and so does one of the frequency sums, taking with them a factor of V and β respectively. And we get:



And if we take the FT in r1 – r2, τ1 – τ2, we will finally obtain, flipping the sign of q, ν to match it up with the standard notation, and changing **q**1 → **k**1, and **q**2 → **k**2:

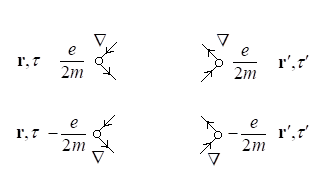


**Approach 3**

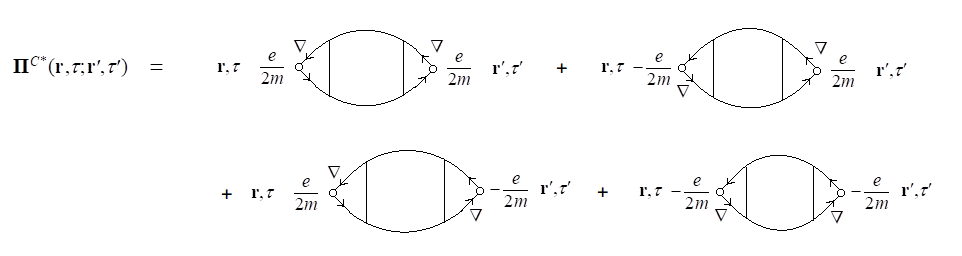
That seemed to take a long time, so I’m looking for a more succinct approach. Consider again (leaving out the spin sum),



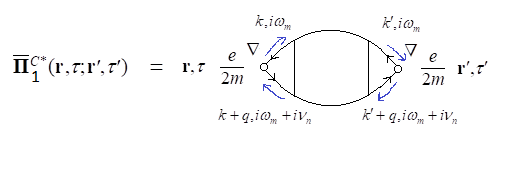
Recognizing that the expectation of the current is zero when traced against the thermal equilibrium background, we can ignore contractions within the brackets themselves, and only worry about contractions between brackets. We can represent the external points in the top/bottom bracket as:



And we’d connect the vertices on the left with those on the right. The gradient operator acts on the GF that gets connected to that leg, and moreover, acts on the argument of the GF connected to the vertex. So basically we’d have:



where all sorts of disorder vertices go inside the blank square. Now let’s consider the upper left diagram translated into terms of the FT of its constituents. We’ll recall the FT file which says we must label all lines with momenta. All internal points, which are integrated over (when disorder average), must conserve ‘momentum’, but the two external points on either side do not. So I’m labeling them as such.



We start with k for the bare GF coming out of the left vertex. Then the internal disorder lines transfer some net momentum upward so that k goes to k´ by the time we get to the GF going into the right vertex. Below that, coming out of the right vertex, we’ll have a new momentum k´+q, ‘cause momentum isn’t conserved here since the vertex isn’t integrated over. Going into the left vertex we have k+q because we know that the net momentum transferred upwards by all those disorder lines was k´-k, and so that means the momentum going into the left vertex will be k´+q-(k´-k) = k+q. So then our diagram would be, more explicitly,



where [….] represents all the internal GF lines and disorder lines in terms of their Fourier components and such. So the FT of our **Π**1 is:



If we do the same with the one on the top row, on the right, we’d get:



and so its FT would be:



Then for the bottom left we have:



And the FT of our **Π**3 is:



Finally for the bottom right guy,



and so its FT would be:



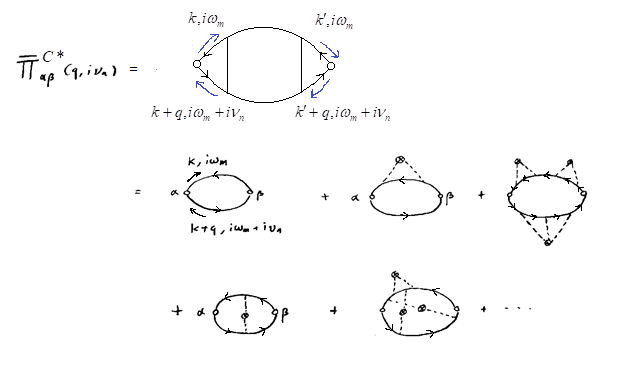
So altogether we clearly have:



So there we go. That’s better.

**Feynman Rules**

Using standard perturbation theory, we can write out the expansion for the current-current correlation function.



Feynman Rules are as follows…

Construct all diagrams with one impurity, two impurities, three impurities, etc. placed one either of the two legs. Connect the impurities together in as many distinct ways as possible remembering that an unconnected impurity line set everything to zero because it would have q = 0 momentum flowing down that line (and we set Vi(q=0)=0).

Start with ‘dummy’ energy–momentum (k,iωn) coming out of the open circle (bare current vertex) into the top line. Note that this won’t necessarily be the momentum going into the bare current vertex on the right from the top line. Impose energy-momentum conservation at each vertex. Add (q,iνn) ’boost’ once cross the other open circle on the right hand. Overall energy-momentum conservation will ensure that energy-momenta ‘below’ the L and R vertices will be (q,iνn) greater than the momenta above the L and R vertices. Each open circle (called the bare current vertex) labeled α connecting unbroken lines labeled k1 and k2 represents one factor of jα = eα = e(k1α + k2α)/2m - this factor is sort of an average current (charge \* average velocity) - the sum of the incoming and out going momenta multiplied by a prefactor. The prefactor comes from the prefactor in the correlation function, and the momenta come from the gradients. Each single/double unbroken line labeled (k,iωn) represents a factor of G0C\*(k,iωn) / GC\*(k,iωn­), as before. Each crossed circle represents a factor of ni and each dashed line labeled q, represents one factor of Vi(q), as before. *The overall Fermion loops doesn’t get a -1 here.*

Sum over all unconstrained momenta and (the one) unconstrained frequency iωm, with the 1/V and 1/β factor as usual. The GF’s carry spin indices, but presuming they’re diagonal in spin indices, then overall sum over spins just result in a net factor of 2 on the outside as well.

Disclaimer: Reasoning straight from a Wick expansion approach, we are accustomed to associating each fermion line/contraction with -G, and each impurity potential with -Vi. But we always have an even number total of these, ‘cause we start with two GF’s. And then each impurity line [meaning one of the dotted lines emanating from impurity star] adds another GF. So we’ll always have an even number of (GF’s + impurity lines). So the negative signs are of no consequence.