**Dielectric Function, Absorptivity, etc.**

**Formula for Dielectric Function and Absorptivity**

We used the RTA approximation to get the electric susceptibility for a metal and an insulator. Let’s do this again. But this time we’ll use quantum Kubo formula discussed earlier. We’ll recall we said that when we have a time-dependent perturbation, then at least to first order, we can calculate the non-equilibrium expectation value of an operator via:



where A = Σiai is a many body operator representing some physical quantity which is the sum of single particle operators, *a*. And |ψn(t)> are the time-dependent single particle wavefunctions. The susceptibility and dielectric function start from an expression for the charge density. And this is:



And the induced charge density would be:



Now let’s look at the first order correction to the wavefunction (spin should be a spectator variable here). We’ll turn the perturbation on adiabatically, so we’ll have something like V(r,t) = eφ(r,t)eηt. But then note we’ll also be adding a blue exponential factor, consistent with how we treat the time-developed quantum distribution function (see Stat Mech/Kubo Formula),



This is necessary so that we eliminate the ephemeral effects of turning the perturbation on suddenly, and isolate the steady state response. We’ll also use the phase convention associated with infinitely timed potentials (see Quantum Mechanics/Time-Dependent/Interaction Picture file), whereby the system’s time evolution in the absence of a potential reduces to what it would look like if evolved at time t = 0. Finally, our potential includes contributions from charges in the system. So it is the total potential. Need to work out what the first order correction looks like in position space,



Okay so now forming the density,



where θ(x) is the Heaviside step function. Let’s take the Fourier transform w/r to time, and space I guess,



Now going to change variables from t,t´ to s = t – t´,t´. This will allow us to do the time-integrals, and gives us,



And I guess I’ll fill in a free electron wavefunction to continue,



Now need to get the second guy,



It’s just the complex conjugate of the first guy, in real space. Filling in the wavefunctions, this amounts to:



Taking the Fourier transform, we’ll find:



So adding these together,



Let’s change variables in second one to k → k + q. Then, we have:



Then doing the trivial spin sum, we have:



which tells us that:



This is called the Lindhardt function. And if we go on to construct the dielectric function, we find (see EM folder),



I’m actually using faux Gaussian units, where ε0 → 1/4π, and μ0 → 4π, and then we also add a factor of 4π to χirr(q,ω) for aesthetic reasons (see Condensed Matter folder/Metals/Free Day for instance). But now, I want to go ahead and calculate the absorptivity. This is (see EM folder),



and using 1/x+iη = 1/x – πiδ(x), this comes to,



See the Condensed Matter Folder for more on these calculations.

**Example. HO in time-dependent external field**

Now let’s say:



And say we want to get the average position of our particle, supposing it starts off in thermal equilibrium (meaning it’s fluctuating over the states according to a thermal equilibrium distribution). So we’d want to calculate:



Well we already know we can do this exactly. So in the single particle QM file, we solved for xH(t), and found,



where , and , are annihilation/creation operators with respect to the unperturbed ground state|0>. It is clear that we get:



We can note that this is exactly,



So our result agrees with Kubo formula. Interesting that thermal averaging plays no role – I guess every state has the same response. If we put in a constant field, then we would get:



So we see oscillations about the equilibrium point. There is no irreversibility here though; shouldn’t it should *settle* at the new equilibrium point? We don’t find irreversibility because we have not included the exponential convergence factors that should be present on GR due to the exponential factor in the distribution function. So taking a step back, we should have:



And then redoing our calculation:



Now we can see that in the t → ∞ limit, we get the correct result. And also, FWIW, if we take the t0 → -∞ limit. We could’ve obtained the constant h, t0 → -∞ result immediately from Fourier space. Generically we’d have:



Using,



We get:

