**Quantum Time Evolution**

What we’re looking for is the time evolution of the statistically averaged characteristics of the sample in response to an external perturbation. In the Drude case, we simply characterize all the particles in the sample by the momentum <p>, give a scattering relaxation time mechanism for re-establishing thermodynamic equilibrium in the absense of the perturbation, and examine the consequences. More sophisticated approaches are to assign the system to a distribution of states (r,p), or (n) if characterizing it via QM. Then we examine the dynamics of the system, starting off in TD equilibrium. It basically amounts to a thermal average of the time evolution of the system via either CM or QM. A key requirement of any description is that when we turn the perturbation off, the system relaxes back to equilibrium with its environment.

**Quantum f(n,t) evolution (density matrix)**

Now let’s suppose we introduce a time-dependent perturbation.

**Operator Approach**

Then the eigenkets will start to evolve with time. And consequently, so will f. We’ll have,



where wj­ is the statistical weight of state |αj>. But I’m going to write this rather as:



which is the formalism I’ve been using elsewhere. I think this captures the real nature of the evolution function, which is the mesoscopic running time average of a system’s states. Here τ would be larger than the thermal relaxation time, whatever that might be. And quantity averages would be given by:



Anyway, differentiating f (recall from thermo folder how we can push derivative in):



Note H(t) and Hbath(t) are in Schrodinger picture. Now we cannot pull H out unless it’s a time-independent operator, or if its time-dependence evolves on a scale much slower than τ. This ought to be the case for H(t), but not Hbath one would think. So then we’d have:



and so it satisfies a *Schrodinger* like equation [the more familiar equation for the time-development of an operator in the Heisenberg picture has the i on the other side of the equality). I don’t know how to handle Hbath. You might think to model it as a dissipative term. But this isn’t done. It’s rather ignored, but then somehow its effects are added back in later with an exponential convergence factor…In what follows, we’re basically trying to determine the time development of the distribution function – like was done in the RTA and Boltzman equation, etc. This is the fundamental calculation, really. Everything else is just working out details. The solution to this equation, sans the bath guy, is:



as we can see since,



Now split H into two parts:



where H012 includes time-independent single and double particle potentials. We presume the former determines the equilibrium state of the system, when V(t) is turned off. So we should have:



I think I’ll call H012 as Heq too, sometimes, maybe. We’ll note it satisfies



Lack of time dependence is the signature of an equilibrium configuration. But unless we know the eigenstates of H012, feq won’t be entirely known either. But anyway, suppose now that the system is perturbed by a Hamiltonian term λV(t) that switches on at time t = 0.. In general we will not have:



unless V(t) is an adiabatic perturbation. Also note that the time dependence of V(t) doesn’t come from the operators. The operators up till now are in the Schrodinger picture. The time dependence would come from a time-dependent potential perhaps. OK, now let’s solve the equation, at least to first order in V. There are two ways. One is to a direct Taylor expansion,



Another way is to define a pseudo-interaction picture operator.



Doing this, we factor out the *quasi*-trivial time dependence of the density matrix because note that the unperturbed hamiltonian, H012, may not necessarily be exactly solvable. So it doesn’t have to be just a kinetic energy, or single particle potential H012, but it can rather contain things like a disorder averaged potential, or e-e interaction, etc. We’re merely separating out the part of hamiltonian that induces a change in some quantity of interest, V, and seeing how f evolves in response to *it* in particular. We may still not know exactly how it evolves according to other terms in H012 that could in themselves be called perturbations. Anyway, obtaining an equation of motion…



And so we have:



Which implies, upon integrating both sides with respect to t,



And now iterating this solution, we get…



And now converting back to the Schrodinger picture…



So our result is, either way:



We should probably put an exponential convergence factor in there exp(-0+(t-t´)). Mello says that we need it here to prevent quantum recurrences (recall recurences will occur on a time scale 1/ΔEgcf, where ΔEgcf is the largest energy unit that will factor out of all of the system’s energy eigenvalues). So this is where the effects of the dissipitive bath are added back in. The use of an infinitesimal convergence factor, 0+, also restricts the formula to the thermodynamic limit (whereby the spacing between energy eigenvalues goes to zero), because otherwise, such a small convergence factor wouldn’t suffice (it would have to go from 0+ to 1/τ, where τ is the now finite time scale for recurrences). This convergence factor is where we get the exponential factors that we we must use on the GF’s, technically. We could also get this factor, if we treated the time development operator a little differently, say by slowly turning on our perturbation (red factor) and also adding a blue e-ηt factor to the time-development operator:



where η is super small. Either way, to accommodate this necessity, we’d write:



It occurs to me that we need to normalize it too, i.e., divide by Trf(t), because it’s supposed to be a probability distribution. What is this?



So I guess we don’t have to worry about this…😊.

**Linear Response: Kubo Formula**

But again, our S operator which determines the time development of the operators will have both Hint and V(t) in it. And a double expansion is inconvenient. So we have to content ourselves usually with just the linear response to V(t). But that is usually all we want.

We can also calculate the thermal averaged linear response of the system to an external perturbation. Many experiments in condensed matter physics measure the response of an observable of the system to an applied perturbation. If the perturbation is small enough, invariably what we’ll have is that

Response = linear response coefficientperturbation

e.g.

|  |  |  |
| --- | --- | --- |
| **Perturbation** | **Response** | **Linear Response Coefficient** |
| E | j (current density) | (conductivity) |
|  | (heat current density) | (thermal conductivity) |
| H | M (magnetization) | (susceptibility) |

In each case, the perturbation drives the system out of thermal equilibrium (i.e., away from a static ensemble described by a time independent state operator). Nonetheless, it turns out that the linear response coefficient can be expressed as an equilibrium correlation function of the unperturbed system.

**Kubo Formula I**

Now let’s calculate the effect of V(t) on some observable A. Note that V depends on t only through some time dependent c-number potential in the definition of V – like a potential v(x,t) or something, not from operators being evaluated at a particular time t – because none are. Below we get time dependence in V as well from the fact that we put the operator in the interaction picture. Note that time dependence of A comes from the time dependence of p(t), not from any intrinsic time dependence in the definition of A. That is to say that the psi’s, and c’s that comprise A don’t have time dependence initially. So note that initially, A and V are both Schrodinger picture operators.



We can write this as:



where in the last step we set λ = 1. Note that you can cycle the operators even through a commutator when taking a trace. The first term is time-independent, and just gives us the equilibrium average. So we have:



If we take the limit t0 → -∞, then we eliminate the transient coming-to-equilibrium response to the perturbation. So the steady-state response can be written:



which is Kubo’s formula. Aeq. means of course to take the expectation of A in the equilibrium ensemble. The retarded Green’s function is evaluated in the ‘unperturbed’ ensemble. But note that feq. will be in general,



and that the operators will evolve according to this unperturbed H as well.



and so this GF may require a perturbative expansion itself. So the first order response of a quantity to a perturbation is a correlation function in the unperturbed ensemble. But the ‘unperturbed’ ensemble may contain other terms in H that aren’t known exactly. Note two special cases of the above. If V(t) = BF(t), then Kubo’s formula reads,



If F(t) is known in the frequency domain, and we want to know A in the frequency domain, we can take the Fourier transform of both sides to get.



so,



**Kubo Formula II**

And we can do it another way, at least to first order (not sure how far beyond that we can go), it turns out that the evolution of f(t) is the same as we would get if we just kept the thermal average w/r to the unperturbed system and yet evolved the wavefunctions according to the perturbed system. In other words (leaving out the convergence factor),



which we can write as:



which is of course our previous result. And if the perturbation doesn’t mix the particles, then we can just calculate corrections to the individual particle wavefunctions. So then we can proceed with the above, and come to the conclusion that:



*A* is the many-body operator, and *a* is the single-body operator. For instance, if calculating the density, then we’d have,



and in the single-body case is:



A problem with this approach is that we have to expand Ψ w/r to the Hint and V(t) perturbations – unless Hint is 0. And this would be rather difficult – but we can go to the interaction picture, like we did w/ f and determine simply the linear response w/r to V(t) perhaps.

**Kubo Formula III**

Instead of evolving the distribution operator, as we ought to be doing, we can get away with simply evolving the observable operator. Not sure if this alternative would match the correct one beyond first order either. Let our Hamiltonian be H = H012 + V(t). Then (leaving out the convergence factor)



where Ueq involves the time-independent part H, and S involves the time-dependent part V(t) in the interaction picture. Now we can write out what S equals, noting that we only need the term in S that is linear in V since we’re looking only at linear response. So we evaluate this expectation to linear order in V. We end up with in short order,



and so we have again,



where we’ve taken 0 to be -∞ again, eliminating the transient response. It remains to be seen whether evolving the density matrix as in approach 1 is the same as evolving the operator directly, as in approach 2, *to all orders*. If it is, then we would just time evolve according to H, but thermally average w/r to the equilibrium – time independent H.

Well I guess it is the same to all orders, because:



So perhaps,



But perhaps the formula is only valid to linear order for some reason? Perhaps it has to do with the fact that we can treat the bath via the exponential convergence factor only to first order?

**Connection between non-equilibrium f and equilibrium f**

If we have a time-independent perturbation, V, then we will expect the system to settle into an equilibrium arrangement, if it can (don’t think this is possible for a system in an electric field with disorder, say). And so I’d expect the non-equilibrium distribution to settle into an equilibrium distribution in the long-time limit. Let’s consider,



(well I guess we already knew this) and if the perturbation is constant in time, then, coupled with the ad hoc exponential factor that was added to f, and should be here too somewhere/somehow, we should find that |ψn(t)> would just settle adiabatically into its new time-independent state.



But the sort of weird thing is that feq. would be e-β(E-μN)/Ξ, and not e-β(E´-μN)Ξ´. But then we could proceed and come to the conclusion that:



where = Σ. Yeah I don’t know – this might work to first order, but I’d be skeptical beyond that. One more thing…we can determine the first order equilibrium response to a constant perturbation, then, from the non-equilibrium distribution function. We’d have, as usual,



and in terms of the FT, this would translate to:



This makes sense – the static response is just the dynamic response, with ω set to 0.