**Excitations**

So now we’ll take a look at some excitations – specializing to one particular case.

Maybe for ease of distinction for these notes, I’d prefer insulator electrons to just be stationary? So basically/not in the conduction band?

**Frohlich Polaron Hamiltonian**

We’ll look at the coupling between electrons and optical phonons.



where,



We’ll specialize to just one electron in the band – if the semiconductor isn’t heavily doped, then we might be able to get away with treating the electrons independently. So the kinetic energy is just 2/2m. And also, n(-q) will be:



And since we’re considering optical bands here, we’ll take Ωk3 = Ω3, i.e., no k-dependence. And I guess we’ll just focus on the longitudinal optical band, Ω3 apropos the free part of the H too, since the other bands don’t couple to the electron. Last, I guess we’ll write g(q) as follows,



So now we have:



This is called the Frohlich Hamiltonian. It describes the interaction between an electron in a solid and phonons. It could very well describe the properties of a macroscopically small amount of electrons in the conduction band of an insulator or semi-conductor. It would be quite inappropriate for a metal since we have to take into account the e-e interaction between conduction electrons, and at the very least, the statistics of the electron fermions.

The unperturbed electron is taken to have free-particle motion with an effective mass m. Since there is only one electron in the problem, the results are independent of the statistics of the particle. The same results are obtained for any particle – boson or fermion. The phonon modes are unaffected by the one electron in the solid so the phonon self energy is 0 (or actually O(1/V)), and the phonon GF is always free. The model also assumes that the motion is isotropic in direction and that the energy bands of the solid are nondegenerate. These rather restricted conditions describe what is called the ***Frohlich polaron problem***.

This problem was important in mathematical physics during the 1950’s. Numerous mathematical techniques were tried out on this problem. Brillouin-Wigner perturbation theory, Rayleigh-Schrödinger perturbation theory, strong coupling theory, and linked cluster/exponential resummation (GF’s). The problem was most accurately solved by Feynman (1955). He introduced a variational method based on path integrals, which reproduced the successes of all the other methods in their respective areas of applicability.

The phonon energy bands will not be changed by the presence of the macroscopically few electrons. But the electron energy levels will change quite a bit from the free particle spectrum, as we’ll see. The classical picture has the particle exerting forces upon the ions which respond and move. The ion motion creates new forces, which act back upon the particle. The nonzero ion frequency makes the reaction forces, of the ions on the particle, retarded in time. The quantum nature of the phonons makes these forces occur in discrete units. In both the classical and quantum pictures, the ion motion is pictured as a polarization of the surrounding medium by the particle. *The e-, as it travels around the solid, will polarize the medium, much like a charge does in an insulating solid. That’s why they’re called polarons*. *This phenomenon is responsible for the increased effective mass of the polaron, as it has to ‘drag’ this polarization with it, which increases its inertia.*

**Electron Self-Energy: Small Coupling Regime**

So we’re going to examine, among other things, the self-energy of the electron, as the coupling strength M0 increases. We’ll often put our results in terms of a dimensionless coupling constant,



**Brillouin-Wigner PT**

So we’d like to see how the energy spectrum of the electron changes. One would usually resort to GF’s to make this calculation. The GF (self-energy) would give us the spectrum of single particle/electron excitations on top of the solid – basically the excitation spectrum of a particle injected into the solid. And this wouldn’t be an exact spectrum in the sense that the injected electron, uncoupled to the phonons, is not a true state of the system, and so it would decay. The GF approach basically gives us the best approximation to a single particle spectrum. If we use RS or BW perturbation theory, then we’re calculating something a little different. Here we are seeing how the unperturbed states of the system are modified by the perturbation, and turn into mixed many-body states. And so the eigenstates and eigenenergies we calculate are the actual many-body states and energies of the system, to that order in PT. But I imagine the results are comparable. Anyway, when we are not dealing with complex fermion statistics, which makes the GF approach more tractable than the PT approach, one usually just uses PT. So we’ll do that first. And we’ll use the BW approach. So let’s go back to our H.



and recall the formula for the energy (see QM folder/Time-Independent/BW perturbation theory)



(note at T = 0, the free particle state with energy less than Ω3 would be an exact eigenstate, as there would be no way for it to decay, as there’d be no phonons it could give off, and there’d be none – b/c T = 0 – that it could absorb). We’ll look at PT up to 2nd order. Our states are |ψ{Nq,p}(0)> = |{Nq}p>, meaning Nq phonons in the q momentum state, and one electron in the p momentum state. The unperturbed energy would be: E(0){Nq},p = p2/2m + ΣqΩ3Nq. So let’s look at the first order correction,



Note {Nq(≠k),Nk-1} means ‘the usual Nq occupation numbers for q ≠ k, and occupation number Nk-1 when q = k’. So we get zero because of the zero overlap between states with different phonon occupation numbers (i.e., N±k on left and N±k∓1 on the right). So now we’ll go to second order. We’ll use,



So,



Now let’s look at the phonon overlaps. These are independent of the eikr term of course.



Maybe do the electron overlap here too, now. We have:



So



We’ll note the two sets of delta functions are mutually incompatible. So when we take the modulus of the numerator, the cross terms must annihilate each other. And we’ll just have:



and,



Now observe that the δp+k-p´ and δp+k´-p´ constrain k and k´ to be equal. So we’ll enforce this first,



And this makes the set of δ functions after the second Π superfluous. So we can write:



And now we’ll employ the δ functions in the sum over {N´q}p´,



So all total, our equation, up to second order, our Brillouin-Wigner PT equation for the energy would read,



This energy is that possessed by the entire system: phonons + electron. But I think we presume the phonon energy levels to be negligibly affected by the presence of the single electron, so that any change in the energy is taken up, rather, by the electron. And we’ll call the energy of the electron εp, as opposed to the unperturbed value εp(0) = p2/2m. So we’ll say,



and so,



And this simplifies to:



Let’s note that physically, our second order equation,



describes a process where by our initial state |{Nq}p> makes a transition to an intermediate state |I>, and then back to the initial state. I can take two forms. It can be the result of absorbing a phonon of momentum k.



or of emitting a phonon of momentum –k.

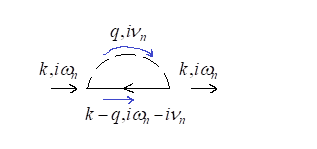


These two processes must be distinguished because they are different. Absorbing a phonon of k is not the same as emitting a phonon of -k because we have different numbers of phonons in the two cases, and so the intermediate state is different. After it is in the intermediate state, it does the inverse process to arrive back at the initial state p. Anyway, this virtual process evokes the self-energy diagrams we did with GF. So let’s compare this calculation to a GF calculation of the electron self energy.

Way back in the Metal’s file, we calculated the self-energy of an electron in the presence of the e-ph interaction. We can do the same here. In fact we’ll just copy that calculation. The form of the Heph interaction is the same in both cases. So we have:



Let’s just write out what the first term above is. So we’d have:



And in symbols,



(the Ωq is implicitly that of the longitudinal branch – see Interaction file) And we could do the Matsubara sum with the contour integral approach, but I’ll not. Maybe I will. So using that identity (see Stat Mech/Math Appendix)



we can do the sum over frequencies, to get:



So we have:



Let’s note the following:



So can say,



Now to compare to our BW result, we’d set nF = 0 everywhere, as we have no electrons to speak of.



So the full expression for the energy would be:



So we have:



where in this line we change variable of summation q → -q, and that take advantage of the fact that Ωq = Ω-q. And so our result matches what we found using BW perturbation theory. So that’s cool! Now let’s go ahead and do this calculation at T = 0. So then nB(Ωq) = Nq = 0, as does nB(Ω-q) = N-q. And we’ll have:



Now have to do that integral.



Okay now what. He says that we can change limits of integration on k to -∞ to 0. Let’s see. I’ll change variables of integration k → -k, and cosθ → -cosθ.



And so we do get the same integrand. So we can say. So we can add both of these together and divide by two.



This makes the integral much easier to do. So now we have:



The term in the square root should be positive, since Ω3 > εp for smallish/normal values of p. We can use residues to get this integral. We’ll close the contour up I guess.



Going to write x = cosθ,



and then change variables to:



which gives us,



So our final result is:



And this equation would need to be solved self-consistently to get εp. If we’re close to the center of the band, then p ≈ 0. So doing Taylor expansion about this, we have approximately,



This is equivalent to a cubic equation for the energy. Turns out though, that this is a poor approximation to the energy. And rather, Raleigh-Schrodinger perturbation theory does a better job. So we’ll turn to that.

**Raleigh-Schrodinger PT approach**

Now let’s repeat the calculation using the RS perturbation theory approach. The energy levels are, to second order:



So out to this order, we see that we can get the RSPT estimate from the BWPT estimate simply by replacing En in BW with En(0) in the 2nd order term.



which is:



We can write this as:



and finally,



We can expand this in powers of p, using sin-1(x) = x + x3/6 + …



And so we get:



The first term is the zero-point energy, the potential energy between the electron and the lattice, which gets polarized in response to the electron. The second term is the kinetic energy. Can see that as the lattice coupling, α, or M0 basically, increases strength, it slows the electron down, effectively localizing it when α = 6, if we can trust the result of second order perturbation theory out that far. Can see that then εp would be negative for sure, and in a bound state. Another way to frame that result is the polarization cloud gives the electron an effective mass:



*The extra mass occurs because the electron has to drag its polarization cloud with it everywhere it goes. So observe that a lattice does renormalize the free particle spectrum of the electrons. Interestingly, m\* blows up in the strong coupling regime, α = 6. An infinite mass would mean infinite inertia – which would indicate that it cannot move. And this is indeed a harbinger of an actual result. The particles become localized in this strong coupling regime.* Interestingly, keeping just this order term does a good job for even intermediate values of coupling, 1 < α < 6. The next non-zero order term is given by:



This integral can also be calculated exactly – although with a bit of difficulty, and we get for the zero point energy, taking a careful limit, or just evaluating directly:



RS gives contributions of all number of phonons at each order. It just gives first order correlations at first order, and second order correlations at second order, etc. He says that RSPT gives excellent results when ImΣ is unimportant, basically because state cannot decay, as would be the case for T < Ω3 in this case. And BW/GF would be more useful otherwise. And GF especially when the exclusion principle is necessary to account for. For another example, recall that the insulating static (single or multi-state) polaron problem in the next file was not solved by finding the exact self energy. This would’ve corresponded to the BW approach but required us to sum an infinite number of diagrams. Rather it was solved by canonical transformation. So the moral of the story is – for getting best results quickly – sometimes BW/GF are easiest, sometimes RS is easiest. For recall how easily the GF method dealt with all of the many body correlations in the perturbative approach involving the Fermi Sea, etc., and how complicated it was with RS to get the right terms. And also, it was simple in some cases to get the exact Σ. So keep both methods in mind!

**Other Raleigh-Schrodinger PT results**

We’ll look at the wavefunction in the RS context. Recall the general first order equation:



Let’s use it to determine what the perturbed ground state wavefunction looks like.



and continuing,



Can split the electron and phonon parts of the wavefunction,



I’t easier to denote |{0q}> as just |0>, and |{0q≠-k,1q=-k}> as a-k†|0>. Then we can write:



And let’s dot both sides against <r|,



Now keeping in mind how the polaron is dragging the polarized medium – the oscillating medium – the phonons with it. Let’s attempt to calculate how many phonons it carries. The total number of phonons in this state is found by taking the expectation of the phonon number operator in this state,



So,



and this is:



Now gotta evaluate this integral….



Now we’ll extend the range of integration like we did above.



And then we’ll complete the square,



We can do this integral by closing the contour up, again. First we’ll note the following to get the residue,



So,



Now do to this integral, we can use:



Now have to do this integral. We’ll be presuming p < √(2mΩ3). I’ll set x = sin(y).



So then,



which is,



So can say,



Interestingly it carries more and more as its energy approaches the phonon mode. We could also calculate the total polaron momentum:



Seems like we’d just get **p**.