**Excitations**

Moving on to strong coupling regime.

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

For the strong coupling case, a non-perturbative approach seems necessary. We’ll use a variational approach.

**Variational approach**

I suppose the e- gets localized b/c it simply get’s trapped by the attractive force the ions exert on it. The bound state approximation isn’t too unlikely since, as the lattice deforms in response to the presence of the electron, it can create a local potential surrounding the electron which might be strong enough to trap it.

The strong coupling theory for polarons was invented by Landau and Pekar. Their theory was the first work on polarons, and even preceded the word. Their theory, and its subsequent improvements is known to be valid at large values of α > 5 or so; hence the current name of strong coupling theory. The Rayleigh-Schrödinger theory is correct for α < 5. α ~ 5 is the crossover regime. The LP theory is basically a variational calculation on a Gaussian wave function. We start with:



And then we rewrite the phonon part in the operators xq and pq. Recall in QM/Many Particles/Distinct folder we worked out the Hamiltonian for coupled harmonic oscillators. We found,



where,



and,



But we’ll restrict our attention to the 3rd (longitudinal) branch λ = 3, for which **ε**q = , which is the only branch which couples to the electron. So we’ll say,



And going to want to put Aq in terms of q, so, as can see from right above,



(λ = 3 implicitly) So this is our H,



And let’s go to position space. So again recall/see from QM/Many Particles/Distinct/HO’s that this will come to:



where,



and xR is the displacement of the oscillator at location R. And of course for us, λ = 3. To be honest, I’m only guessing that eik·r→ Re(eik·r) in that last Heph term, cause it has to be real. So they assume a trial wavefunction for the system.



where xn are the displacements of the oscillators at position Rn. And Xk is related to these via the preceding equation. And the phonon mode wavefunctions are the usual HO wavefunctions in Xk (see QM/Many Particles/Distinct/N 1D HO’s file), but with a non-zero equilibrium point, and where,



β is a variational parameter. Do note Xk, r are real numbers, not operators now. So now we need to take the expectation of the energy,



Let’s do the first one,



Ugh. Okay, well this is:



Next, let’s do the Eph term.



To evaluate this, we can just make the shift Xk → Xk – δXk in all the Xk integrals. This won’t affect the kinetic energy term. It will change the potential energy, by effectuating Xk2 → (Xk – δXk)2 = Xk2 – 2XkδXk + (δXk)2. The first term is just the usual potential energy term. The middle term should go to zero, as the wavefunctions are even in Xk. And the last term is just a constant. So we should have:



(all sums over q are restricted to BZ by the way) This is just the usual HO energy with an additional potential energy term due to the displacement of the oscillator/particle. And then we have the Eeph term.



We’ll make the same Xk → Xk – δXk substitution in all the d3Xk integrals. Then the Xq term will be mapped to Xq – δXq of course. And the Xq term will go away as it’s odd. And so we’ll be left with:



Working this out,



So altogether,



and we want to figure what δXq and β are, to minimize this energy. First let’s do the δXq guy. So we do,



And now fill this into E,



And now need to minimize w/r to β. But Mahan actually evaluates this first. So,



Can put this in terms of α,



So,



*Now* we’ll minimize w/r to β,



Finally, we plug this back into the energy,



So our final result is:



So can see our energy is negative (besides the phonons). So the electron is definitely in a *bound* state. And for large α, it goes as α2, not as α, as the RSPT result predicted, not that we can trust the RSPT result out that far – though to be fair, the next order RSPT term did predict coupling ~ -α2, and with a coefficient very close to 1/3π. Can also see from previous line that the potential energy of the electron in the lattice is (negative) twice its kinetic energy, consistent with the virial theorem, says Mahan.

The electron can have excited states in its ‘potential well’ that it feels from the phonons. One can calculate such states. The first would have p-wave symmetry (i.e. ℓ = 1). But this excited state isn’t stable (I suppose b/c its energy is technically higher than the well created by the lattice potential), but nonetheless optical experiments have demonstrated transitions from the s-wave to p-wave states and back. I suppose one can tell because the optical transitions would be sensitive to the angular momentum of the ingoing states – just like we saw in the QM scattering folder, where we have partial cross sections for different ℓ values. So the strongly coupled polaron can create its own internal structure. In the strong coupling limit the electron has sufficient binding energy that its oscillatory motion in the potential well is much faster than the vibrational frequency of the phonons. The phonons do not have time to adjust to the individual oscillations of the electron. Instead they adjust to the average motion of the electrons. The ions are treated as a rigid potential well, in which the electron adiabatically oscillates. A quite different picture applies to the weak coupling limit. There the phonon energy is larger than that of the electrons. The picture is that the phonons, or ion polarization, follow the electron during its motion.