**Excitations**

Moving on, we’ll look at the medium coupling regime.

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

Now let’s look at a diagrammatic approach to calculating the polaron behavior. Since we’ll be using GF formalism, let’s write H in fully 2nd quantized form,



where,



and,



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:



I guess we’ll look at the expansion for the electron causal GF. But this necessarily involves the expansion of three other GF’s. Recall from the Stat Mech/GF Perturbative Expansion in Real Time, the generic rules for expanding an electron GF:

**Fourier Space/Real Time Rules**

Our four electron GF’s are represented with bold lines:

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and are four phonon GF’s are similarly,

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And the perturbative series for the electron GF works as follows. So we start with the external points. We represent the two arguments/operators in the GF we’re trying to get with external points. We use the first if we want G+-, the next for G-+, the next for G—and the last for G++.

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Then at each order of PT, we bring down the same number of vertices (discussed in a second) and connect with bare iGF’s. The bare (unperturbed) iGF’s are represented with non-bold lines,

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and,

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The unperturbed electron GF’s are:



But since we can say that nkσ is practically zero, these simplify to:



and the unperturbed phonon GF’s are:



And we are taking nqλ to be constant N0. Additionally, only longitudinal optical phonons (Ω3) are involved in the interaction, and are taken to not depend on q. So we can say,



Now to the vertex. So we have two vertices, corresponding to the two S-operators in the expansion (can compare to stated rules for e-ph interaction and GC\*, DC\* in metals, as well as generic rules for real time GC’s in Quantum Mechanics/Multiple Particles folder):

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where,



So we construct the diagrams, and then we sum over all internal σ, λ. And sum (1/V)Σq over all internal wavevectors, and integrate ∫dt over all internal times. As a practical matter, we can avoid dealing with internal σ and λ d.o.f. The electron GF is diagonal in spin index, and so it will just force all spins to be the same. So we can take everything to be spin-independent. And the gλ guy is proportional to δ3λ, so we can just take all λ’s to be 3.

**First non-vanishing order Expansion of GF**

So the general expansion of our causal GF will be something like:

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where we construct all diagrams with arbitrary numbers of + and – vertices, to our two external legs. So to first nonvanishing (second) order, we have the following GF’s (note the restriction q ≠ 0 eliminates those balloon/tadpole diagrams):

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But note that since G-+ and G++ are zero, these reduce to the following set.

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So let’s go ahead and calculate these. The first is:

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which is:



We’re clearly going to want to put this in terms of temporal Fourier transform. So taking temporal Fourier transform of both sides, we have:



What are the Fourier transforms?



So filling these in…actually gonna fill in the blue line,



Now gotta do those ν integrals. I guess I’ll close the first ν integral up. The second ν integral has poles only in the u.h.p. So if we close it down, we’ll simply get zero. So,



Don’t think we’re going to bother with the q-integral. Let’s just do the inverse Fourier transform and get G(k,t).



We can combine the first and last terms,



For each of these if t > 0, then must close down, and if t < 0, then must close up. But there are no poles in the u.h.p. for any of the three terms, so the t < 0 term is just 0. So we have:



This seems substantially correct. Now just have to get the other terms. It’s actually the same as we just did: just take Ω3 → -Ω3. So,



So altogether,



which simplifies to:



Looks like Mahan’s result differs from mine by a minus sign. So maybe I made a mistake somewhere. Whatever. By the way, I guess we’d set the chemical potential μ = 0. There is a more concise way to get the GF expansion, afforded by the simplification that we have only one/few electrons in the band. Let’s go back to the generic formula for the causal GF (see Stat Mech folder/Real Time expansion of GF file).



where the contour is:

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And,



The unperturbed states that comprise eigenstates of K0 have any number of phonons, but zero electrons – it’s an electron vacuum state. This being the case, powers of V(t) will annihilate the vacuum. And so the expression for the GF will simplify,



and so the contour just simplifies to a causal one,

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and we can write,



and so the expansion for the causal GF only involves other causal GF’s. We saw evidence of this above in that all the diagrams with non-causal GF’s present vanished.

**Exponential Resummation**

It seems that when we are taking expectations against the vacuum, and thereby have minimal correlations with the background expectation state, a good/better alternative to the Dyson self-energy approach to GF’s is the exponential resummation approach. Looks like this approach works well in the small-intermediate coupling range α < 5 or so. Basically, we just posit.



And we’ll expand F(p,t) in orders of V.



One of the advantages here is that the Fn(p,t) will directly tell us about the energy and lifetime of our state. And then we compare this to Dyson’s expansion,



where,



(but only even powers of n will survive, ‘cause need even powers of phonon operator A) And so we equate these two, order by order, and find,



So we find,



For us, W1 = W3 = 0. So the first term of interest is:



which we already calculated of course. We found,



and so F2 = eiξ\_k·tW2 = ieiξ\_k·tG—2/θ(t), which is:



Might recall we found the polaron self-energy in the previous file,



and can see the bottom two terms of F2(k,t) correspond to this. And we could go on to evaluate F4, etc. Turns out this term is a good bit smaller than F2. So F2 provides a good approximation. So our GF is approximately,



Even this first non-zero F-term provides a good description of the GF at small-intermediate coupling. Let’s look at the spectral function. This would be:



And what is the retarded GF? Well, we can use:



But G< = 0, right? If go back to Stat Mech folder, and look at formal properties of GF’s, then can see G< = 2πiεnF/B(ω)A(ω), and so we might think that saying G< = 0 → A(ω) = 0. But actually it is nF/B(ω) which is zero for us; if we redo the derivation with our restricted subset of vacuum states, we can see that what corresponds to nF/B(ω) will be zero. This point is even clearer if we go back to the QM folder and look at the ‘state’ averaged GF’s. In that case, a general f(ω) replaces nF/B(ω), and the (vacuum) state against which we’re taking expectations makes f(ω) = 0. Okay, so GC = GR. And we can say,



When the spectral function is calculated for k = 0, it reveals peaks at multiples of Ω3.

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This is interpreted as the electron absorbing multiples of phonons. And this coupling was also reflected in the RSPT calculation of the polaron energy in the previous file. So the exponential resummation approach works pretty well in this case. In contrast many terms of Σ would have to be evaluated to give a good description of GF in Dyson’s approach – as we’ll recall from the BW perturbation theory calculation. But beyond the first order these are too difficult to calculate. The only way to determine if the first term is adequate is to basically look at the second term’s relative size. It is found that in this case the second term, which would describe correlations between phonons, is quite small. Thus the series converges quite rapidly.

**Interesting aside: exact exponential resummation on a linear electron energy spectrum**

We could solve for the properties of the electron exactly, if we assumed a linear excitation spectrum. Of course then for this to be appropriate we’d need a metal. And if *that* were the case, then we’d have to consider the e’s effects on the lattice in order to be realistic, and we wouldn’t be averaging against a vacuum state, but a thermal equilibrium metal state (w/ lots of electrons). Nonetheless, consider the model below:



If we attempt to solve for the electron single particle causal GF, then we’d run into the expansion,



Consider the density operator,



If it were the case that the energy dependence were linear in momentum, then we may have,



Pulling out the time factors we’d have,



The operation of the density operators on the right is:



This will be equal to k if the sum of the q-vectors is zero. This must be the case for a non-zero expectation, and so we’ll have,



So now we have,



This can be evaluated exactly. Note that all the time-ordered products/contractions can have their time-arguments changed to match up exactly with any *one* of them, since we’re integrating over all times, and so all times are dummy variables. For instance,



Then in the ‘last’ contraction, do: sm → s2, s2 → sm-1, sm-1 → sm. Then we have:



Furthermore, the qj’s are all dummy variables, as can see from the summation over q in expression for GC up above. So we can switch these around. Crucially, the eiε\_q·tMq terms are all invariant w/r to this operation. And so let’s to the same mapping on the q’s as we did to the s’s: qm → q2, q2 → qm-1, qm-1 → qm. Then we have:



So we see we just have copies of the same term. How many copies? Well, (m-1)(m-3)… 3·1 = (m-1)!! So now we can say,



Will note that the GF’s will enforce the two momenta are the same: q1 = -q2, qm-1 = -qm, etc. Filling this into our GF expression,



And continuing to simplify. Apparently, (m-1)!! = m!/(2m/2(m/2)!). And we can take out the i from the iD0C term,



Finally, the entire GF is:



(since only even m will contribute). And noting M-q = Mq, we can say our GF is:



Evidently, had we done the exponential resummation technique, we would’ve found the first term was the only non-zero term. So this sort of analysis would apply to particles with a linear spectrum, for example. Note how Maslov was able to come to such a form for his interacting GF – and his work was predicated upon having a linear spectrum.