Electron-phonon interactions

So far, we considered the motion of electrons in the static periodic potential that would arise if the ions were frozen in their equilibrium positions. Then we looked just at the ions, and discussed the lattice vibrations – phonons – while ignoring the existence of valence electrons (apart from the fact that they screen ion-ion interactions to make them shorter-range). Now we have to go back and consider what is the influence of the existence of phonons on the behavior of the valence electrons? And of course, we also have to consider the other side of the coin: what is the effect of the valence electrons on the phonons?

Both these issues are addressed by studying the so-called **electron-phonon coupling**. Let us first see how this comes about, and then we will discuss its effects. If you look back at our CM "theory of everything", clearly the term that depends both on electrons and ions is the one that describes their interactions:

$$\hat{H}_{e-ion} = \sum_{i,a} V(\hat{\vec{r}}_i - \hat{\vec{R}}_a)$$

Here, $V(r)$ should be the same screened potential like we used for the e-e and ion-ion interactions.

Now let's start to specialize this general term to our actual situation, namely that the ions are performing small oscillations about their equilibrium positions. Like in the last section, we'll use $\vec{R}_{n,\alpha} = \vec{R}^{(0)}_{n,\alpha} + \vec{u}_{n,\alpha}$ to describe the location of the ion $\alpha = 1, ..., r$ belonging to unit cell $n = 1, ..., N$. This is written as the equilibrium position plus its small displacement out of equilibrium. We again use a Taylor expansion to simplify things, and stop at the first non-trivial contribution:

$$\hat{H}_{el-ion} = \sum_{i=1}^{N} \sum_{n,\alpha} V_\alpha(\hat{\vec{r}}_i - \hat{\vec{R}}_{n,\alpha}) \approx \sum_{i=1}^{N} \sum_{n,\alpha} V_\alpha(\hat{\vec{r}}_i - \hat{\vec{R}}^{(0)}_{n,\alpha}) - \sum_{i=1}^{N} \sum_{n,\alpha} \hat{\vec{u}}_{n,\alpha} \frac{\partial V_\alpha(\vec{r}_i - \vec{R}_{n,\alpha})}{\partial \vec{R}_{n,\alpha}}$$

The first term in this equation is the interaction of the electrons with the static, frozen lattice. This part was already included in the electronic Hamiltonian, so we do not need to consider it again. The second term is the extra part describing the electron-phonon interaction. Let's consider it carefully. First, we need to write this in the second quantization, to be similar to the electronic and phonon parts.

We already know how $\hat{\vec{u}}_{n,\alpha}$ depends on the phonon creation and annihilation operators, so that part is easy. For the electrons, we need to choose in which basis we quantize, i.e. what creation and annihilation operators we use. Let us assume that our material has weak-enough e-e interaction that the quasiparticle picture is good. In other words, that we can approximate with good accuracy:

$$\hat{H}_e \approx \sum_{b,\vec{k},\sigma} E_{b,\sigma}(\vec{k}) c^\dagger_{b,k,\sigma} c_{b,k,\sigma}$$

where b is the band index (I'm running out of letters; I can't use n because that is now labeling the unit cells); $\vec{k}$ is the momentum and is restricted to the BZ, and σ is the spin. Then $c^\dagger_{b,k,\sigma}$ creates an electron (quasiparticle, actually) in this one-particle state, whose energy is $E_{b,\sigma}(\vec{k})$. We assume these quantities to be known – presumably we have already solved the electronic part of the problem.

Note that we can use any other basis we like for what follows below. For instance, if we have a Hubbard-like model with strong interactions and do not know how to deal with them, we could use the $c^\dagger_{n,\alpha,\sigma}$ operators, which create an electron on the (orbital of interest of) ion n, α. Well,

we would use their Fourier transforms in order to take advantage of the translation symmetry, but that doesn't really change their nature. Of course, we would get different expressions if we did that, and that makes sense: what we are asking is how are phonons influencing electrons if the electrons are occupying the states we used for second-quantization. The expression we get will differ depending on the nature of these states. However, if we were able to solve the problem exactly, the final answer would be the same no matter what basis we chose. In reality, however, we must make approximations ... so one has to be as careful as possible.

Enough talk, let's do some work. According to our general prescriptions, and given that from the point of view of the electrons this is a one-particle operator, in the second-quantization we have:

$$\mathcal{H}_{el-ph} = \sum_{\substack{b,k,\sigma \\ b',k',\sigma'}} \langle b,k,\sigma|...|b',k',\sigma'\rangle c^\dagger_{b,k,\sigma} c_{b',k',\sigma'}$$

where

$$\langle b,k,\sigma|...|b',k',\sigma'\rangle = -\int d\vec{r}\phi^*_{bk\sigma}(\vec{r}) \sum_{n,\alpha} \hat{\vec{u}}_{n,\alpha} \frac{\partial V_\alpha(\vec{r}-\vec{R}_{n,\alpha})}{\partial \vec{R}_{n,\alpha}} \phi_{b'k'\sigma'}(\vec{r})$$

To calculate this, we express the potential V in terms of its Fourier transform, $V_\alpha(\vec{r}-\vec{R}_{n,\alpha}) = \frac{1}{V}\sum_Q e^{i\vec{Q}(\vec{r}-\vec{R}_{n,\alpha})} V_{\vec{Q}}$; the gradient is now trivial to take, and we are left with:

$$\langle b,k,\sigma|...|b',k',\sigma'\rangle = i\sum_{n,\alpha} \vec{Q}\cdot\hat{\vec{u}}_{n\alpha} \frac{1}{V}\sum_Q e^{-i\vec{Q}\vec{R}_{n,\alpha}} V_{\vec{Q}} \int d\vec{r}\phi^*_{bk\sigma}(\vec{r}) e^{i\vec{Q}\vec{r}} \phi_{b'k'\sigma'}(\vec{r})$$

To do this integral, remember that any Bloch state can be written as

$$\phi_{bk\sigma}(\vec{r}) = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{V}} u_{b\vec{k}}(\vec{r})\chi_\sigma$$

where $u_{b\vec{k}}(\vec{r}) = u_{b\vec{k}}(\vec{r}+\vec{R}_n)$ is periodic with respect to lattice translations. Assuming that the potential is independent of spin, then we must have $\sigma = \sigma'$: the electron-phonon interaction cannot change the electron spin. The integral can now be evaluated by breaking the integral over the whole crystal into a sum of integrals over each individual unit cell:

$$\int d\vec{r}\frac{e^{-i\vec{k}\vec{r}}}{\sqrt{V}} u^*_{b\vec{k}}(\vec{r}) e^{i\vec{Q}\vec{r}} \frac{e^{i\vec{k}'\vec{r}}}{\sqrt{V}} u_{b'\vec{k}'}(\vec{r}) = \sum_m \int_{unit-cell} d\vec{\rho}\frac{e^{-i\vec{k}(\vec{\rho}+\vec{R}_m)}}{\sqrt{V}} u^*_{b\vec{k}}(\vec{\rho}) e^{i\vec{Q}(\vec{\rho}+\vec{R}_m)} \frac{e^{i\vec{k}'(\vec{\rho}+\vec{R}_m)}}{\sqrt{V}} u_{b'\vec{k}'}(\vec{\rho})$$

But

$$\sum_m e^{i(-\vec{k}+\vec{Q}+\vec{k}')\vec{R}_m} = N\sum_G \delta_{\vec{G},-\vec{k}+\vec{Q}+\vec{k}'}$$

where $N = V/\Omega$ is the total no. of unit cells, Ω is the unit cell volume, and the $\vec{G}$ are the reciprocal lattice vectors.

Now, remember that:

$$\hat{\vec{u}}_{n\alpha} = \sum_{j,\vec{q}} \sqrt{\frac{\hbar}{2M_\alpha\omega_j(\vec{q})}} \vec{e}^{(j)}_\alpha(\vec{q}) \frac{e^{i\vec{q}\vec{R}_n}}{\sqrt{N}} \left(b_{j,\vec{q}} + b^\dagger_{j,-\vec{q}}\right)$$

This allows us to carry the sum over all unit cells indexed by n, using:

$$\sum_n e^{i(\vec{q}-\vec{Q})\vec{R}_n} = N\delta_{\vec{q},\vec{Q}}$$

where $\vec{q}$ is the momentum carried by phonons, and $\vec{Q}$ was the Fourier component of the potential (no Umklapp is possible in this case). Also, let me denote by:

$$\alpha_{\vec{G};b\vec{k};b'\vec{k}'} = \frac{1}{\Omega}\int_{unit-cell} d\vec{\rho} e^{i\vec{G}\vec{\rho}} u^*_{b\vec{k}}(\vec{\rho}) u_{b'\vec{k}'}(\vec{r}) \tag{1}$$

the remaining integral over the unit cell. This can be calculated if the Bloch wavefunctions are known - so these α's are just some numbers. In general, one makes the assumption that these integrals are negligible unless $b = b'$, i.e. that electron-phonon interactions cannot excite an electron from one band to a different band. This is usually justified by the fact that the typical phonon energies are much smaller than the gaps between bands – but in materials where this is not true, one must keep inter-band transitions as well. Let us keep the whole expression, for completeness.

Putting all these pieces together, we find that the electron-phonon interaction Hamiltonian has the general form:

$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N}} \sum_{\substack{\vec{k},\vec{G},\vec{q},\\ j,b,b',\sigma}} v_{\vec{k},\vec{G},\vec{q};j,b,b'} \left(b^\dagger_{j,-\vec{q}} + b_{j\vec{q}}\right) c^\dagger_{b,\vec{k}+\vec{q}+\vec{G},\sigma} c_{b',\vec{k},\sigma} \tag{2}$$

where I've included all the multiplying constants in the $v_{\vec{k},\vec{G},\vec{q};j,b,b'}$ vertex. This Hamiltonian describes processes where an electron in band b' and with momentum $\vec{k}$ either absorbs a phonon of mode j with momentum $\vec{q}$ or emits a phonon of mode j with momentum $-\vec{q}$, and as a result it changes its state to one in the band b, with momentum $\vec{k}+\vec{q}+\vec{G}$, and same spin. In practice, one does not write the sum over $\vec{G}$ explicitly: remember that that it is there just so that if $\vec{k}+\vec{q}$ is outside the first Brillouin zone, we choose the proper $\vec{G}$ so that $\vec{k}+\vec{q}+\vec{G}$ is inside the BZ. With this convention, and limiting ourselves only to the band b which hosts the Fermi level (assuming that we deal with a metal), we get the more customary form:

$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N}} \sum_{\vec{k},\vec{q},j,\sigma} v_{\vec{k},\vec{q};j} \left(b^\dagger_{j,-\vec{q}} + b_{j\vec{q}}\right) c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} \tag{3}$$

where $c^\dagger_{\vec{k},\sigma}$ are now understood to be the operators for states in this partially filled valence band.

Furthermore, if we assume that there is a single phonon mode (there are always more than one, but depending on the material of interest, one mode may interact a lot more strongly with the electrons than the others, so we can ignore the other ones to first order), we get the even simpler form:

$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N}} \sum_{\vec{k},\vec{q},\sigma} v_{\vec{k},\vec{q}} (b^\dagger_{-\vec{q}} + b_{\vec{q}}) c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma}$$

where now the phonon operators are for the phonon mode most strongly coupled to electrons in this band.

All these approximations might make you weary. The reason we're making them is because (as you might expect) we cannot solve such problems exactly, and the simpler the Hamiltonians, the

easier it is to gain some idea on how to make good approximations. As always, it is a matter of whether we are trying to understand the general consequences of such a term (which is our goal here), in which case any generic model is good enough; or are we trying to be as precise as we can in calculating properties for a specific material (in which case, we will include all the details relevant for that specific case). Also, remember that even the general form we had on the previous page is, actually, the result of keeping only terms linear in u in the expansion (this is known as **a linear approximation**). If the displacements are not all that small, then higher order terms need to be included, and that will complicate things even more.

1 Famous examples

Here are some specific models of electron-phonon coupling that have been studied extensively.

1.1 The Fröhlich Hamiltonian

This describes free electrons (no underlying lattice, i.e. a jellium model) coupled to the longitudinal acoustic phonons through unscreened Coulomb interactions:

$$\hat{H} = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} b^\dagger_{\vec{q}} b_{\vec{q}} + \frac{1}{\sqrt{N}} \sum_{\vec{k},\vec{q}} M(q)(b^\dagger_{-\vec{q}} + b_{\vec{q}}) c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} \tag{4}$$

where, if you repeat the calculation above but for plane-waves, the vertex turns out to be $M(q) = \sqrt{\frac{\hbar}{2M\omega_{\vec{q}}}} q V(q)$. Note that because of the $\vec{q}\cdot\vec{u}$ part, only the longitudinal acoustic phonon contributes; for the transverse ones this dot product vanishes.

If we use the unscreened Coulomb potential $V(q) \sim \frac{1}{q^2}$ and the dispersion for acoustic phonons $\hbar\omega_{\vec{q}} = c_s q$ for small enough q (or in a Debye model), we find that $M(q) \sim 1/q^{\frac{3}{2}}$. Clearly, the small-$q$ divergence is because of the unscreened $V(q)$, so any unphysical consequences coming from here can be dismissed because we know that there is screening in real systems.

1.2 The Holstein Hamiltonian

This is the most studied lattice model for electron-phonon coupling, because it is the simplest model one we can write. From this point of view, you can think of it as the counterpart of what the Hubbard model is for the study of strongly correlated electrons. Like there, we assume a lattice containing identical ions, and that only one orbital per ion is of interest for the valence electrons. Let $c_{n,\sigma}, c^\dagger_{n,\sigma}$ be the operators to remove or add an electron (in that orbital) at site n with spin σ. The model also assumes that the coupling is to a single branch of optical phonons, which are described by an Einstein model: $\hbar\omega_{\vec{q}} = \Omega$. It reads:

$$\hat{H} = -\sum_{n,m,\sigma} t_{n,m} c^\dagger_{n,\sigma} c_{m,\sigma} + \hbar\Omega \sum_n b^\dagger_n b_n + g \sum_{n,\sigma} c^\dagger_{n,\sigma} c_{n,\sigma} (b^\dagger_n + b_n) \tag{5}$$

The first term describes the hopping of the electrons on the lattice (usually restricted to nearest-neighbor hopping only); the second is the phonons and the third is the Holstein coupling. If you Fourier transform, you'll find that it has the standard form written above with $v_{\vec{k},\vec{q}} \to g$, i.e. it is a constant (so indeed, the simplest possible form).

But if you actually think about this Hamiltonian (which many people don't bother to do), it is really strange. First of all, why would there be an optical phonon in a crystal with a one-atom basis? But more importantly, how can the coupling possibly have this form?! Remember that for Einstein phonons, $b_n^\dagger + b_n \sim u_n$ is the displacement of site n from its equilibrium value. Of course, $\sum_\sigma c_{n,\sigma}^\dagger c_{n,\sigma} = \hat{n}_n$ is the number of electrons at that site. Assume $g > 0$. Then this interaction says that if there is an electron at one of the sites, then the energy of system goes up if that site moves to the right and $\langle u \rangle > 0$, and down if it moves to the left. But that site has identical ions on both sides so that makes no physical sense; and moreover, what is "right" and what is "left", especially in a 3D system?

The answer to these puzzles is that the model was written for a so-called "molecular crystal", where each "site" is actually a polar molecule. If an electron is added to this molecule, it distorts to a new equilibrium configuration (say, it gets longer). So the phonon is actually a vibron, it describes this internal oscillation of each molecule about its equilibrium configuration, NOT the displacement out of equilibrium of the molecule as a whole. This explains what the Einstein "phonon" is. Then, indeed, the coupling will favor the energy to increase/decrease when the molecule becomes shorter/longer, so this form of the coupling now makes perfect physical sense.

Even this model, which is as simple as one can write, cannot be solved exactly except when either $t = 0$ (no hopping) or $g = 0$ (no coupling). It can be generalized to describe longer range coupling (between an electron at site n and phonons at site m); if that coupling decreases like $1/r$, and if the electron density is fairly small (remember that states at the bottom of the band have quadratic dispersion), then this mimics quite well the Fröhlich Hamiltonian.

1.3 The Peierls/SSH Hamiltonian

The two models above had a vertex that does not depend on $\vec{k}$, despite the general form saying that that dependence is generically expected. For lattice models like Holstein (and its longer range counterparts) it is easy to see that this comes from the fact that the dependence on electrons operators comes through their density, $\sum_\sigma c_{n,\sigma}^\dagger c_{n,\sigma}$. This, in turn, comes from the fact that interactions between electrons and ions (whether screened or not) originate in the Coulomb interaction which depends on the electron density, hence the electron number operator. So one has to wonder if dependence of $\vec{k}$ is ever possible in such models.

The answer, of course, is yes, but it must be due to a different origin of the electron-phonon coupling. Remember that for a lattice model, the hopping t between two sites depends on the distance between the sites – the closer they are, the larger the overlap and bigger (the magnitude of) the hopping. If the sites oscillate, then this oscillation will modulate the hopping. If we assume small oscillations, then we could make again a Taylor expansion:

$$t_{nm} = t(\vec{R}_n - \vec{R}_m) = t(\vec{R}_n^{(0)} - \vec{R}_m^{(0)}) \left[1 \pm \alpha(|\vec{u}_n| - |\vec{u}_m|) + ...\right]$$

(the $\pm$ sign is chosen such that the hopping increases if the sites move closer together, and decreases is they move further apart.) If we make a linear approximation, then we ignore higher order terms. The fist term here is the usual hopping that appears in electronic Hamiltonians. The second part shows how the phonons affect it, i.e. it describes a form of electron-phonon coupling. This is know as Peierls (but this is more general), or Su-Schrieffer-Heeger (SSH) – although the SSH model is specifically written for polyacetylene, so this name is a bit too specific. In any event, if we keep only nearest-neighbor hopping and set $t(\vec{R}_n^{(0)} - \vec{R}_m^{(0)}) = t$ if n, m are nearest neighbors, then in this

case:

$$\mathcal{H}_{el-ph} = -g \sum_{n,\sigma} \left(c^\dagger_{n\sigma} c_{n+1,\sigma} + h.c. \right) \left(b^\dagger_n + b_n - b^\dagger_{n+1} - b_{n+1} \right)$$

where the factor in front collects all the constants, $g = t\alpha\sqrt{\frac{\hbar}{2M\Omega}}$, and for simplicity I wrote this for a 1D chain. If you Fourier transform this one, it will have the standard form with explicit dependence on both the electron's and the phonon's momenta, k and q, respectively.

Given that I spent the last decade studying electron-phonon couplings and their consequences on the polaron spectrum, let me say that the discussion that follows, although it's standard textbook stuff and would be perceived by most condensed matter physicists as giving a fair idea of about all the important/interesting aspects of this problem, it is in fact rather specialized to models of the first type, where the coupling came through the potential energy (not the kinetic energy, like in SSH). The second class of models is just now beginning to be investigated more thoroughly and oftentimes leads to qualitatively different behavior. But this is not a course specialized on polarons and there really isn't time to go into such detailed discussions.

2 Effects of the electron-phonon coupling

Here we will assume that the electron-phonon coupling is weak enough that we can treat it perturbatively. To go beyond this level we need to know diagrammatics and even non-perturbative approaches, and you will only learn those in more advanced courses. The goal for now is simply to gain some intuition about what this coupling is likely to do.

The Hamiltonian we will study is:

$$\hat{H} = \hat{H}_0 + \hat{H}_{el-ph} = \sum_{k,\sigma} E(k) c^\dagger_{k\sigma} c_{k,\sigma} + \sum_q \hbar\omega_q b^\dagger_q b_q + \frac{1}{\sqrt{N}} \sum_{k,q,\sigma} g(q) \left[b^\dagger_{-q} + b_q \right] c^\dagger_{k+q,\sigma} c_{k\sigma} \qquad (6)$$

Here all k, q should be assumed to be vectors corresponding to the dimension we are working in, but I won't bother to put the vectors on them. If we have a lattice model, then the sums over quasimomenta are restricted to the Brillouin zone. If we have free electrons then their momentum can be anything, but for phonons we still have a restriction to $|q| \leq q_D$, where q_D is the Debye radius. Clearly, we assume that the e-e interactions are weak-enough that it is a good approximation to express the electronic part in terms of free electrons (quasiparticles), but possibly with a dispersion $E(k)$ quite different from that of free electrons, $\epsilon(k) = \frac{\hbar^2 k^2}{2m}$. For simplicity, we also assume a single phonon mode – generalization to many modes is straightforward.

The coupling $g(q)$ is assumed to be "small", so that we can use perturbation theory with some confidence. How "small" is defined quantitatively depends of the quantity of interest and details of the model. One way to check that it is small enough is to calculate the next order correction, in perturbation theory, and make sure that it is at least an order of magnitude smaller than the one we stopped at. We won't do this because the calculations become rather boring, but if you want some practice, you should try it.

In any event, if the eigenstate of $\hat{H}_0$ of interest is $|\Psi_0\rangle$ (assumed to be non-degenerate) and its energy is E_0, then perturbation theory tells us that the eigenstate and energy become:

$$|\Psi_1\rangle = |\Psi_0\rangle + \frac{1 - P_0}{E_0 - \hat{H}_0} \hat{H}_{el-ph} |\Psi_0\rangle + ...$$

and

$$E_2 = E_0 + \langle\Psi_0|\hat{H}_{el-ph}\Psi_0\rangle + \langle\Psi_0|\hat{H}_{el-ph}\frac{1-P_0}{E_0-\hat{H}_0}\hat{H}_{el-ph}|\Psi_0\rangle + ...$$

where $1-P_0 = 1-|\Psi_0\rangle\langle\Psi_0|$ makes sure we are projecting out the state $|\Psi_0\rangle$ (else the denominators blow up). Note: the formula above can be straightforwardly generalized to deal with low-energy degenerate manifolds, like discussed in one of the homework problems.

2.1 Polaron and mass enhancement

Let us first study the effect of the electron-phonon coupling on the electron's (quasiparticle) dispersion. For simplicity, let's assume that we are at $T = 0$, so that there are no thermally excited phonons in the system (you can repeat this at finite-T and see what is the difference). So we start with some zero-phonon eigenstate of $\hat{H}_0$ and want to see the effect of the electron-phonon coupling on it.

The simplest case we can consider is when we have a *single electron* in the system, i.e. the zeroth order state and energy are $|\Psi_0\rangle = c^\dagger_{k,\sigma}|0\rangle$ and $E_0 = E(k)$, respectively. Let's focus on the effect of the e-ph coupling on the quasiparticle energy:

$$\tilde{E}(k) = E(k) + \langle 0|c_{k\sigma}\hat{H}_{el-ph}\frac{1-P_0}{E_0-\hat{H}_0}\hat{H}_{el-ph}c^\dagger_{k\sigma}|0\rangle + ...$$

It is clear that we have to go to second order: the first order contribution vanishes because the coupling changes the number of phonons:

$$\hat{H}_{el-ph}c^\dagger_{k\sigma}|0\rangle = \frac{1}{\sqrt{N}}\sum_q g(q)b^\dagger_{-q}c^\dagger_{k+q,\sigma}|0\rangle$$

so we can't have a finite matrix element between zero-phonon states. However, there is a second-order correction. The energy of this intermediate state is $E(k+q)+\hbar\omega_q$, so the denominator is straightforward and we find:

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{E(k+q)+\hbar\omega_q - E(k)} + ...$$

To make some more progress, let's assume we are at the bottom of a tight-binding band (or in a free electron model) where we can approximate $E(k) = \frac{\hbar^2k^2}{2m}$, where in the former case, m already contains corrections due to interactions with the static lattice and possibly e-e interactions, at a mean-field level. For simplicity, let me also assume that the phonon is optical and we model it as an Einstein mode with $\omega_q = \Omega$. Then:

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{\hbar\Omega + E(q) + \frac{\hbar^2}{m}\vec{k}\vec{q}} + ... = E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{\hbar\Omega+E(q)}\left[1 - \frac{\frac{\hbar^2}{m}\vec{k}\vec{q}}{\hbar\Omega+E(q)} + \left[\frac{\frac{\hbar^2}{m}\vec{k}\vec{q}}{\hbar\Omega+E(q)}\right]^2 + ..\right] + ..$$

if $\vec{k}$ is small enough so that we can treat it term perturbatively, as well. If we again do the trick with distorting the BZ in a sphere of radius q_D, we see that the integral proportional to $\vec{q}$ will vanish by symmetry, while in the one proportional to $k_iq_ik_jq_j$ only terms with $i = j$ are non-zero (and equal to one another). In other words, we find:

$$\tilde{E}(k) = E(k) - E_P - \frac{\hbar^2k^2}{2m}\lambda + ...$$

where $E_P = \frac{1}{N}\sum_q \frac{|g(q)|^2}{\hbar\Omega + E(q)} > 0$ and $\lambda = \frac{2\hbar^2}{3mN}\sum_q \frac{|g(q)|^2 q^2}{[\hbar\Omega + E(q)]^3} \ll 1$ (if the coupling is small) are some positive energy and dimensionless number, respectively, which can be calculated if we know $g(q)$. Using $1 - \lambda \approx \frac{1}{1+\lambda}$, we find:

$$\tilde{E}(k) = -E_P + \frac{\hbar^2 k^2}{2m(1+\lambda)} = -E_P + \frac{\hbar^2 k^2}{2m^*}$$

In other words, the coupling to the phonons has (a) lowered the energy by some overall constant E_P, and (b) enhanced the effective mass $m \to m^* = m(1+\lambda)$. This shows that we can still speak about a quasiparticle, but one that is somewhat heavier and has lower energy than the *bare particle*, i.e. if the coupling wasn't there.

This quasiparticle is called a **polaron**, and you should think of it as being the original quasiparticle surrounded by a cloud of phonons that propagates coherently with it (the particle keeps emitting and absorbing phonons and thus generates this cloud of phonons that accompanies it). The quasiparticle itself was the original electron together with a cloud of electron-hole pairs (if the original model included e-e interactions; if not, it was just the bare electron), so now we're adding phonons to this "dressing" cloud. So the quasiparticle becomes a more complex composite object, but overall we can still think of it as one single whole object, which has a certain energy that depends in a certain way on its momentum.

How do we know that there are phonons moving with the polaron? Very easily, from its wavefunction:

$$|\Psi(k)\rangle = c^\dagger_{k\sigma}|0\rangle + \frac{1}{\sqrt{N}}\sum_q \frac{g(q)}{E(k+q) + \hbar\omega_q - E(k)} b^\dagger_{-q} c^\dagger_{k+q,\sigma}|0\rangle + ...$$

which shows that with some probability, there is a phonon together with the electron (of course, in higher orders we'll find terms with more phonons).

So the simple picture here is this: if you place the electron somewhere in the system, because of the interaction with the ions, the nearby ions are pulled out from their equilibrium positions, in other words the electron locally distorts the lattice (this distortion can be decomposed as a sum of phonons). This lowers the energy overall, and that explains the E_P term, also known as the polaron formation energy. Now, if the electron moves slowly through the crystal, this lattice distortion moves with it (hence the polaron) but slows it down somewhat because it takes some time for a new distortion to form at the new location of the electron, and the old distortion to relax back to equilibrium after the electron moved away.

Based on this, it seems reasonable to assume that as we increase the electron-phonon coupling even beyond the range where we can use perturbation theory, the distortion grows and therefore the effective mass grows as well. Indeed, in models with $g(q)$ coupling, this turns out to be true. For instance, one can show that at large couplings, the Holstein model polaron becomes exponentially heavy (probably homework).

However, you can see that it was very important in all this that $g(q)$ did not also depend on k. If it did, then what we just said may or may not be valid depending on the specific form of that dependence. As I said, recent work shows that models with $g(k,q)$ coupling can have polarons that are lighter (even at strong coupling) than the particle would be without coupling. That should not be that surprising because remember that $g(k,q)$ coupling is due to changing the hopping integrals, in other words the presence of phonons here can enhance the hopping and thus make the polaron more mobile (lighter).

2.2 Polaron revisited

What we've just discussed is fine if we have a single electron (quasiparticle) in the system. That would be relevant, for instance, if we study a very weakly doped insulator. But what about if we have a metal?

Warning: this discussion is somewhat different from that appearing in standard textbooks, eg. Taylor and Heinonen, or Madelung. The bottom line is that this problem is complex enough that even perturbational calculations can only be done correctly (without any hand-waving) using diagrammatics. That is something you will discuss in Phys503. The textbooks are trying to pretend they're doing a proper complete calculation without having the proper formalism for it, and I think it fairer to not pretend we can do more than we can. Of course, the gist is the same and we'll reach the same conclusions about what is the effect of el-ph coupling (at least in this weakly-coupling regime).

So back to our problem. First, let's assume we have an inert Fermi sea: $|FS\rangle = \prod_{|\vec{k}|<k_F,\sigma} c^\dagger_{\vec{k},\sigma}|0\rangle$. By inert, I mean that these electrons do not interact with the phonons, they just sit there as spectators. Now assume that I add an extra electron above the Fermi sea, so that the state is $c^\dagger_{\vec{k},\sigma}|FS\rangle$ with $k > k_F$. This additional electron is allowed to emit and absorb phonons. If we repeat the calculation just like before, assuming that only this particular electron is allowed to scatter and emit the phonon, we find its energy to be:

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{(1-\langle n_{k+q}\rangle)|g(q)|^2}{\hbar\Omega + E(k+q) - E(k)}$$

where the $(1-\langle n_{k+q}\rangle)$ factor is because we can move an electron from state k into state $k+q$ only if that second state was empty to begin with! So we have an additional phase-space restriction, because of the Pauli principle and the presence of the Fermi sea.

You can now see that something must happen to $\tilde{E}(k)$ for k such that $E(k) \approx E_F + \hbar\Omega$, because in this case there are empty $k+q$ states for which the denominator vanishes. Indeed, following some rather brutal approximations (mirroring the ones in the textbook), one can see that the speed $\vec{v}_k = \frac{1}{\hbar}\nabla_{\vec{k}}\tilde{E}(\vec{k})$ diverges here (the expression from the textbook also diverges although that expression is a bit different, see discussion below). Of course, at this point we should worry that we can't use perturbation theory anymore, a singularity is not a "small correction" by any means. Again, I'll return to this in a bit.

Given that the energies of quasiparticles added above the Fermi sea are changed, we should wonder what happens to those in the Fermi sea (because of course those electrons aren't inert). We could investigate that, for instance, just picking one electron out of all in the Fermi sea, and allowing $\hat{H}_{el-ph}$ to act only on it to scatter it above the Fermi sea, and then back. The expression will be just like the one above. This shows that the el-ph coupling doesn't have much effect on the energy of quasiparticles lying well below the Fermi energy, because these scattering processes become less and less likely (the denominator increases so the correction is smaller).

However, we could look at this in another way, by starting with a hole in the Fermi sea: $c_{\vec{k},\sigma}|FS\rangle$ and seeing how its energy (which is $-E(k)$, missing object) changes at is scatters on phonons. In this case, another electron from the Fermi sea must be involved (it scatters into this hole state leaving a phonon behind, and then the process is reversed) - so we can't even talk about an inert Fermi sea. In any event, we now find:

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{\langle n_{k-q}\rangle|g(q)|^2}{E(k-q) - E(k) - \hbar\Omega}$$

Unlike the expression above, this suggests that something non-trivial happens at $|k| < k_F$ such that $E(k) = E_F - \hbar\Omega$ because here the denominator can again vanish for the appropriate q. BUT: how can we get two different expressions for $\tilde{E}(k)$ when $k < k_F$, and what does that mean? Well, the different expressions are because we are comparing different situations. In one case we had N_e electrons, in the other $N_e - 1$, so this tells us we better be very careful how we define things. The reason why the number of quasiparticles matter (as obvious from the various occupation numbers) is that phonons actually induce effective electron-electron interactions, as we'll see in a bit. As soon as we have interactions, we cannot think of the total energy as being a sum of quasiparticle energies, like we're trying to do here, so the whole procedure we are following here becomes suspect.

The correction in textbooks is basically the sum of these two expressions discussed here. The proper calculation done with diagrammatics will take into consideration the fact that the Fermi sea is not inert, instead all those electrons are turned into polarons themselves; this further complicates what happens when we remove or add an extra particle, but diagrammatics allows us to calculate changes systematically upon addition or removal of one particle.

The result (in agreement with experiment), looks something like in the next figure: there is a so-called "kink" in the slope of the energy at $\hbar\Omega$ below the Fermi energy (I'm assuming $E_F \gg \hbar\Omega$, which is usually the case). This can be measured through photoemission spectroscopy, when an electron with momentum $\vec{k}$ is kicked out of the Fermi sea to create a hole, like in the case discussed above. Energies above E_F are measured by inverse photoemission spectroscopy, when an electron is injected above the Fermi sea (the first case we discussed). One should not put both curves in one figure, like many textbooks do, because they represent very different states (electron removal vs. electron addition, i.e. they are in different Hilbert sectors). So things are quite complicated, but the bottom line is that we expect a change in the slope of quasiparticles within $\hbar\Omega$ of E_F – these quasiparticles can scatter easily by emitting and absorbing phonons, so they become "heavier" than the quasiparticles that are far from the Fermi energy.

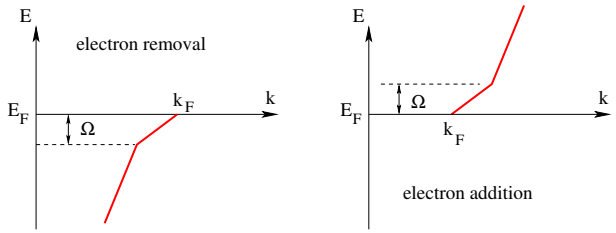

Figure 1: Change in slope of the energy $E(k)$ for states below and above the Fermi energy.

2.3 Phonon-induced electron-electron interaction

As mentioned above, one major reason for the complications that arise here is that the coupling to phonons does not only change the quasiparticle energies (the quadratic part of the Hamiltonian), but also gives rise to effective interactions between them. In other words, even if the original quasiparticles could be assumed to be non-interacting (eg, because of very effective screening), coupling to phonons will make them interacting again!

How such interactions come about it is very simple: one electron scatters from $k \to k + q$ while emitting a phonon, and then another electron absorbs that phonon to scatter from $k' \to k' - q$ (this is referred to as an exchange of phonons between the polaron clouds). Overall it looks like

we started with two electrons with momenta k, k' and ended up with two electrons with momenta $k+q, k'-q$, i.e. a process described by a standard interaction (quartic) term:

$$V = \frac{1}{2N} \sum_{\substack{k,k',q \\ \sigma,\sigma'}} V_{k,k'}(q) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}$$

which describes the same overall process. We would like to know how is $V_{k,k'}(q)$ related to the electron-phonon coupling. To second order in perturbation theory, our Hamiltonian is:

$$\hat{H} \approx \hat{H}_0 + \hat{H}_{el-ph} \frac{1-P_0}{E_0 - \hat{H}_0} \hat{H}_{el-ph}$$

and we're trying to put this in the effective form:

$$\hat{H} = \sum_{k,\sigma} \tilde{E}(k) c^\dagger_{k,\sigma} c_{k,\sigma} + \frac{1}{N} \sum_{\substack{k,k',q \\ \sigma,\sigma'}} V_{k,k'}(q) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}$$

As discussed previously, we can find $\tilde{E}(k)$ by collecting terms where the perturbation involves a single electron (or hole). To find the value of $V_{k,k'}(q)$, we should ask that matrix elements between all states where 2 particles have scattered also be equal. For instance, assume first that we only have two electrons in the system. Then, asking that all $\langle 0 | c_{k'-q,\sigma'} c_{k+q,\sigma} ... c^\dagger_{k,\sigma} c^\dagger_{k',\sigma'} | 0 \rangle$ be equal for both expressions, we can identify:

$$V_{k,k'}(q) = 2|g(q))|^2 \left[\frac{1}{E(k) - E(k+q) - \hbar\Omega} + \frac{1}{E(k') - E(k'-q) - \hbar\Omega} \right]$$

There are two terms because either electron can be the one that emits the phonon, i.e. scatters first. If these two electrons are above a filled Fermi sea, then this changes to:

$$V_{k,k'}(q) = 2|g(q))|^2 \left[\frac{1 - \langle n_{k+q} \rangle}{E(k) - E(k+q) - \hbar\Omega} + \frac{1 - \langle n_{k'-q} \rangle}{E(k') - E(k'-q) - \hbar\Omega} \right]$$

where the occupation numbers show that those final states must also be above the Fermi sea, else the scattering is not allowed. This leads to the extraordinary prediction that if these electrons are within a small energy Ω above the Fermi sea, specifically if $E_F < E(k), E(k') < E_F + \hbar\Omega$, then the phonon-mediated interaction between them is **attractive** because both those terms are definitely negative! ($E_{k+q} > E_F$ if $k+q$ is empty). Similarly, you can check that two holes that are within $\hbar\Omega$ below E_F also experience effective attraction due to phonon-exchange. As we'll see soon, this attraction, no matter how small it is, has extraordinary effects on the state of the system: it makes it turn superconducting at low enough temperatures!

Before going on to superconductivity, let us also see what is the effect of the electron-phonon coupling on the phonons. And before doing that, let me mention that for a Hamiltonian like the one at the top of the page, one has to be careful when assigning a quasiparticle energy. The expression for $\tilde{E}(k)$ was the one obtained from perturbation theory, however we know that this gets further renormalized in the presence of interactions (think about Hartree-Fock for jellium model). The expression for the quasiparticle energy given in textbooks includes this mean-field like correction, hence the difference from the expressions I listed (but this has no qualitative effects, both show that "kink" in the energy at $\hbar\Omega$ of E_F). Again, the bottom line is to realize that untangling what is happening here is not trivial, and that a more powerful formalism is needed to sort out the proper way of doing things.

2.4 Phonon renormalization and the Kohn anomaly

So now let us assume that we have a filled Fermi sea plus a phonon of momentum $\vec{q}$, to see how the interaction with the electrons changes its energy. So we take again a diagonal matrix element and we attribute the new terms that come from the processes where this phonons is absorbed by an electron (which is therefore excited above the Fermi sea) and then re-emitted with the same frequency back. It is also possible that a second identical phonon is first emitted, and then the original phonon is absorbed. Taken together, these lead to:

$$\hbar\tilde{\omega}_q = \hbar\Omega + \frac{|(g(q)|^2}{N}\sum_k \left[\frac{\langle n_k(1-n_{k+q})\rangle}{\hbar\Omega + E_k - E_{k+q}} + \frac{\langle n_k(1-n_{k-q})\rangle}{E_k - E_{k-q} - \hbar\Omega}\right]$$

If we change in the second sum $k \to k+q$ the denominators become equal and we can simplify the expression to:

$$\hbar\tilde{\omega}_q = \hbar\Omega + \frac{|(g(q)|^2}{N}\sum_k \frac{\langle n_k\rangle - \langle n_{k+q}\rangle}{\hbar\Omega + E_k - E_{k+q}}$$

where we recognize the Lindhart function on the right hand side. This shows that even if we started with a dispersionless Einstein mode, the interaction with the valence electrons makes it acquire a momentum dependence (if the phonons were acoustic, we should have used $\hbar\omega_q$ everywhere on the rhs). As we know, the Lindhart function can be calculated analytically. The result I gave you was valid when we could set $\hbar\Omega \approx 0$ in the denominator, which is reasonable if the phonon frequency is much smaller than the Fermi energy. Then, the Lindhart function becomes a function with a singularity in the slope at $q = 2k_F$. Physically, this is because phonons with this momentum can always excite an electron from below the Fermi sea (say, just below $-k_F$) to above the Fermi sea (just above k_F).

Indeed, phonon spectra show a "kink" in their dispersion near $q = 2k_F$, as sketched below. This is known as **the Kohn anomaly**, and its strength gives an idea about how small or large is the electron-phonon coupling.

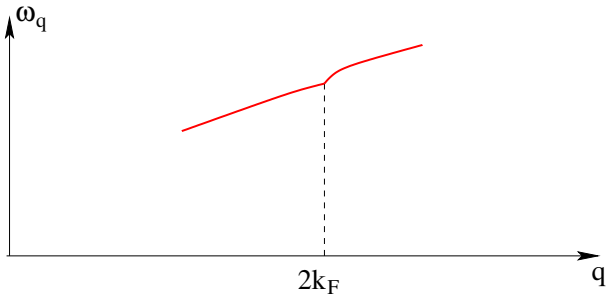

Figure 2: Kohn anomaly in the phonon dispersion at $q = 2k_F$.

Is this all there is (at weak coupling)? The answer is no. If we had more than one phonon, they could scatter on one another through particle-hole pairs creation and annihilation. That would add anharmonic terms to the effective Hamiltonian (which, again, is why we should find a better way to identify these terms in a systematic way). But even if we stop here in terms of possible processes, note that we specialized the analysis to a $g(q)$ coupling for most of the discussion. If instead the coupling depended on both k and q, the results could be very very different.

To conclude, I hope this gives you a flavor of the complications that arise when electron-phonon interactions are added in the Hamiltonian: even though we started with non-interacting electrons and phonons (i.e., we assumed those to be good approximations) we see that electron-phonon coupling induces such effective interactions, which we then have to deal with. Not only that, but these phonon-induced e-e interactions can be attractive! As I said, we can use diagrammatics to deal with this problem in a more systematic way (when the coupling is week). However, I think it is fair to say that this problem is still very far from being understood in the general case. We understand well the so-called Migdal limit, when $E_F \gg \hbar\Omega$ and the el-ph coupling is weak (this is where the Kohn anomaly and everything else we discussed above holds). We also have a pretty good understanding of the single polaron limit (i.e. $E_F = 0$), at both weak and strong coupling. The behavior in all other regimes is essentially unknown.