**Electron-Phonon Interaction**

Now we’ll add in phonons – lattice oscillations.

**Beginning**

Now we want to consider the effects of the electrons interacting with a mobile lattice in our semiconductor. We can borrow the generic e-ph Hamiltonian we derived in the Metals folder. The free electron and phonon Hamiltonians are together,



And k for the phonons is restricted to the Brillouin zone. With metals, we eventually saw (see Interacting Electrons and Phonons file) that the effective acoustic lattice oscillation frequencies, Ωkλ, were linear in k, due to screening electrons. But in a semiconductor, we often don’t have so many electrons that the ion-ion interaction gets effectively screened, and so the acoustic branch will have a *finite* minimum at k = 0. The branches will look something like this (3 acoustic branches and 3 optical branches pictured):

Chart, surface chart

Description automatically generated

In an isotropic solid, I guess one acoustic branch will be longitudinal (pointing along **q**), and two will be transverse (perpendicular to **q**). Anyway, now we’d like to explore the form of the e-ph interaction Hamiltonian, as we did in metals. Many of the results will be similar.

**Acoustic Coupling**

First we’ll look at coupling between electrons and the electric field created by the motion of the lattice basis as a whole. Oscillations of lattice atoms which are in phase w/in the basis are called acoustic oscillations. The interaction between electrons and acoustic oscillations is the dominant form of interaction in metals and we treated it pretty thoroughly there. But one difference between metals and semiconductors is that we’ll not treat the potential between an individual ‘ion’ in the lattice and a given electron as the Coulomb potential. We can’t really justify that approach per se´ because while in metals, each atom (or basis, more generally) contributes one or two electrons to the conduction band, and makes itself an ion therefore, each atom of a semiconductor doesn’t do this. At normal temperatures, there are far fewer electrons in the condunction band than that. The convention is to treat it phenomenologically as some of short ranged ‘deformation’ potential. And previous protestations notwithstanding, we’ll suppose it to be centered at every lattice site.



So I’ll just review. So we have:



And then we’ll expand the potential in powers of x.



The first term is our crystal potential. The second is what we’ll call the e-ph interaction (ph being vibrating lattice). We’ll ignore higher order terms. So now we have:



I guess I’ll put the electron/crystal part in 2nd quantized notation, as is standard, presuming the crystal potential just renormalizes the electron mass. And refering back to our work on the free lattice, we saw that (with our CMT phase convention for a, a†):



where the a’s are the annihilation operators of lattice excitations. Note one reason the phase convention we’re using is prefered is that the i out front cancels the i in Veph. If we plug those into the lattice part of H, then altogether we have, for the free part,



I’m making it explicitly clear that our sum runs over the BZ when pertaining to phonons. Now let’s continue to work out Veph,



Doing the integral over r,



Now split the q sum into the part that ranges over BZ and simultaneously over the reciprocal lattice vectors, and do the sum over **R**. That gives us Nδq´q´´. Oh yeah, and ei**K**·**R** = 1 by definition of reciprocal lattice vector **K**…



I think I’ll change primes to unprimes, and going to leave just a factor of 1/√V on the outside.



and recall from Quantum Mechanics/Identical Particles/2nd quantization files,



At this point, we can combine the sum over **q** ∈ BZ, and **K** ∈ RLV into just a sum over all q, provided we stipulate that Ωqλ, **ε**qλ, and Aqλ (and later the associated GF) is a periodic function of **q**, so that when **q** extends past the BZ, we just map it back to the BZ by subtracting off the requisite number of RLV, **K**. Kind of like this (illustrated for acoustic spectrum, which we don’t necessarily have, but you get the idea):

Chart, line chart

Description automatically generated

So then we’ll have:



where ρion = MionN/V, and nion = N/V. And we eliminate the q = 0 mode from the interaction as q = 0 corresponds to uniform displacements, which we do not consider. Let’s specialize to an isotropic system. Then **ε**kλ is either parallel or perpendicular to **k,** corresponding to longitudinal or transverse phonon branches, respectively. We’ll call λ = 3 the mode parallel to k (or q whatever you call it).



And so we have:



And finally, we can fill in our phenomenological approximation to the e-ion potential,



to get,



**Piezoelectric coupling (sketchy)**

The piezoelectric effect is an electric field is generated in certain semi-conductors when squeezed. So it’s a type of acoustic e-ph interaction. Semi-conductors must lack an inversion center to be piezoelectric. We can derive an expression for the induced electric field generated by squeezing the crystal, and once we have, we can obtain the potential induced everywhere in the crystal consequently. And once we have that, we can determine the energy of the electrons from being placed in this potential. Then that gives us the effective e-ph. Hamiltonian for these crystals. The induced electric field is:



where S is the stress-tensor. Where **U** is the displacement variable formerly known as **x**, and given by:



Filling this in, we have:



And so,



So anyway, that gives us the induced field in terms of the tensor M. Mahan says that doing some work on the form of Mijk (somewhere), we can show it reduces to something like,



So then we have:



And now we can determine the potential derivable from this field via (kind of extending q sum over BZ to all q):



Comparing the two, we come to a formula for the effective potential:



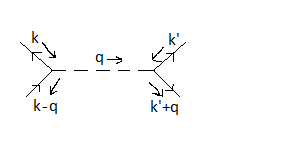
And we can now write down the effective e-ph. interaction for these piezoelectric semiconductors. Borrowing a little work from above,



Can write this as:



where ρion = MionN/V. Apparently Mλ(q) depends very much on the direction of q. Evidenttally, in order for Heph to be Hermitian, we at least need Mλ(-q) = Mλ(q). But otherwise, it seems most people just approximate it as a constant. We can estimate this value in the following way. We consider the effective e-e interaction mediated by the phonon. We can see what this is simply by observing that the effective potential comes from the value of the diagram shown below. So if we just put two phonon vertices together to get a Feynman diagram representation of the e-ph-e interaction.



If this were e-e graph, then this would be G0(k)G0(k-q)[-V(q)]G0(kʹ)G­0(-kʹ-q), where V(q) is the e-e interaction. For the phonon graph, this would be G0(k)G0(k-q)(-g(q))[-D0(q)](-g(-q))G0(kʹ)G0(-kʹ-q), where D0(q) = -2/Ωq in the small frequency limit. So we can identify the effective phonon-mediated interaction between electrons as:



If we take the acoustic frequency spectrum to be acoustic-like, then can say Ωq ~ vsq, in which case we have:



Then taking the inverse Fourier transform:



And so we have an effective (attractive) Coulomb interaction between the electrons, mediated by the these piezoelectric/acoustic phonons. And we come to the same sort of interpretation. Two electrons polarize the medium changasing the energy of the situation, which can be interpreted as an effective interaction between the electrons. When the electrons come closer, they polarize the medium more, hence the dependence on r. So we can write, to lowest order in η,



where ε is the dielectric constant. So we can estimate M from the dielectric constant.

**Polar Coupling**

Let’s now specialize to a lattice with a polar basis (GaAs is a semiconductor with a two-atom basis, but not sure if it’s polar). And we’ll consider specifically the optical branch of lattice oscillations. Since optical branch oscillations have the basis atoms moving out of phase, this means that the dipole moment of the basis will be created/changing. And this means an electric field will be created, similar to how we modelled the induced electric field created in insulators due to displacment of an insulating atom’s electron cloud w/r to its nucleus. Note the basis atoms’ deviations from their equilibrium positions is described by plane waves with some k in BZ, so it is periodic. We can be quantitative. We’ll go back to EM folder and write (fake Gaussian units here, see Units file perhaps]:



Thus the induced E-field, coming from the basis atoms, that interacts with the electrons is proportional to the polarization. And the polarization is proportional to Δ**x**(r), where Δ**x**(r) is the separation between atoms in the basis, in some sense. Taking the Fouerier transform of this, we have,



where a3 is the unit cell volume, and η is some proportionality constant. Now recall from the Classical Mechanics folder that the formula for the positions of the atoms in a basis is:



where i denotes the lattice site, and δ denotes the atom in the basis. So Δx would be, in some sense,



I feel like we can just redefine the Akλ’s and **ε**kλδ’s, to write this in the usual form:



And can get rid of the δ index if just have two of these guys. So,



And this is just the usual acoustic form. So I think we can just appropriate the usual 2nd version of the position operators for acoustic waves. Now recall from the Metal e-ph interaction file we found the acoustic ionic oscillations were given by:



Now taking the Fourier transform, (where we’ve kind of taken a limit that R → r so we have a continuous **x** field)



Then we have:



We may determine a potential from this. Consider that:



So,



and then comparing, we have



Evidently, for this to work out we need εqλ to point in direction q. Typically there is a longitudinal polarization **ε**­q3, which does this, and two transverse polarizations **ε**q1, **ε**q2 which don’t. So we’ll go with λ = 3. And we’ll write ε­­q3­­ = . And then we can say,



And now we integrate this times the e charge density over all space and obtain the e-ph Hamiltonian. We find:



where,



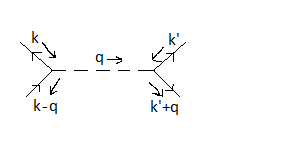
If we say that a3 = V/N, then we can write this as:



which is the same as the form of the metal interaction, coincidentally. Can write this is:



Note if η = 1, we would have the exact same expression as we had for the metallic case. But we can estimate the proportionality constant by estimating the effective e-e interaction by adding both the bare e-e potential term and phonon mediated potential term. We did this same calculation in the Metal e-ph interaction file. So if we just put two phonon vertices together to get a Feynman diagram representation of the e-ph-e interaction.



If this were e-e graph, then this would be G0(k)G0(k-q)[-V(q)]G0(kʹ)G­0(-kʹ-q), where V(q) is the e-e interaction. For the phonon graph, this would be G0(k)G0(k-q)(-g(q))[-D0(q)](-g(q))G0(kʹ)G0(-kʹ-q), where D0(q) = -2/Ωq in the small frequency limit. So we can identify the effective phonon-mediated interaction between electrons as:



Then taking the inverse Fourier transform:



(if we take the optical limit for our Ω’s, making them constant thereby) And so we have an effective (attractive) Coulomb interaction between the electrons, mediated by the optical phonons. So we can write, to lowest order in η,



where ε is the dielectric constant. So then,



where n = N/V.

**Tight Binding Model**

Semiconductor bands are probably *best* modelled using the tight binding approach. So let’s give this a consideration. We’ll look at using it to model an interaction with acoustic phonons. So the Hamiltonian of a single electron part would be:



where the sum runs over all lattice sites, **x**j is the deviation (it’s a vector) of the jth atom from its lattice site. And we’ll take the tightbinding states |jν> ~ φν(r-Rj) to be eigenstates of:



with eigenvalues εν. And so the 2nd quantized H would be for all electrons in the crystal would be:



Let’s expand for small x,



The first term is the Hamiltonian of the electron in the periodic crystal field. And the second term is the e-ph interaction term. I guess I’ll do a little more work on the former,



where we have defined:



which is the potential at site j coming from all the other sites’s potentials. Now ΔVei,j(r) should not actually depend on j, due to the crystal’s periodicity. And further, the expectation <jν|ΔVei,j(r)|kν´> should only depend on the relative position of the two sites, i.e., on **R**k – **R**j = **R**δ. So I’m going to write reparameterize |k> as |j+δ>, and write:



So going back to:



So then we have:



Now let’s look at the e-ph part. Note we can slide the |kν´> past the xℓ operator, as they exist in different Hilbert Spaces.



Let’s split this up into j = k and j ≠ k terms,



We can write the j = k guy as:



What about that potential term?



Filling this in,



If we were to define,



Then we’d have:



Now let’s look at:



And I think we’ll say k = j + δ, where δ roams over nearest neighbors. Also, as far as the potential is concerned, I think we’ll specialize to the case where ℓ = j or ℓ = k = j + δ. These should be the predominant contributions.



…making a few changes of variables. We’ll note the second term is the Hermitian conjugate of the first. So we can write this as:



The matrix element shouldn’t depend on j, just ν, ν´, and δ. So we can say,



And we can say,



I’d think that Vei(r) probably has something like spherical symmetry. So we’d get something like:



Now without the φν´ term, we’d just get zero. Or if δ were not there, we’d get zero. Otherwise, the integrand will be largest where φν(r-δ) is largest, which is at **r** = **δ**. So I think **r** = **δ** will get the most contribution from the integrand. So we should be able to approximately say,



So altogether we might say,



where,



This isn’t want Mahan gets. I don’t know how he ends up with his result. And I don’t. care.