The electron-phonon interaction

- The Frölich Hamiltonian
- Perturbation theory
- Polarons
- the effective attraction between electrons

The Fröhlich Hamiltonian

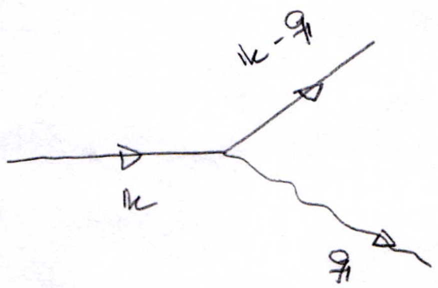
In a crystal, the electrons and the ions rely heavily on each other. The electrons form energy bands due to the periodic potential created by the ions. And the ions are held together and may vibrate due to the presence of the electrons, which mediate the interatomic interaction.

But so far we have treated these two effects as independent (which is called the Born - Oppenheimer approximation). As a first approximation, this is not too bad. The masses of the electrons and ions are quite different so the time scales of their motion are usually well sepparated: the electrons adapt themselves quickly, so during a vibration of the ions, the electrons simply go along adiabatically.

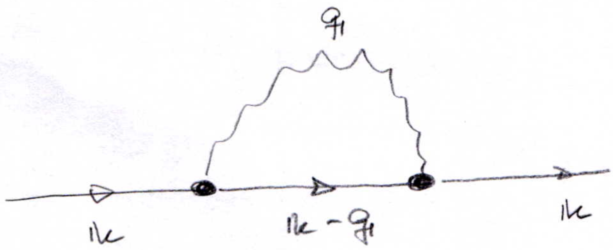
Notwithstanding, there are situations where the electron-phonon interaction plays an important role. The simplest effect is the introduction of a temperature dependence on the electrical conductivity of metals. In ionic crystals, like NaCl (salt), the interaction of an electron with optical phonons cause the electron to carry with it a cloud of charge due to the ions (which is what we call a polaron). This modifies the mass of the electron considerably.

Finally, electrons may interact with each other by the exchange of virtual phonons. For the electrons close to the Fermi surface, this interaction turns out to be attractive. this causes the electrons to bound themselves into cooper pairs, which is the microscopic origin of superconductivity

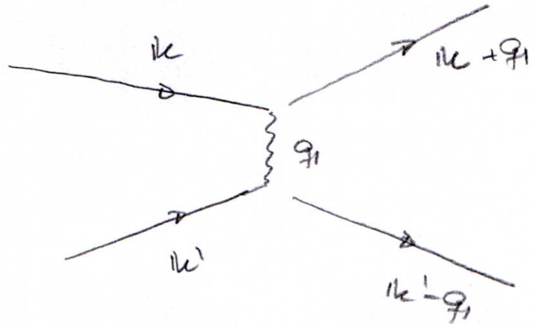
we can represent these 3 effects I just mentioned by diagrams of the electron-phonon interactions



Electrons are scattered by phonons, increasing the resistivity. the number of phonons changes with T, which introduces a temperature dependence in the resistivity



Emission and absorption of a virtual phonon by the electron. this causes a change in mass for the electron.



Exchange of a virtual phonon by a pair of electrons. this can give rise to an attractive force, binding them into cooper pairs.

Consider a lattice with ions at equilibrium positions $\mathbb{R}_m$. The potential energy felt by an electron at position $\mathbb{r}$ due to all ions in the crystal will then be

$$V_{ei}(\hat{\mathbb{r}}) \sum_m v(\hat{\mathbb{r}} - \mathbb{R}_m) \qquad (1)$$

where $v(\mathbb{r})$ is the attractive (and perhaps screened) coulomb potential

$$v(\mathbb{r}) = -Ze^2 \frac{e^{-\mu r}}{r} \qquad (2)$$

The Hamiltonian of a single electron will then be

$$H = \frac{\mathbb{p}^2}{2m} + V_{ei}(\mathbb{r}) \qquad (3)$$

It is this periodic potential $V_{ei}(\mathbb{r})$ that gives rise to the appearance of energy bands and Bloch wavefunctions.

The new ingredient we now introduce is the possibility for the ions to vibrate around their equilibrium positions. Thus, the atomic positions are no longer $\mathbb{R}_m$ but $\mathbb{R}_m + \mathbb{u}_m$, where $\mathbb{u}_m$ is the displacement from equilibrium. When the ions are displaced from equilibrium, the total potential becomes

$$V_{ei}(\hat{\mathbb{r}}) = \sum_m v(\hat{\mathbb{r}} - \mathbb{R}_m - \mathbb{u}_m) \qquad (4)$$

By the way, I'm writting $\hat{\mathbb{r}}$ just to emphasize that $\hat{\mathbb{r}}$ is the position operator for the electron.

We now move to second quantization using the standard recipe for single particle Hamiltonians:

$$\mathcal{A} = \sum_{\alpha,\beta} \langle \alpha | A | \beta \rangle \, c_\alpha^\dagger c_\beta \tag{5}$$

We use for the single-particle basis the momentum states $|k\rangle$. then V_{ei} becomes

$$\mathcal{V}_{ei} = \sum_{\mathbb{k}\mathbb{k}'n} \langle \mathbb{k} | V(\mathbb{r} - \mathbb{R}_n - \mathbb{u}_n) | \mathbb{k}' \rangle \, c_{\mathbb{k}}^\dagger c_{\mathbb{k}'} \tag{6}$$

We now define the Fourier transform

$$\langle \mathbb{k} | V(\mathbb{r} - \mathbb{R}_n - \mathbb{u}_n) | \mathbb{k}' \rangle = \frac{1}{v_0} \int d^3\mathbb{r} \; V(\mathbb{r} - \mathbb{R}_n - \mathbb{u}_n) \, e^{i(\mathbb{k}' - \mathbb{k}) \cdot \mathbb{r}}$$

change variables to $\mathbb{x} = \mathbb{r} - \mathbb{R}_n - \mathbb{u}_n$. then

$$\langle \mathbb{k} | V(\mathbb{r} - \mathbb{R}_n - \mathbb{u}_n) | \mathbb{k}' \rangle = \frac{1}{v_0} \int d^3\mathbb{x} \, V(\mathbb{x}) \, e^{i(\mathbb{k}' - \mathbb{k}) \cdot (\mathbb{x} + \mathbb{R}_n + \mathbb{u}_n)}$$

$$= e^{i(\mathbb{k}' - \mathbb{k}) \cdot (\mathbb{R}_n + \mathbb{u}_n)} \, V(\mathbb{k} - \mathbb{k}') \tag{7}$$

where

$$V(\mathbb{p}) = \frac{1}{v_0} \int d^3\mathbb{x} \;\; V(\mathbb{x}) \, e^{-i\mathbb{p} \cdot \mathbb{x}} \tag{8}$$

Eq (6) then becomes

$$\mathcal{V}_{ei} = \sum_{\substack{\mathbb{k},\mathbb{k}' \\ m}} e^{i(\mathbb{k}'-\mathbb{k})\cdot(\mathbb{R}_m + \mathbb{u}_m)} V(\mathbb{k}-\mathbb{k}') c^{\dagger}_{\mathbb{k}} c_{\mathbb{k}'} \tag{9}$$

we now assume the displacements $\mathbb{u}_m$ are small, allowing us to expand

$$e^{i(\mathbb{k}'-\mathbb{k})\cdot\mathbb{u}_m} \simeq 1 + i(\mathbb{k}'-\mathbb{k})\cdot\mathbb{u}_m \tag{10}$$

we also introduce the Fourier transform

$$\mathbb{u}_m = \frac{1}{\sqrt{N}} \sum_{\mathbb{q}} e^{i\mathbb{q}\cdot\mathbb{R}_m} \mathbb{u}_{\mathbb{q}} \tag{11}$$

then

$$e^{i(\mathbb{k}'-\mathbb{k})\cdot\mathbb{u}_m} \simeq 1 + \frac{i}{\sqrt{N}} (\mathbb{k}'-\mathbb{k}) \cdot \sum_{\mathbb{q}} e^{i\mathbb{q}\cdot\mathbb{R}} \mathbb{u}_{\mathbb{q}} \tag{12}$$

this then allows us to sepparate (9) into two terms

$$\mathcal{V}_{ei} = \mathcal{V}_{ei}^{(0)} + H_{ep} \tag{13}$$

where

$$\mathcal{V}_{ei}^{(0)} = \sum_{\mathbb{k}\,\mathbb{k}'\,m} e^{i(\mathbb{k}'-\mathbb{k})\cdot\mathbb{R}_m} V(\mathbb{k}-\mathbb{k}') c^{\dagger}_{\mathbb{k}} c_{\mathbb{k}'} \tag{14}$$

$$H_{ep} = \frac{i}{\sqrt{N}} \sum_{\substack{\mathbb{k}\,\mathbb{k}' \\ \mathbb{q},\, m}} e^{i(\mathbb{k}'-\mathbb{k}+\mathbb{q})\cdot\mathbb{R}_m} (\mathbb{k}'-\mathbb{k})\cdot\mathbb{u}_{\mathbb{q}}\, V(\mathbb{k}-\mathbb{k}') c^{\dagger}_{\mathbb{k}} c_{\mathbb{k}'} \tag{15}$$

The operator $V_{ei}^{(0)}$ is just the ionic potential in the absence of vibrations. This is the usual periodic potential that gives rise to the energy bands. We can combine $V_{ei}^{(0)}$ with the kinetic energy to obtain the electron Hamiltonian

$$H_0 = \sum_{k} \frac{k^2}{2m} c_k^{\dagger} c_k + V_{ei}^{(0)} \qquad (16)$$

We will not worry about this guy too much. We know that what it does is split the energies into bands. But we also saw that, within these bands, the electrons move freely with dispersion relations of the form $k^2/2m$, but with m being an effective mass. Thus, henceforth we will simply assume that

$$H_0 = \sum_{k} \epsilon_k c_k^{\dagger} c_k \qquad (17)$$

where $\epsilon_k = k^2/2m$.

Next we turn to H_{ep} in (15), which is the electron-phonon interaction. We can carry out the sum over n, which will give a $\delta_{q, k-k'}$. Thus we get

$$H_{ep} = i\sqrt{N} \sum_{k k'} (k'-k)\cdot u_{k-k'} V(k-k') \, c_k^{\dagger} c_{k'} \qquad (18)$$

This couples the electron momenta $c_k^{\dagger} c_{k'}$ with the ion displacements $u_{k-k'}$

Change variables as $k = k' + q$, then we get

$$H_{ep} = -i\sqrt{N} \sum_{k' q_1} q_1 \cdot u_q \, V(q) \, C^{\dagger}_{k'+q_1} C_{k'} \tag{19}$$

Finally we relate u_q with the phonon creation and annihilation operators $a^{\dagger}_{q_1 \lambda}$ and $a_{q\lambda}$, where λ distinguishes the different phonon branches. They are related by

$$u_{q_1} = \sum_{\lambda} \frac{\hat{e}_{q\lambda}}{\sqrt{2M\omega_{q\lambda}}} \left(a_{q\lambda} + a^{\dagger}_{-q\lambda} \right) \tag{20}$$

where $\hat{e}_{q\lambda}$ is the polarization vector.

We see in (19) the appearance of $q_1 \cdot u_{q_1}$. Thus, only the longitudinal phonon branch will contribute. We then finally obtain

$$\boxed{H_{ep} = \sum_{kq} g_q \, C^{\dagger}_{k+q_1} C_k \left(a_q + a^{\dagger}_{-q} \right)} \tag{21}$$

where

$$\boxed{g_q = -i\sqrt{N} \frac{|q|}{\sqrt{2M\omega_q}} V(q)} \tag{22}$$

We therefore see that the electron-phonon interaction is interpreted as a 3-body process. One electron comes in with momentum $\mathbb{k}$ and either creates or destroys a phonon with momentum q, leaving with momentum $\mathbb{k}+q$.

The amplitude for each process to occur is g_q. Assuming $v(r)$ is a Yukawa potential (screened coulomb)

$$v(r) = -Ze^2 \frac{e^{-\mu r}}{r} \rightsquigarrow V(q) = -\frac{Ze^2}{q^2+\mu^2} \tag{23}$$

we then get

$$g_q = \frac{i\sqrt{N}}{\sqrt{2M\omega_q}} \, Ze^2 \, \frac{q}{q^2+\mu^2} \tag{24}$$

For acoustic phonons, $\omega_q \sim q$ and thus $g_q \sim 1/q^{3/2}$.

For optical phonons $\omega_q \sim 1$ so $g_q \sim 1/q$.

Perturbation theory

The total Hamiltonian of the electron-phonon system is

$$\boxed{H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q a_q^\dagger a_q + \sum_{kq} g_q c_{k-q}^\dagger c_k (a_q + a_{-q}^\dagger)} \qquad (25)$$

If $g_q = 0$ then the electrons and phonons do not interact at all. Thus, if we let $H = H_0 + H_{ep}$, then we know all the eigenstates of H_0: they are the Foch states for the electrons and phonons.

Now we are going to treat H_{ep} as a perturbation. Let me first make a comment about perturbation theory. You have probably seen the formula

$$E_m = E_m^{(0)} + \langle m | V | m \rangle + \sum_{m \neq m} \frac{|\langle m | V | m \rangle|^2}{E_m^{(0)} - E_m^{(0)}}$$

This can be written in a slightly nicer way as

$$E_m = E_m^{(0)} + \langle m | V | m \rangle + \langle m | V \frac{1}{E_m^{(0)} - H_0} V | m \rangle \qquad (26)$$

provided we take the assumption that, in the last term, we avoid any terms which diverge.

This formula is interesting for many reasons. First, as we will see, it gives a neat physical interpretation in terms of Feynmann diagrams. Second, it tells us how to extend the perturbation to higher orders. For instance, the third order term will be

$$\langle m | V \frac{1}{E_m^{(0)} - H_0} V \frac{1}{E_m^{(0)} - H_0} V | m \rangle \qquad (27)$$

and so on. Finally, Eq (26) allows us to extend the calculations to mixed states by taking on an additional thermal average in the end.

Now let $|\psi\rangle$ be a state with n_q phonons with mom. q and n_k ($=0,1$) electrons with momentum k. That is

$$|\psi\rangle = \text{some Fock state w/ different electron and phonon numbers.} \qquad (28)$$

Then the correction to the energy will be

$$\boxed{\mathcal{E} = \mathcal{E}_0 + \langle \psi | H_{ep} | \psi \rangle + \langle \psi | H_{ep} \frac{1}{\mathcal{E}_0 - H_0} H_{ep} | \psi \rangle} \qquad (29)$$

The first order term is zero because H_{ep} changes the number of phonons in the system, so $\langle\psi|$ and $H_{ep}|\psi\rangle$ will be orthogonal. The 2nd order term will be, using (21)

$$\mathcal{E}_2 = \langle\psi|\Big[\sum_{kq} g_q\, c^{+}_{k+q} c_k (a_q + a^{+}_{-q})\Big] \frac{1}{\mathcal{E}_0 - H_0}$$

$$\cdot\Big[\sum_{k'q'} g_{q'}\, c^{+}_{k'+q'} c_{k'} (a_{q'} + a^{+}_{-q'})\Big]|\psi\rangle$$

Out of the 4 terms that appear, the only that survive are those with $\langle\psi|a_q(\dots)a^{+}_{-q'}|\psi\rangle$ and $\langle\psi|a^{+}_{-q}(\dots)a_{q'}|\psi\rangle$. The other two will have sandwiches with different numbers of phonons. Thus we get

$$\mathcal{E}_2 = \sum_{\substack{kq\\k'q'}} g_q g_{q'} \Big\{\langle\psi|c^{+}_{k+q} c_k a_q (\mathcal{E}_0 - H_0)^{-1} c^{+}_{k'+q'} c_{k'} a^{+}_{-q'}|\psi\rangle$$
$$+ \langle\psi|c^{+}_{k+q} c_k a^{+}_{-q} (\mathcal{E}_0 - H_0)^{-1} c^{+}_{k'+q'} c_{k'} a_{q'}|\psi\rangle\Big\} \qquad (30)$$

Since H_0 does not affect the phonon number, these terms will only be non-zero when $-q' = q$. Thus we get

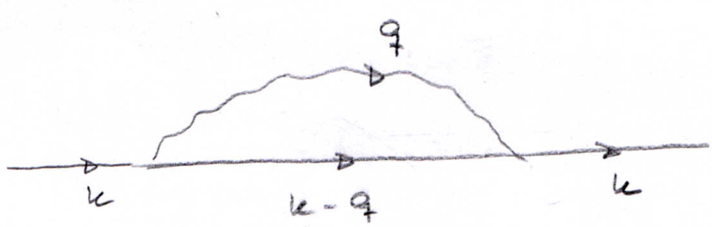
$$\mathcal{E}_2 = \sum_{kk'q} g_q g_{-q} \Big\{\langle\psi|c^{+}_{k+q} c_k a_q (\mathcal{E}_0 - H_0)^{-1} c^{+}_{k'-q} c_{k'} a^{+}_{q}|\psi\rangle$$
$$+ \langle\psi|c^{+}_{k+q} c_k a^{+}_{-q} (\mathcal{E}_0 - H_0)^{-1} c^{+}_{k'-q} c_{k'} a_{-q}|\psi\rangle\Big\} \qquad (31)$$

In each term, the only non-zero elements will be those which conserve momentum. this means that $k' = k - q$. thus

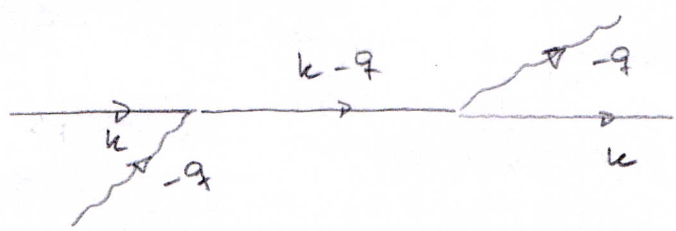
$$\boxed{\begin{aligned} \mathcal{E}_2 = \sum_{kq} |g_q|^2 \Big\{ &\langle \psi | c_k^{\dagger} c_{k-q} a_q (\mathcal{E}_0 - H_0)^{-1} c_{k-q}^{\dagger} c_k a_q^{\dagger} | \psi \rangle \\ &+ \langle \psi | c_k^{\dagger} c_{k-q} a_{-q}^{\dagger} (\mathcal{E}_0 - H_0)^{-1} c_{k-q}^{\dagger} c_k a_{-q} | \psi \rangle \Big\} \end{aligned}} \qquad (32)$$

these two terms may be represented graphically as follows

1st term:



2nd term:



In the first term an electron is scattered from k to k-q by the creation of a phonon. the term $(\mathcal{E}_0 - H_0)^{-1}$ is a measure of the time the electron-phonon pair coexists. then the electron eventually reabsorbs the phonon and recovers the momentum k.

In the 1^{st} term of (32) the operator $(\mathcal{E}_0 - H_0)^{-1}$ is sandwiched between the ket $|\psi'\rangle = c^+_{k-q} c_k a^+_q |\psi\rangle$. Since $\mathcal{E}_0 - H_0$ gives the energy difference between the configuration $|\psi\rangle$ and $|\psi'\rangle$ we see that

$$\langle \psi' | (\mathcal{E}_0 - H_0)^{-1} | \psi' \rangle = \frac{-1}{\epsilon_{k-q} - \epsilon_k + \omega_q}$$

In the second term $|\psi'\rangle = c^+_{k-q} c_k a_{-q} |\psi\rangle$ so

$$\langle \psi' | (\mathcal{E}_0 - H_0)^{-1} | \psi' \rangle = \frac{-1}{\epsilon_{k-q} - \epsilon_k - \omega_q}$$

where I used the fact that $\omega_{-q} = \omega_q$. Thus, (32) becomes

$$\mathcal{E}_2 = -\sum_{kq} |g_q|^2 \left\{ \frac{\langle \psi | c^+_k c_{k-q} a_q c^+_{k-q} c_k a^+_q | \psi \rangle}{\epsilon_{k-q} - \epsilon_k + \omega_q} + \frac{\langle \psi | c^+_k c_{k-q} a^+_{-q} c^+_{k-q} c_k a_{-q} | \psi \rangle}{\epsilon_{k-q} - \epsilon_k - \omega_q} \right\} \tag{33}$$

Finally, we rearrange the operators to write them on a more convenient way.

$$\langle \psi | c_k^\dagger c_{k-q}\, a_q\, c_{k-q}^\dagger\, c_k\, a_q^\dagger | \psi \rangle = \langle \psi | c_k^\dagger c_k\, c_{k-q}\, c_{k-q}^\dagger\, a_q\, a_q^\dagger | \psi \rangle$$

$$= \langle c_k^\dagger c_k (1 - c_{k-q}^\dagger c_{k-q}) (a_q^\dagger a_q + 1) \rangle$$

Let

$$\hat{n}_k = c_k^\dagger c_k \qquad \hat{n}_q = a_q^\dagger a_q .$$

then we get

$$\boxed{\mathcal{E}_2 = -\sum_{kq} |g_q|^2 \langle \hat{n}_k (1 - \hat{n}_{k-q}) \rangle \left\{ \frac{\langle \hat{n}_q \rangle + 1}{\epsilon_{k-q} - \epsilon_k + \omega_q} + \frac{\langle \hat{n}_{-q} \rangle}{\epsilon_{k-q} - \epsilon_k - \omega_q} \right\}} \tag{34}$$

this result is true for any Fock state $|\psi\rangle$. Now we may perform an additional average over thermal states. then

$$\langle \hat{n}_q \rangle = \langle \hat{n}_{-q} \rangle = \frac{1}{e^{\beta \omega_q} - 1} \tag{35}$$

and

$$\langle \hat{n}_k \rangle = \frac{1}{e^{\beta \epsilon_k} + 1} \tag{36}$$

Moreover, provided $q \neq 0$, $\langle \hat{n}_k (1 - \hat{n}_{k-q}) \rangle = \langle n_k \rangle \langle 1 - \hat{n}_{k-q} \rangle$.

thus (34) becomes

$$\varepsilon_2 = -\sum_{kq} |g_q|^2 \langle \hat{n}_k \rangle \langle 1 - \hat{n}_{k-q} \rangle \left\{ \frac{1}{\epsilon_{k-q} - \epsilon_k + \omega_q} + \right.$$

$$\left. + \frac{2 \langle \hat{m}_q \rangle (\epsilon_{k+q} - \epsilon_k)}{(\epsilon_{k-q} - \epsilon_k)^2 - \omega_q^2} \right\} \qquad (35)$$

A final detail: there will be a term which is

$$\sum_{kq} \langle \hat{n}_k \rangle \langle n_{k-q} \rangle \langle m_q \rangle (\epsilon_{k+q} - \epsilon_k)$$

this term will be zero by symmetry since we are summing over k, q. thus we finally write

$$\boxed{\varepsilon_2 = -\sum_{kq} |g_q|^2 \frac{\langle \hat{n}_k \rangle \langle 1 - \hat{n}_{k-q} \rangle}{\epsilon_{k-q} - \epsilon_k + \omega_q} + - \sum_{kq} |g_q|^2 \frac{2 \langle \hat{n}_k \rangle \langle \hat{m}_q \rangle (\epsilon_{k-q} - \epsilon_k)}{(\epsilon_{k-q} - \epsilon_k)^2 - \omega_q^2}} \qquad (36)$$

this is the first correction to the energy of the system due to the electron-phonon interaction.

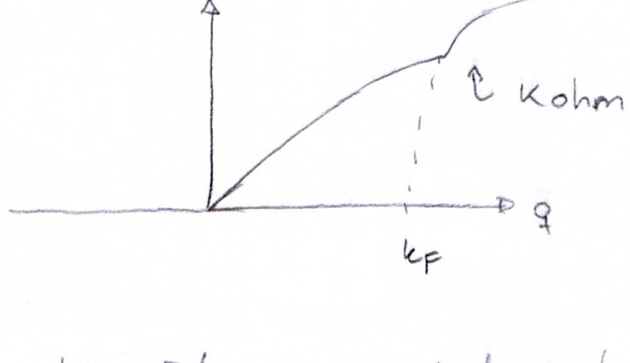
The phonon energy in equilibrium is $\sum_q' \omega_q \langle m_q \rangle$. We see now that we get a new term in (36) due to the electron-phonon interaction. Thus, the phonon dispersion relation is renormalized according to

$$\boxed{\tilde{\omega}_q = \omega_q - \sum_k' |g_q|^2 \frac{2\langle \hat{n}_k \rangle (\epsilon_{k-q} - \epsilon_k)}{(\epsilon_{k-q} - \epsilon_k)^2 - \omega_q^2}} \tag{37}$$

Assuming $\omega_q \ll |\epsilon_{k+q} - \epsilon_k|$ we may approximate this as

$$\tilde{\omega}_q = \omega_q - 2|g_q|^2 \sum_k' \frac{\langle \hat{n}_k \rangle}{(\epsilon_{k-q} - \epsilon_k)} \tag{38}$$

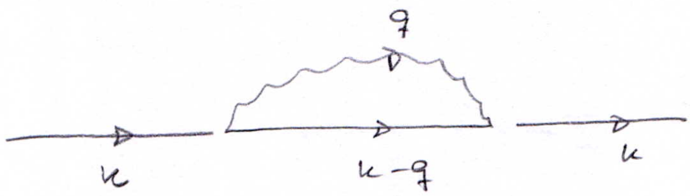
This contribution will introduce an anomaly in $\tilde{\omega}_q$ when q is close to the Fermi momentum k_F. For, it is only around k_F that $\langle \hat{n}_k \rangle$ changes substantially. This is known as a Kohn anomaly



This should not exist in insulators, but only in metals.

Polarons

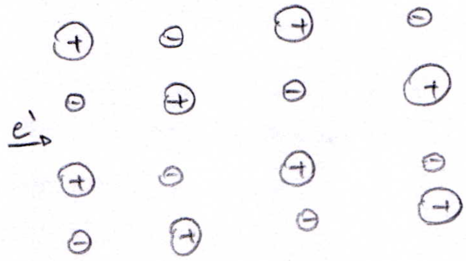
Returning to the processes I drew in page 12, we see that even if we have just one electron moving in a lattice with no phonons, the electron-phonon interaction will still have an effect:



when the electron moves it may create and reabsorb phonons as it moves along. To obtain that from (36) we set $\langle n_q \rangle = 0$. we then get

$$E_2 = -\sum_{kq} |g_q|^2 \frac{\langle n_k \rangle \langle 1 - \hat{n}_{k-q} \rangle}{\epsilon_{k-q} - \epsilon_k + \omega_q} \tag{39}$$

this effect becomes particularly interesting in ionic crystals, like NaCl, where the electron couples strongly with the longitudinal optical mode.



As the electron moves around, the positive ions are attracted to it and the negative ions are repelled. This creates a cloud of charge that follows the electron around. The electron plus its cloud is called a <u>polaron</u>.

In ionic crystals $\omega_q \simeq \omega_0 = \text{const}$. Moreover, as discussed around Eq (29), $g_q \sim 1/q$. It is customary to define

$$g_q = i\left[\frac{(2\sqrt{2}\,\pi\alpha)}{v_0}\right]^{1/2}\frac{1}{q}$$

where v_0 is the volume and α is a constant measuring the strength of the interaction. These weird constants in front are chosen so that things come out pretty in the end.

Returning now to (39), we assume we have only 1 electron with momentum p, so $\langle \hat{n}_k\rangle = \delta_{kp}$. Then the correction to the energy of this electron will be

$$\Delta\epsilon = -\frac{2\sqrt{2}\,\pi\alpha}{v_0}\sum_q \frac{1}{q^2}\,\frac{1}{\frac{(p-q)^2}{2m}-\frac{p^2}{2m}+\omega_0} \tag{40}$$

It will be fun to compute this sum. The final result will be quite interesting.

For simplicity we set $m = \omega_0 = 1$. Then, converting the sum to an integral we get

$$\Delta E = -2\sqrt{2}\,\pi\alpha \int \frac{d^3 q_1}{(2\pi)^3} \frac{1}{q^2} \frac{1}{\frac{q^2}{2} - p \cdot q_1 + 1}$$

$$\Delta E = -4\sqrt{2}\,\pi\alpha \int \frac{d^3 q_1}{(2\pi)^3} \frac{1}{q^2} \frac{1}{q^2 - 2p \cdot q_1 + 2} \qquad (41)$$

Now we use an awesome trick due to Feynman, based on the following identity

$$\frac{1}{ab} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2} \qquad (42)$$

We use this with $b = q^2$ and $a = q^2 - 2q_1 \cdot p + 2$. We then get

$$\Delta E = -4\sqrt{2}\,\pi\alpha \int_0^1 dx \int \frac{d^3 q_1}{(2\pi)^3} \frac{1}{\left[(q^2 - 2q_1 \cdot p + 2)x + q^2(1-x)\right]^2}$$

We simplify the denominator to

$$q^2 - 2x\, q_1 \cdot p + 2x = (q_1 - xp)^2 + 2x - x^2 p^2$$

Now let $\lambda = 2x - x^2 p^2$ and change the q variable to $q \to q_1 - x p$. We then get

$$\Delta\epsilon = -4\sqrt{2}\,\pi\,\alpha \int_0^1 dx \int \frac{d^3 q_1}{(2\pi)^3} \frac{1}{(\lambda + q^2)^2}$$

We can now compute the q integral

$$\int \frac{d^3 q_1}{(2\pi)^3} \frac{1}{(\lambda^2 + q^2)^2} = \frac{1}{8\pi\sqrt{\lambda}}$$

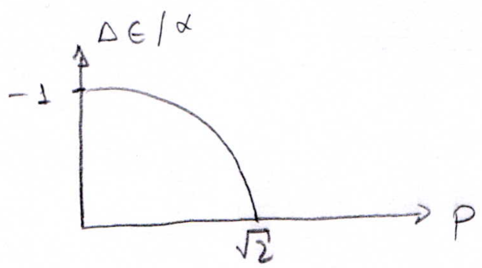
Thus

$$\Delta\epsilon = -\frac{4\sqrt{2}\,\pi\,\alpha}{8\pi} \int_0^1 dx \frac{1}{\sqrt{2x - x^2 p^2}}$$

This integral can also be computed exactly:

$$\boxed{\Delta\epsilon = -\frac{\alpha\sqrt{2}}{p} \arcsin\left(\frac{p}{\sqrt{2}}\right)} \qquad (43)$$

This looks like this



Two points stand out from this result. First, when p is small we get

$$\Delta E \simeq -\alpha - \frac{\alpha}{12} p^2 \qquad (44)$$

We add this to the kinetic energy $p^2/2$ (recall that $m = 1$). We then get

$$\epsilon_p \simeq -\alpha + \frac{p^2}{2}\left(1 - \frac{\alpha}{6}\right)$$

$$\simeq -\alpha + \frac{1}{2} \frac{p^2}{1 + \frac{\alpha}{6}}$$

Thus we see that the mass of the electron changes as

$$\frac{m_{eff}}{m} = 1 + \frac{\alpha}{6} \qquad (45)$$

the electron-phonon interaction increases the mass of the electron: since the polaron has to carry a charge cloud with it, it becomes heavier. Here are some typical values of α:

	KCl	KBr	AgCl	AgBr	ZnO	PbS	GaAs	InSb
α	4.0	3.5	2.0	1.7	0.85	0.16	0.06	0.014

Another interesting point about (21) is that the energy becomes imaginary when $p > \sqrt{2}$. This can be interpreted as dissipation of energy by Cherenkov radiation. If you inject an electron with a really high momentum into the crystal it will simply emit radiation and eventually stop.

The effective attraction between electrons

Let us return once again to our perturbative correction (36). We see that there is a term which is proportional to $\langle \hat{m}_k \rangle \langle \hat{m}_{k-q} \rangle$:

$$\mathcal{E}_2 = \sum_{k,q} |g_q|^2 \frac{\langle \hat{m}_k \rangle \langle \hat{m}_{k-q} \rangle}{\epsilon_{k-q} - \epsilon_k + \omega_q} \tag{46}$$

This term can be interpreted as an effective interaction between electrons. We can also write it in a more convenient way as follows. Exchang the summation variables

$$k = k' - q' \qquad \Rightarrow \qquad q = k - k' = -q'$$
$$k - q = k'$$

Since $\omega_{-q} = \omega_q$ we get

$$\mathcal{E}_2 = \sum_{k'q'} |g_{q'}|^2 \frac{\langle m_{k'-q'} \rangle \langle m_{k'} \rangle}{\epsilon_{k'} - \epsilon_{k'-q'} + \omega_{q'}} \tag{47}$$

Now we write $\mathcal{E}_2$ as the average of (46) and (47)

$$\mathcal{E}_2 = \sum_{k,q} \frac{|g_q|^2}{2} \langle n_k \rangle \langle n_{k-q} \rangle \left[\frac{1}{\epsilon_{k-q} - \epsilon_k + \omega_q} + \frac{1}{\epsilon_k - \epsilon_{k-q} + \omega_q} \right]$$

$$= \sum_{k,q} \frac{|g_q|^2}{2} \langle n_k \rangle \langle n_{k-q} \rangle \frac{2\omega_q}{\omega_q^2 - (\epsilon_{k-q} - \epsilon_k)^2}$$

or

$$\boxed{\mathcal{E}_2 = \sum_{kq} |g_q|^2 \langle n_k \rangle \langle n_{k-q} \rangle \frac{\omega_q}{\omega_q^2 - (\epsilon_{k-q} - \epsilon_k)^2}} \tag{48}$$

This result has a very very very very important interpretation. Even though ϵ_k may be very different from ω_q, the <u>sign</u> of the energy correction is determined by a comparison between ω_q^2 and an energy difference $(\epsilon_{k-q} - \epsilon_k)^2$. It is therefore possible that the phonons may mediate an <u>attractive</u> <u>interaction</u> between the electrons. This is the origin of <u>superconductivity</u>.

To make this more consistent, let us return to the full Frölich Hamiltonian

$$H = H_0 + H_{ep} \tag{49}$$

where

$$H_0 = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q a_q^\dagger a_q \tag{50}$$

$$H_{ep} = \sum_{k,q} g_q \, c_{k+q}^\dagger c_k \left(a_q + a_{-q}^\dagger \right) \tag{51}$$

We now perform a similarity transformation

$$H' = e^S H e^{-S} \tag{52}$$

where S is an operator. Using the BCH formula we get

$$\begin{aligned} H' &= H + [S, H] + \frac{1}{2}[S, [S, H]] + \cdots \\ &= H_0 + H_{ep} + [S, H_0] + [S, H_{ep}] + \\ &\quad + \frac{1}{2}[S, [S, H_0]] + \frac{1}{2}[S, [S, H_{ep}]] + \cdots \end{aligned} \tag{53}$$

We now choose S such that

$$H_{ep} + [S, H_0] = 0 \tag{54}$$

We are then left with

$$H' = H_0 + [S, H_{ep}] - \frac{1}{2}[S, H_{ep}] + \frac{1}{2}[S,[S,H_{ep}]] + \dots$$

or

$$H' \simeq H_0 + \frac{1}{2}[S, H_{ep}] \quad (55)$$

we take as ansatz

$$S = \sum_{k,q} g_q \, c^{\dagger}_{k+q} c_k \left(A a_q + B a^{\dagger}_{-q} \right) \quad (56)$$

where A, B are coefficients to be determined. Now we play with some commutation relations:

$$\begin{aligned}
[H_0, c_k] &= -\epsilon_k c_k \\
[H_0, c_k^{\dagger}] &= \epsilon_k c_k^{\dagger} \\
[H_0, a_q] &= -\omega_q a_q \\
[H_0, a_q^{\dagger}] &= \omega_q a_q^{\dagger}
\end{aligned} \quad (57)$$

Thus

$$\begin{aligned}
[H_0, c^{\dagger}_{k+q} c_k a_q] &= c^{\dagger}_{k+q}[H_0, c_k a_q] + [H_0, c^{\dagger}_{k+q}] c_k a_q \\
&= c^{\dagger}_{k+q}\left(c_k [H_0, a_q] + [H_0, c_k] a_q \right) \\
&\quad + [H_0, c^{\dagger}_{k+q}] c_k a_q \\
&= (\epsilon_{k+q} - \epsilon_k - \omega_q) c^{\dagger}_{k+q} c_k a_q
\end{aligned}$$

and

$$[H_0, c^\dagger_{k+q} c_k a^\dagger_{-q}] = (\epsilon_{k+q} - \epsilon_k + \omega_q)\, c^\dagger_{k+q} c_k a^\dagger_{-q}$$

Thus, given our ansatz (56), we get

$$[S, H_0] = \sum_{k,q} g_q \Big\{ A(\omega_q - \epsilon_{k+q} + \epsilon_k)\, c^\dagger_{k+q} c_k a_q$$
$$+ B(-\omega_q - \epsilon_{k+q} + \epsilon_k)\, c^\dagger_{k+q} c_k a^\dagger_{-q} \Big\}$$

Comparing with (54) and (51) we see that in order for (54) to be satisfied, we must have

$$A = \frac{1}{\omega_q - \epsilon_{k+q} + \epsilon_k} \qquad (58)$$

$$B = \frac{1}{-\omega_q - \epsilon_{k+q} + \epsilon_k}$$

Thus

$$\boxed{S = \sum_{k,q} g_q \left\{ \frac{c^\dagger_{k+q} c_k a_q}{\epsilon_k - \epsilon_{k+q} + \omega_q} + \frac{c^\dagger_{k+q} c_k a^\dagger_{-q}}{\epsilon_k - \epsilon_{k+q} - \omega_q} \right\}} \qquad (59)$$

Finally we plug this into (55). We get

$$\frac{1}{2}[S, H_{ep}] = \sum_{\substack{k,q \\ k'q'}} \frac{g_q g_{q'}}{2} \Big[A\, c^{\dagger}_{k+q} c_k a_q + B\, c^{\dagger}_{k+q} c_k a^{\dagger}_{-q} \,,$$
$$c^{\dagger}_{k'+q'} c_{k'} a_{q'} + c^{\dagger}_{k'+q'} c_{k'} a^{\dagger}_{-q'} \Big]$$

This commutator will be quite messy. But there are two terms which are quite special. Namely, those where there are no phonon operators. They will be

$$\frac{1}{2}[S, H_{ep}] = \sum_{\substack{kq \\ k'q'}} \frac{g_q g_{q'}}{2} \Big\{ A\, c^{\dagger}_{k+q} c_k [a_q, a^{\dagger}_{-q'}] c^{\dagger}_{k'+q'} c_{k'}$$
$$+ B\, c^{\dagger}_{k+q} c_k [a^{\dagger}_{-q}, a_{q'}] c^{\dagger}_{k'+q'} c_{k'} \Big\}$$
$$+ (\dots)$$

All other terms will still contain a's in them. Thus, they would be zero if we work within states of zero phonons. Now, this pretty term of ours, which I will call Hee, becomes

$$H_{ee} = \sum_{kqk'} \frac{|g_q|^2}{2} (A - B)\, c^{\dagger}_{k+q} c_k c^{\dagger}_{k'-q} c_{k'}$$

Making some final adjustments:

$$A - B = \frac{1}{\epsilon_k - \epsilon_{k+q} + \omega_q} - \frac{1}{\epsilon_k - \epsilon_{k+q} - \omega_q}$$

$$= \frac{2\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - \omega_q^2}$$

we may now finally write

$$\boxed{H_{ee} = \sum_{kk'q} V_q \, c^\dagger_{k+q} c^\dagger_{k'-q} c_{k'} c_k} \qquad (60)$$

where

$$\boxed{V_q = \frac{|g_q|^2 \omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - \omega_q^2}} \qquad (61)$$

we therefore see that, indeed, the electron-phonon interaction may be interpreted as an effective electron-electron interaction (a 4-body Hamiltonian) with an effective interaction V_q. And, what is most important, this interaction may be attractive for certain values of q.