Theorie der Kondensierten Materie II SS 2015

Prof. Dr. A. Shnirman
Dr. B. Narozhny

Blatt 4
Besprechung 22.05.2015

---

1. Polarons

We consider electrons in the conduction band of a semiconductor. The dispersion relation is $E(\vec{p}) = (\vec{p})^2/2m$, where m is the effective (band) mass and the energy is measured from the bottom of the conduction band. The electronic gas in the conduction band is non-degenerate, i.e., the chemical potential is in the gap between the valence and the conduction bands, i.e., $\mu < 0$.

Consider a situation in which electrons interact only via emission and absorption of virtual phonons (no direct Coulomb interaction). Effectively this means that the "wavy" line in our diagrammatic expansion is now replaced by a phononic line. The latter is proportional to the phonon Green's function:

$$U(\omega, \vec{q}) = g^2 \frac{\omega_0^2(\vec{q})}{\omega^2 - \omega_0^2(\vec{q}) + i0} \; . \tag{1}$$

Only acoustic phonons with the dispersion relation $\omega_0(\vec{q}) = c|\vec{q}|$ and $|\vec{q}| < q_D$ are taken into account. Here c is the sound velocity, q_D is the Debye momentum, and g is the coupling constant (deformation potential).

(a) **Calculate the lowest order contribution to the self-energy of the electrons, $\Sigma(\epsilon, \vec{p})$. The resulting Green's function describes now polarons (electrons dressed by phonons).**

The Feynman diagram corresponding to the lowest order self-energy is shown in Fig. 1.

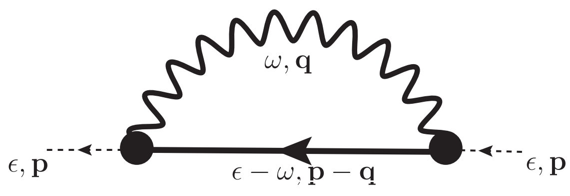


Abbildung 1: Lowest order diagram for self-energy

Using the diagrammatic rules we obtain

$$\Sigma(\epsilon, \mathbf{p}) = i \int \frac{d^d\mathbf{q}}{(2\pi)^d} \frac{d\omega}{2\pi} \, G_0(\epsilon - \omega, \mathbf{p} - \mathbf{q}) U(\omega, \mathbf{q}) \; ,$$

where

$$G_0 = \frac{1}{\epsilon - \epsilon_p + i0\,\mathrm{sign}\,\epsilon_p} \ .$$

Here $\epsilon_p \equiv E(\mathbf{p}) - \mu$. Since $\mu < 0$, we have $\epsilon_p > 0$. Thus,

$$G_0 = \frac{1}{\epsilon - \epsilon_p + i0} \ .$$

We obtain

$$\Sigma(\epsilon, \mathbf{p}) = ig^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} \frac{d\omega}{2\pi} \frac{1}{\left(\epsilon - \omega - \left[\frac{(\mathbf{p}-\mathbf{q})^2}{2m} - \mu\right] + i0\right)} \frac{c^2\mathbf{q}^2}{(\omega^2 - c^2\mathbf{q}^2 + i0)} \ ,$$

We use

$$\frac{c^2\mathbf{q}^2}{(\omega^2 - c^2\mathbf{q}^2 + i0)} = \frac{cq}{2}\left[\frac{1}{\omega - cq + i0} - \frac{1}{\omega + cq - i0}\right] \ , \tag{2}$$

where $q \equiv |\mathbf{q}|$.

We, first, perform the integration over ω. Only the first term in (2) contributes, as its pole is on the other side as compared to that of G_0. This gives

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} \frac{cq}{\left(\epsilon - \left[\frac{(\mathbf{p}-\mathbf{q})^2}{2m} - \mu\right] - cq + i0\right)} \ .$$

From now one we use $d = 3$. We use the spherical coordinates for $\mathbf{q}$ such that the angle θ is measured from the direction of $\mathbf{p}$. Then

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2}{2} \int \frac{q^2 dq \sin\theta d\theta}{(2\pi)^2} \frac{cq}{\left(\epsilon + \mu - \left[\frac{p^2}{2m} + \frac{q^2}{2m} + \frac{pq\cos\theta}{m}\right] - cq + i0\right)} \ .$$

We introduce $x = -\cos\theta$ and obtain

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 c}{8\pi^2} \int_0^{q_D} q^3 dq \int_{-1}^{1} dx \frac{1}{\left(\epsilon + \mu - \left[\frac{p^2}{2m} + \frac{q^2}{2m} - \frac{pqx}{m}\right] - cq + i0\right)} \ . \tag{3}$$

(b) **From** $\mathrm{Re}\Sigma(\epsilon, \vec{p})$ **extract the dispersion relation of the polaron. Find the binding energy and the effective mass of the polaron.** *Tip: show that near the mass shell ($\epsilon \approx E(\vec{p}) - \mu$) and for $|\vec{p}| \ll mc$ the self energy reads*

$$\Sigma(\epsilon, \vec{p}) = \epsilon_0 - \alpha_1 \left(\epsilon + \mu - E(\vec{p})\right) - \alpha_2 E(\vec{p}) \ .$$

Near the mass shell (of the bare electron) , i.e., for $\epsilon \approx \frac{p^2}{2m} - \mu$ the denominator of (3) is given by $\approx (\frac{pqx}{m} - \frac{q^2}{2m} - cq + i0)$. Since $q > 0$ we conclude that for $p \ll mc$ the denominator cannot vanish. Thus, in this regime ($\epsilon \approx p^2/(2m) - \mu$ and $p \ll mc$) the self-energy is purely real and we can disregard $i0$ in (3). The integral over x can be easily calculated, as it is a logarithmic one:

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 cm}{8\pi^2 p} \int_0^{q_D} q^2 dq \ln\left(\frac{\epsilon + \mu - \frac{(p-q)^2}{2m} - cq}{\epsilon + \mu - \frac{(p+q)^2}{2m} - cq}\right) \ .$$

Let us introduce two small parameters: $\Delta \equiv \epsilon + \mu - p^2/(2m)$ (has dimensions of energy) and $v = p/m$ (has dimensions of velocity). Then

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 cm}{8\pi^2 p} \int_0^{q_D} q^2 dq \ln \left(\frac{\frac{q^2}{2m} + q(c-v) - \Delta}{\frac{q^2}{2m} + q(c+v) - \Delta} \right) .$$

Let us first consider the situation exactly on-shell, $\Delta = 0$. Then, since $v \ll c$, we can expand in v/c and obtain

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 cm}{8\pi^2 p} \int_0^{q_D} q^2 dq \left(- \frac{2qv}{\frac{q^2}{2m} + qc} \right) = - \frac{g^2 c}{4\pi^2} \int_0^{q_D} \frac{q^3 dq}{\frac{q^2}{2m} + qc} .$$

Usually, q_D is of order of the inverse lattice constant, i.e., is large. Therefore, $q_D/m \gg c$. Thus, we can neglect cq in comparison to $q^2/(2m)$ in the most of the integration domain. This gives

$$\Sigma = \epsilon_0 \approx - \frac{g^2 cm q_D^2}{4\pi^2} .$$

This is the binding energy of the polaron. That is a polaron with $p = 0$ has a negative energy, lower that the bottom of the conduction band. Next, we expand to the power v^3 and reinstall Δ. We obtain

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 cm}{8\pi^2 p} \int_0^{q_D} q^2 dq \left(- \frac{2qv}{\frac{q^2}{2m} + qc - \Delta} - \frac{2(qv)^3}{3\left(\frac{q^2}{2m} + qc - \Delta\right)^3} + \ldots \right) .$$

Next we expand in Δ

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 cm}{8\pi^2 p} \int_0^{q_D} q^2 dq \left(- \frac{2qv}{\frac{q^2}{2m} + qc} - \frac{2qv\Delta}{\left(\frac{q^2}{2m} + qc\right)^2} - \frac{2(qv)^3}{3\left(\frac{q^2}{2m} + qc\right)^3} + \ldots \right) .$$

We again neglect qc in comparison with $q^2/(2m)$. The resulting logarithmic integrals should be cut off from below at $q \approx mc$

$$\Sigma(\epsilon, \mathbf{p}) = \frac{g^2 c}{8\pi^2} \int_{mc}^{q_D} dq \left(-4mq - \frac{8m^2\Delta}{q} - \frac{16m^3 v^2}{3q} \ldots \right) .$$

Thus, we obtain

$$\Sigma(\epsilon, \mathbf{p}) = \epsilon_0 - \alpha_1 \Delta - \alpha_2 \frac{p^2}{2m} ,$$

where

$$\alpha_1 = \frac{g^2 m^2 c}{\pi^2} \ln \left(\frac{q_D}{mc} \right) \quad \text{and} \quad \alpha_2 = (4/3)\alpha_1 .$$

We find the new dispersion relation by solving

$$\Delta - \Sigma(\epsilon, \mathbf{p}) = 0 .$$

This gives

$$(1+\alpha_1)\left(\epsilon+\mu-\frac{p^2}{2m}\right)-\epsilon_0+\alpha_2\,\frac{p^2}{2m}=0\ ,$$

and

$$\epsilon=\frac{p^2}{2m}\left(1-\frac{\alpha_2}{1+\alpha_1}\right)-\mu+\frac{\epsilon_0}{1+\alpha_1}\ .$$

We obtain the new mass

$$m^*=\frac{m}{1-\frac{\alpha_2}{1+\alpha_1}}\ .$$

The new mass is higher than the bare mass: the electron is "dressed by phonons".

(c) **Consider** $\mathrm{Im}\Sigma(\epsilon,\vec{p})$ **and find the life-time of a polaron with momentum** $\vec{p}$**.**

We start again with

$$\Sigma(\epsilon,\mathbf{p})=\frac{g^2c}{8\pi^2}\int_0^{q_D}q^3dq\int_{-1}^{1}dx\,\frac{1}{\left(\epsilon+\mu-\left[\frac{p^2}{2m}+\frac{q^2}{2m}-\frac{pqx}{m}\right]-cq+i0\right)}\ .$$

This gives

$$\mathrm{Im}\Sigma=-\frac{g^2c}{8\pi}\int_0^{q_D}q^3dq\int_{-1}^{1}dx\ \delta\left(\epsilon+\mu-\left[\frac{p^2}{2m}+\frac{q^2}{2m}-\frac{pqx}{m}\right]-cq\right)\ .$$

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{4\pi}\int_0^{q_D}q^3dq\int_{-1}^{1}dx\ \delta\left(2m(\epsilon+\mu-cq)-\left[p^2+q^2-2pqx\right]\right)\ .$$

We define $y=p^2+q^2-2pqx$. Then

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{8\pi p}\int_0^{q_D}q^2dq\int_{(p-q)^2}^{(p+q)^2}dy\ \delta\left(y-2m(\epsilon+\mu-cq)\right)\ .$$

Consider on-shell situation $\epsilon+\mu=p^2/(2m)$. Then, the argument of the delta-function can become zero if

$$\frac{(p+q)^2}{2m}>\frac{p^2}{2m}-cq>\frac{(p-q)^2}{2m}$$

(recall that $p>0$ and $q>0$). With $v=p/m$ this gives

$$\frac{q^2}{2m}+qv>-cq>\frac{q^2}{2m}-qv\ .$$

The left inequality is automatically fulfilled, whereas the right one gives

$$q<2m(v-c)\ .$$

Thus, the polaron has a finite life-time only if $v>c$. In this case we obtain

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{8\pi p}\int_0^{2m(v-c)}q^2dq=-\frac{g^2cm^3}{3\pi v}\,(v-c)^3\ .$$

This is the inverse life-time of the polaron (with velocity $v>c$).

2. Fermionic chain (Kitaev model)

Consider spinless fermions on a one-dimensional chain of sites, numbered by an index n. The Hamiltonian reads $H = H_0 + V$, where

$$H_0 = \sum_n \left(t a_n^\dagger a_{n+1} + t a_{n+1}^\dagger a_n - \mu a_n^\dagger a_n \right)$$

and

$$V = \sum_n \left(\Delta a_n a_{n+1} + \Delta a_{n+1}^\dagger a_n^\dagger \right) \ .$$

Here t, Δ and μ are real constants.

(a) **Find the Green's function G_0 corresponding to H_0.** *Tip: use the Fourier representation.*
The Fourier transformation yields

$$H_0 = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \epsilon_q a_q^\dagger a_q, \qquad V = i\Delta \int_{-\pi}^{\pi} \frac{dq}{2\pi} \sin q (a_{-q} a_q + a_{-q}^\dagger a_q^\dagger),$$

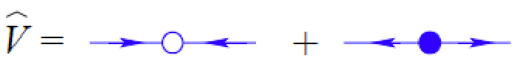
with

$$\epsilon_q = 2t \cos q - \mu.$$

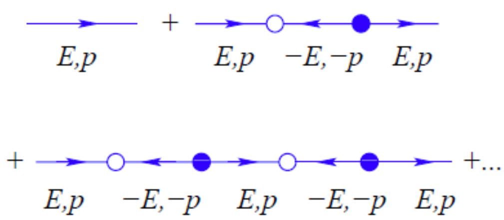
The "non-interacting" problem is characterized by the "free" Green's function

$$G_0(\epsilon, q) = \frac{1}{\epsilon - \epsilon_q + i\delta \mathrm{sign}\epsilon}.$$

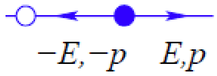
(b) **Consider the perturbation series for the Green's function G of the full problem. Develop the diagrammatic rules. Sum up the series and determine the dispersion relation of the new excitations.**
The interaction potential V corresponds to two vertices in the diagram technique:



The expressions corresponding to the two vertices are $2i\Delta \sin q$ and $-2i\Delta \sin q$, respectively.
The perturbative corrections to the Green's function form the following series:



Notice, that the signs alternate. This follows form the momentum conservation. Because of this, only "even-order" corrections appear in the series. The elementary block is represented by the pair of vertices and a pair of Green's functions.



In terms of this block, the series is a simple geometric progression. This can be summed up using the standard rule. Thus we find

$$G(\epsilon, q) = \frac{G_0(\epsilon, q)}{1 + 4\Delta^2 \sin^2 q G_0(\epsilon, q) G_0(-\epsilon, -q)} = \frac{\epsilon + 2t\cos q - \mu}{\epsilon^2 - [(2t\cos q - \mu)^2 + 4\Delta^2 \sin^2 q] + i\delta}.$$

The poles of the full Green's function give the excitation spectrum:

$$\epsilon = \pm\sqrt{(2t\cos q - \mu)^2 + 4\Delta^2 \sin^2 q}.$$

The sign of the imaginary term $i\delta$ in $G(\epsilon, q)$ points out that the upper branch of the spectrum is empty, while the lower branchis fully occupied.

(c) **Could the solution be found without perturbation theory?**

Since the Hamiltonian is quadratic, one can also use the Bogolyubov trnasformation known from the theory of superconductivity to solve the problem. This will be discussed in more detail in one of the next assignments.