Karlsruher Institut für Technologie

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Theorie der Kondensierten Materie II SS 2017

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Blatt 6
Lösungsvorschlag

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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.

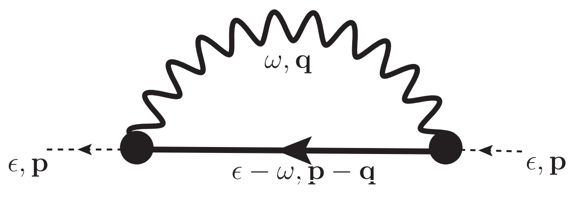

Abbildung 1: Lowest order diagram for self-energy

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

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

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

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

(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

$$\Sigma(\epsilon,\mathbf{p})=\frac{g^2c}{8\pi^2}\int\limits_0^{q_D}q^3dq\int\limits_{-1}^{1}dx\,\frac{1}{\left(\epsilon+\mu-\left[\frac{p^2}{2m}+\frac{q^2}{2m}-\frac{pqx}{m}\right]-cq+i0\right)}\ .$$

This gives

$$\mathrm{Im}\Sigma=-\frac{g^2c}{8\pi}\int\limits_0^{q_D}q^3dq\int\limits_{-1}^{1}dx\ \delta\left(\epsilon+\mu-\left[\frac{p^2}{2m}+\frac{q^2}{2m}-\frac{pqx}{m}\right]-cq\right)\ .$$

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{4\pi}\int\limits_0^{q_D}q^3dq\int\limits_{-1}^{1}dx\ \delta\left(2m(\epsilon+\mu-cq)-\left[p^2+q^2-2pqx\right]\right)\ .$$

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

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{8\pi p}\int\limits_0^{q_D}q^2dq\int\limits_{(p-q)^2}^{(p+q)^2}dy\ \delta\left(y-2m(\epsilon+\mu-cq)\right)\ .$$

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

$$\mathrm{Im}\Sigma=-\frac{g^2cm}{8\pi p}\int\limits_0^{2m(v-c)}q^2dq=-\frac{g^2cm^3}{3\pi v}\,(v-c)^3\ .$$

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

2. Jordan-Wigner Transformation:

(a) Using the trivial property $(\sigma_m^z)^2 = 1$, we express the fermion operators in terms of the Pauli matrices

$$a_n = \sigma_n^- \prod_{m<n} \sigma_m^z, \quad a_n^\dagger = \sigma_n^+ \prod_{m<n} \sigma_m^z.$$

Note, that since the products do not contain any Pauli matrices at the site n, the products commute with $\sigma_n^\pm$. Consequently,

$$a_n^\dagger a_n = \sigma_n^+ \sigma_n^-, \quad a_n a_n^\dagger = \sigma_n^- \sigma_n^+.$$

Using explicit form of the Pauli matrices we now find

$$\sigma_n^+ \sigma_n^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \sigma_n^- \sigma_n^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

and thus we recover the anticommutation relation

$$a_n^\dagger a_n + a_n a_n^\dagger = 1.$$

Similarly,

$$a_n^2 = \left(\sigma_n^-\right)^2 = 0, \quad \left(a_n^\dagger\right)^2 = \left(\sigma_n^+\right)^2 = 0.$$

For operators belonging to different sites, we can (without loss of generality) consider two sites $n_1 < n_2$. Then

$$a_{n_1}^\dagger a_{n_2} = \sigma_{n_1}^+ \prod_{m<n_1} \sigma_m^z \prod_{m<n_2} \sigma_m^z \, \sigma_{n_2}^- = \sigma_{n_1}^+ \sigma_{n_2}^- \prod_{m=n_1}^{n_2-1} \sigma_m^z.$$

For the opposite order of the operators we find

$$a_{n_2} a_{n_1}^\dagger = \sigma_{n_2}^- \prod_{m<n_2} \sigma_m^z \prod_{m<n_1} \sigma_m^z \, \sigma_{n_1}^+ = \sigma_{n_2}^- \prod_{m=n_1}^{n_2-1} \sigma_m^z \, \sigma_{n_1}^+ = \sigma_{n_2}^- \sigma_{n_1}^z \sigma_{n_1}^+ \prod_{m=n_1+1}^{n_2-1} \sigma_m^z$$

Now, the remaining commutation we'll perform explicitly:

$$\sigma_{n_1}^z \sigma_{n_1}^+ = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \sigma_{n_1}^+,$$

$$\sigma_{n_1}^+ \sigma_{n_1}^z = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = -\sigma_{n_1}^+,$$

and hence

$$a_{n_2} a_{n_1}^\dagger = -\sigma_{n_2}^- \sigma_{n_1}^+ \prod_{m=n_1}^{n_2-1} \sigma_m^z = -a_{n_1}^\dagger a_{n_2},$$

proving the anticommutation for fermionic operators on different sites. Other pairs of operators can be considered in the same fashion.

(b) Consider the product of operators on adjacent sites:

$$a_n^\dagger a_{n+1} = \sigma_n^+ \prod_{m<n} \sigma_m^z \prod_{m<n+1} \sigma_m^z \, \sigma_{n+1}^- = \sigma_n^+ \sigma_{n+1}^z \sigma_{n+1}^- = -\sigma_n^+ \sigma_{n+1}^-;$$

$$a_n a_{n+1}^\dagger = \sigma_n^- \prod_{m<n} \sigma_m^z \, \sigma_{n+1}^+ \prod_{m<n+1} \sigma_m^z = \sigma_n^- \sigma_{n+1}^+ \sigma_n^z = \sigma_n^- \sigma_{n+1}^+;$$

$$a_n^\dagger a_{n+1}^\dagger = \sigma_n^+ \prod_{m<n} \sigma_m^z \, \sigma_{n+1}^+ \prod_{m<n+1} \sigma_m^z = \sigma_n^+ \sigma_{n+1}^+ \sigma_n^z = -\sigma_n^+ \sigma_{n+1}^+;$$

$$a_n a_{n+1} = \sigma_n^- \prod_{m<n} \sigma_m^z \prod_{m<n+1} \sigma_m^z \, \sigma_{n+1}^- = \sigma_n^- \sigma_n^z \sigma_{n+1}^- = \sigma_n^- \sigma_{n+1}^-.$$

Now we can use the above relations to transform the terms in the Hamiltonian:

$$\sigma_n^x \sigma_{n+1}^x = \left[\sigma_n^+ + \sigma_n^-\right]\left[\sigma_{n+1}^+ + \sigma_{n+1}^-\right] = -a_n^\dagger a_{n+1}^\dagger - a_n^\dagger a_{n+1} + a_n a_{n+1}^\dagger + a_n a_{n+1}$$

$$= -\left[a_n^\dagger - a_n\right]\left[a_{n+1}^\dagger + a_{n+1}\right],$$

$$\sigma_n^y \sigma_{n+1}^y = -\left[\sigma_n^+ - \sigma_n^-\right]\left[\sigma_{n+1}^+ - \sigma_{n+1}^-\right] = a_n^\dagger a_{n+1}^\dagger - a_n^\dagger a_{n+1} + a_n a_{n+1}^\dagger - a_n a_{n+1}$$

$$= \left[a_n^\dagger + a_n\right]\left[a_{n+1}^\dagger - a_{n+1}\right],$$

As a result, the Hamiltonian of a generic spin chain takes the form

$$\hat{H} = -\sum_{n=-\infty}^{\infty} \Big\{ J_x \left[a_n^\dagger - a_n\right]\left[a_{n+1}^\dagger + a_{n+1}\right] - J_y \left[a_n^\dagger + a_n\right]\left[a_{n+1}^\dagger - a_{n+1}\right]$$

$$-J_z \left[2a_n^\dagger a_n - 1\right]\left[2a_{n+1}^\dagger a_{n+1} - 1\right] + B\left[2a_n^\dagger a_n - 1\right] \Big\}$$