Karlsruhe Institute of Technology | Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I   WS 2022/2023

Prof. Dr. A. Shnirman
Dr. D. Shapiro, Dr. H. Perrin

Sheet 13
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Category A

1. Phonon-mediated interaction of electrons, Schrieffer-Wolf-transformation ($5+5+5+15=30$ points)

In this task, we propose to show that the electron-phonon interaction induces an effective electron-electron interaction using the canonical transformation (Schrieffer-Wolf transformation)

(a) A canonical transformation of an operator H is defined by

$$\tilde{H} = e^{-S} H e^{S}$$

Show that, up to order 2 in S, the above transformation is equivalent to

$$\tilde{H} = H + [H,S] + \frac{1}{2}\left[[H,S],S\right] + \mathcal{O}(S^3)$$

Solution:

Using the Taylor expansion:

$$e^{S} = 1 + S + \frac{1}{2}S^2 + \mathcal{O}(S^3)$$

we obtain:

$$\begin{aligned}
\tilde{H} &= \left(1 - S + \frac{1}{2}S^2 + \mathcal{O}(S^3)\right) H \left(1 + S + \frac{1}{2}S^2 + \mathcal{O}(S^3)\right) \\
&= H + (HS - SH) + \frac{1}{2}\left(HS^2 + S^2H - 2SHS\right) + \mathcal{O}(S^3) \\
&= H + [H,S] + \frac{1}{2}\Big((HS - SH)S + S(SH - HS)\Big) + \mathcal{O}(S^3), \\
&= H + [H,S] + \frac{1}{2}\left[[H,S],S\right] + \mathcal{O}(S^3).
\end{aligned}$$

(b) Now, we consider an Hamiltonian H_0 with a small perturbation V

$$H = H_0 + V$$

The idea of the canonical transformation is to choose the operator S such that the modified Hamiltonian $\tilde{H}$ does not contains terms linear with respect to V.
For $S \ll H_0$, show that this condition is equivalent to

$$V + [H_0, S] = 0$$

Solution: Cancellation of the linear in V term means that $S \sim V$. Performing the expansion we find:

$$\tilde{H} = e^{-S}\left(H_0 + V\right)e^{S} = H_0 + V + [(H_0 + V), S] + \frac{1}{2}\left[[H_0, S], S\right] + \mathcal{O}(S^3)$$

In order to cancel the linear term, the following condition must be fulfilled:

$$V + [H_0, S] = 0. \tag{1}$$

Finally, we have

$$\tilde{H} = H_0 + [V, S] + \frac{1}{2}\left[[H_0, S], S\right] + \mathcal{O}(V^3) = H_0 + \frac{1}{2}[V, S] + \mathcal{O}(V^3).$$

(c) Use the eigenstates of the unperturbed Hamiltonian $\langle n|$ and show that S can be written as

$$\langle n|S|m\rangle = \frac{\langle n|V|m\rangle}{E_m - E_n}$$

where E_n is the energy corresponding to the state $|n\rangle$ of the unperturbed Hamiltonian and show that for the modified Hamiltonian, now, holds the equality:

$$\tilde{H} = H_0 + \frac{1}{2}[V, S] + O(V^3)$$

Solution: From Eq. (1), we find :

$$\langle n|\left(V + [H, S]\right)|m\rangle = 0 \quad \Rightarrow \quad V_{nm} + E_n S_{nm} - E_m S_{nm} = 0,$$

and (if $E_n \neq E_m$)

$$S_{nm} = \frac{V_{nm}}{E_m - E_n}.$$

(d) Let's now consider the Frölich Hamiltonian

$$H_{e-ph} = \sum_{p,q,\sigma} V(q) c^{\dagger}_{p+q,\sigma} c_{p,\sigma}\left(a_q + a^{\dagger}_{-q}\right),$$

which describes the electron-phonon interaction, as a perturbation for the Hamiltonian

$$H_0 = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a^{\dagger}_{\mathbf{q}} a_{\mathbf{q}},$$

with $c(c^{\dagger})$ are the annihilation (creation) operators for electrons, $a(a^{\dagger})$ are phonons operators, $(a_q + a^{\dagger}_{-q}) \propto u(q)$ where u is the displacement of the ions, and $\omega_{-q} = \omega_q$.

Using a canonical transformation, derive the effective electron-electron Hamiltonian at zero T. To do this, evaluate the matrix elements of S. Since we are only interested in the low-temperature behavior, the relevant matrix elements in S are determined by transitions between states $|0\rangle_{ph}|1_{\mathbf{p}}\rangle_e$ (zero phonons and an electron with the momentum $\mathbf{p}$) and $|1_{\mathbf{q}}\rangle_{ph}|1_{\mathbf{p-q}}\rangle_e$ (extra phonon with a momentum $\mathbf{q}$, and a fermion with the momentum $\mathbf{p}-\mathbf{q}$). Rewrite S in the form $S = \sum\limits_{p,q,\sigma} V(q) c^\dagger_{p+q,\sigma} c_{p,\sigma}\left(\alpha_{p,q} a_q + \beta_{p,q} a^\dagger_{-q}\right)$ which is true for low-excitation limit of low T. Then, the matrix elements with respect to phonons, $\langle 1_q|[H_{e-ph}, S]|0\rangle_{ph}$, for the correction to the unperturbed Hamiltonian ($[H_{e-ph}, S]$) can be considered as an effective electron-electron interaction.

Solution: We calculate first the matrix elements of H_{e-ph} averaged with respect to states with zero and one phonon $|n\rangle = |0\rangle_{ph}|1_{\mathbf{p}}\rangle_e$ and $|m\rangle = |1_{\mathbf{q}}\rangle_{ph}|1_{\mathbf{k}}\rangle_e$:

$$[\hat{H}_{e-ph}]_{nm} = {}_e\langle 1_{\mathbf{p}}|_{ph}\langle 0|\hat{H}_{e-ph}|1_{\mathbf{q}}\rangle_{ph}|1_{\mathbf{k}}\rangle_e =$$

$$= \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')_e\langle 1_{\mathbf{p}}|\hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}',\sigma}\hat{c}_{\mathbf{p}',\sigma}|1_{\mathbf{k}}\rangle_e \;\; {}_{ph}\langle 0|\left(\hat{a}_{\mathbf{q}'} + \hat{a}^\dagger_{-\mathbf{q}'}\right)|1_{\mathbf{q}}\rangle_{ph}$$

$$= \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')\delta_{\mathbf{p}',\mathbf{k}}\delta_{\mathbf{p},\mathbf{p}'+\mathbf{q}'}\delta_{\mathbf{q}',\mathbf{q}} = V(\mathbf{q})\delta_{\mathbf{p},\mathbf{k}+\mathbf{q}}$$

and

$$V_{mn} = {}_e\langle 1_{\mathbf{p}}|_{ph}\langle 1_{\mathbf{q}}|\hat{H}_{e-ph}|0\rangle_{ph}|1_{\mathbf{k}}\rangle_e =$$

$$= \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')_e\langle 1_{\mathbf{p}}|\hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}',\sigma}\hat{c}_{\mathbf{p}',\sigma}|1_{\mathbf{k}}\rangle_e \;\; {}_{ph}\langle 1_{\mathbf{q}}|\left(\hat{a}_{\mathbf{q}'} + \hat{a}^\dagger_{-\mathbf{q}'}\right)|0\rangle_{ph}$$

$$= \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')\delta_{\mathbf{p}',\mathbf{k}}\delta_{\mathbf{p},\mathbf{p}'+\mathbf{q}'}\delta_{-\mathbf{q}',\mathbf{q}} = V(-\mathbf{q})\delta_{\mathbf{p},\mathbf{k}-\mathbf{q}}.$$

Therefore, we find the matrix elements S_{nm}:

$$S_{nm} = \frac{V(\mathbf{q})\delta_{\mathbf{p},\mathbf{k}+\mathbf{q}}}{\varepsilon_{\mathbf{k}} + \hbar\omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}}}, \quad S_{mn} = \frac{V(-\mathbf{q})\delta_{\mathbf{p},\mathbf{k}-\mathbf{q}}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} - \hbar\omega_{\mathbf{q}}}.$$

We reinstate the operator $\hat{S}$ that reproduces S_{nm} in a single phonon case written above:

$$\hat{S} = \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')\hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}',\sigma}\hat{c}_{\mathbf{p}',\sigma}\left(\frac{\hat{a}_{\mathbf{q}'}}{\varepsilon_{\mathbf{p}'} + \hbar\omega_{\mathbf{q}'} - \varepsilon_{\mathbf{p}'+\mathbf{q}'}} + \frac{\hat{a}^\dagger_{-\mathbf{q}'}}{\varepsilon_{\mathbf{p}'} - \varepsilon_{\mathbf{p}'+\mathbf{q}'} - \hbar\omega_{-\mathbf{q}'}}\right).$$

Let us define it as follows

$$\hat{S} = \sum_{\mathbf{p}',\mathbf{q}',\sigma} V(\mathbf{q}')\hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}',\sigma}\hat{c}_{\mathbf{p}',\sigma}\left(\hat{a}_{\mathbf{q}'}\alpha_{\mathbf{p}',\mathbf{q}'} + \hat{a}^\dagger_{-\mathbf{q}'}\beta_{\mathbf{p}',\mathbf{q}'}\right)$$

where $\alpha(\beta)_{\mathbf{p},\mathbf{q}} = \dfrac{1}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} \pm \hbar\omega_{\mathbf{q}}}$. (We used $\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$ here.) The effective electron-electron interaction at zero temperature is given by

$$\hat{H}_{e-e} = \frac{1}{2}\,{}_{ph}\langle 0|[\hat{H}_{e-ph}, \hat{S}]|0\rangle_{ph}$$

where the average is taken with respect to phonon ground state. We have:

$$
{}_{ph}\langle 0|\hat{H}_{e-ph}\hat{S}|0\rangle_{ph} = \sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}',\sigma,\sigma'} V(\mathbf{q}')V(\mathbf{q})\hat{c}^{\dagger}_{\mathbf{p}'+\mathbf{q}',\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma}\, {}_{ph}\langle 0|\left(\hat{a}_{\mathbf{q}'}+\hat{a}^{\dagger}_{-\mathbf{q}'}\right)\left(\hat{a}_{\mathbf{q}}\alpha_{\mathbf{p},\mathbf{q}}+\hat{a}^{\dagger}_{-\mathbf{q}}\beta_{\mathbf{p},\mathbf{q}}\right)|0\rangle_{ph} =
$$

$$
= \sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\sigma',\sigma} \beta_{\mathbf{p},\mathbf{q}}|V(\mathbf{q})|^2\hat{c}^{\dagger}_{\mathbf{p}'-\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma} \quad (2)
$$

and

$$
{}_{ph}\langle 0|\hat{S}\hat{H}_{e-ph}|0\rangle_{ph} = \sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}',\sigma,\sigma'} V(\mathbf{q}')V(\mathbf{q})\hat{c}^{\dagger}_{\mathbf{p}'+\mathbf{q}',\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma}\, {}_{ph}\langle 0|\left(\hat{a}_{\mathbf{q}'}\alpha_{\mathbf{p}',\mathbf{q}'}+\hat{a}^{\dagger}_{-\mathbf{q}'}\beta_{\mathbf{p}',\mathbf{q}'}\right)\left(\hat{a}_{\mathbf{q}}+\hat{a}^{\dagger}_{-\mathbf{q}}\right)|0\rangle_{ph} =
$$

$$
= \sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\sigma',\sigma} \alpha_{\mathbf{p}',-\mathbf{q}}|V(\mathbf{q})|^2\hat{c}^{\dagger}_{\mathbf{p}'-\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma}. \quad (3)
$$

In the last line in (3) we permute fermion bilinear terms $\sim \hat{c}^{\dagger}\hat{c}$ and obtain for the quartic fermion term, $\hat{c}^{\dagger}_{\mathbf{p}'-\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma} \to \hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma}\hat{c}^{\dagger}_{\mathbf{p}'-\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}$. (Quadratic terms that appear after the permutation are absorbed by $\hat{H}_0$ and are not important.) After that we replace $\mathbf{p}' \to \mathbf{p}$ and $\mathbf{q} \to -\mathbf{q}$. As a result, we find for the electron-electron Hamiltonian:

$$
H_{e-e} = \frac{1}{2}\sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\sigma',\sigma}(\beta_{\mathbf{p},\mathbf{q}}-\alpha_{\mathbf{p},\mathbf{q}})|V(\mathbf{q})|^2\hat{c}^{\dagger}_{\mathbf{p}'-\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma} =
$$

$$
= \frac{1}{2}\sum_{\mathbf{p},\mathbf{q},\mathbf{p}',\sigma',\sigma}\frac{\hbar\omega_{\mathbf{q}}|V(\mathbf{q})|^2}{(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}-\mathbf{q}})^2-\hbar^2\omega_{\mathbf{q}}^2}\hat{c}^{\dagger}_{\mathbf{p}'+\mathbf{q},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}^{\dagger}_{\mathbf{p}-\mathbf{q},\sigma}\hat{c}_{\mathbf{p},\sigma}.
$$

The effective interaction is attractive, if $|\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}-\mathbf{q}}| < \hbar\omega_{\mathbf{q}}$.

Category B

2. Cooper problem (20 Points)

It was shown in the lecture that electrons above the Fermi sea can form bounded pairs even for vanishingly small attractive interactions. We extend this example taking into account holes excitations below the Fermi level.

The electron-electron interaction is reduced to

$$
g_{k,q} = \begin{cases} -g & |\epsilon_k - \epsilon_{k-q}| \leqslant \omega_D \\ 0 & |\epsilon_k - \epsilon_{k-q}| > \omega_D \end{cases},
$$

i.e., in the interval of the width $2\omega_D$ the interaction constant and attractive, and vanishes beyond. Dispersion of the quasiparticles in the vicinity of the Fermi level is linearly approximated.

Analogous to the lecture, calculate the energy of the state with two quasiparticles (electrons or holes) and find the binding energy Δ per quasiparticle.

Solution: Analogous to the lecture, we choose the wave function in the form

$$|\Psi\rangle = \sum_{-\hbar\omega_D<\epsilon_k} \alpha(k)\chi(\sigma_1,\sigma_2)c_{k,\sigma_1}c_{-k,\sigma_2}|\Psi_0\rangle + \sum_{\epsilon_k<\hbar\omega_D} \alpha(k)\chi(\sigma_1,\sigma_2)c^\dagger_{k,\sigma_1}c^\dagger_{-k,\sigma_2}|\Psi_0\rangle \quad (4)$$

where $|\Psi_0\rangle = \prod_{k\leq k_F} c^\dagger_{k,\sigma}|0\rangle$ represents a Fermi sea.

In contrast to the lecture, Eq. (4) contains not only the electron-like quasiparticles but the hole-like ones as well. We measure the energies E and ϵ_k relative to the Fermi level E_F. The further argumentation is based directly on the lecture script and runs completely analogous to the example in there.

The Schrödinger equation $E|\Psi\rangle = (H_0 + H_{el-el-ph})|\Psi\rangle$ yields

$$(2|\epsilon_k| - E)\,\alpha(k) = \frac{g}{V} \sum_{-\hbar\omega_D<\epsilon_{k_1}< \ hbar\omega_D} \alpha(k_1)\,,$$

where $\alpha(k)$ describes now hole excitations for $\epsilon_k < 0$ and particle excitations for $\epsilon_k > 0$.

We introduce

$$C = \frac{1}{V} \sum_{-\hbar\omega_D<\epsilon_{k_1}<\hbar\omega_D} \alpha(k)\,,$$

and insert it into the self-consistency equation for E:

$$1 = \int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon \frac{\nu(\epsilon)g}{2|\epsilon| - E}\ . \quad (5)$$

We have already converted the sum into an integral, $1/V\sum_k \to \int \nu(\epsilon)d\epsilon$. The density of states per spin $\nu(\epsilon)$ is approximated by a constant, $\nu(\epsilon) \approx \nu_0$, near the Fermi level. The integration (5) gives the same result as in the lecture, multiplied by a factor of 2. So we get the equation on E:

$$\frac{1}{g\nu_0} = \ln\frac{\hbar\omega_D - E/2}{-E/2}.$$

The binding energy per electron is $\Delta = -E/2$. In the weak coupling limit $g\nu_0 \ll 1$ we find

$$\Delta = \hbar\omega_D e^{-\frac{1}{g\nu_0}}\ .$$