

Condensed Matter Theory II: Many-Body Theory (TKM II) SoSe 2023

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Homework assignment 5
 Deadline: 26 May 2023

1. Electron-phonon interaction: (5 + 7 + 8 + 5 = 25 points)

The Hamiltonian describing the interaction of electrons with longitudinal phonons in 3D is given by

$$\hat{H}_{\text{e-ph}} = g \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\Phi}(\mathbf{r}),$$

where $\hat{\Phi}(\mathbf{r})$ denotes the phonon field operator. The Green's function of this phonon field is given by

$$D_0(\mathbf{q}, \omega) = \frac{\omega_{\mathbf{q}}^2}{\omega^2 - \omega_{\mathbf{q}}^2 + i0},$$

where $\omega_{\mathbf{q}} = s|\mathbf{q}|$ is the spectrum for acoustic phonons with the sound velocity s . This expression holds for $|\mathbf{q}| < k_D$, where k_D is the Debye wave-vector which determines cutoff at the Debye frequency $\omega_D = sk_D$.

- (a) Consider the electron self-energy $\Sigma(\mathbf{p}, \varepsilon)$ resulting from the interaction of electrons with phonons in leading order in g and draw the self-energy diagrams. Justify why one of these diagrams does not contribute to Σ . Write down an expression for $\Sigma(\mathbf{p}, \varepsilon)$ using the Feynman rules and perform the energy integration in this expression.

Solution: In this task, we want to calculate the self energy for the fermionic Green's function

$$G(\mathbf{r}, t; \mathbf{r}', t') = -i \langle \phi_0 | \mathcal{T} \psi(\mathbf{r}, t) \psi^\dagger(\mathbf{r}', t') | \phi_0 \rangle \quad (1)$$

where the time evolution takes into account the electron-phonon interaction. The diagrammatic treatment of the electron-phonon interaction proceeds similarly to the diagrammatic treatment of the interaction between electrons. The difference is the presence of phonon field operators in the perturbative expansion. The phonon Green's function is defined as

$$D(\mathbf{r}, t; \mathbf{r}', t') = -i \langle 0 | \mathcal{T} \hat{\Phi}(\mathbf{r}, t) \hat{\Phi}(\mathbf{r}', t') | 0 \rangle \quad (2)$$

where the phonon operator is

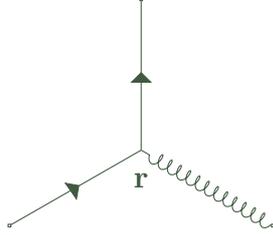
$$\hat{\Phi}(\mathbf{r}, t) = i \sum_{\mathbf{k}} \sqrt{\frac{\omega_{\mathbf{k}}}{2V}} \left(b_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r} - i\omega_{\mathbf{k}}t) - b_{\mathbf{k}}^\dagger \exp(-i\mathbf{k}\mathbf{r} + i\omega_{\mathbf{k}}t) \right) \quad (3)$$

thus

$$\langle 0 | \hat{\Phi}(\mathbf{r}, t) \hat{\Phi}(\mathbf{r}', t') | 0 \rangle = iD(\mathbf{r}, t; \mathbf{r}', t') \quad (4)$$

and contractions between phonon operators and fermion operators vanish. This means that we get non-zero contributions only from diagrams where phonon operators are fully contracted amongst each other.

For the interaction potential we introduce the following vertex:



The phonon Green's function is translational invariant, which means that we can still introduce the self-energy in energy-momentum space as

$$G(\mathbf{q}, \omega) = \frac{1}{[G^{(0)}]^{-1}(\mathbf{q}, \omega) - \Sigma(\mathbf{q}, \omega)}. \quad (5)$$

The lowest order contribution to the self-energy is $\mathcal{O}(g^2)$ and consists of Hartree- and Fock diagrams:

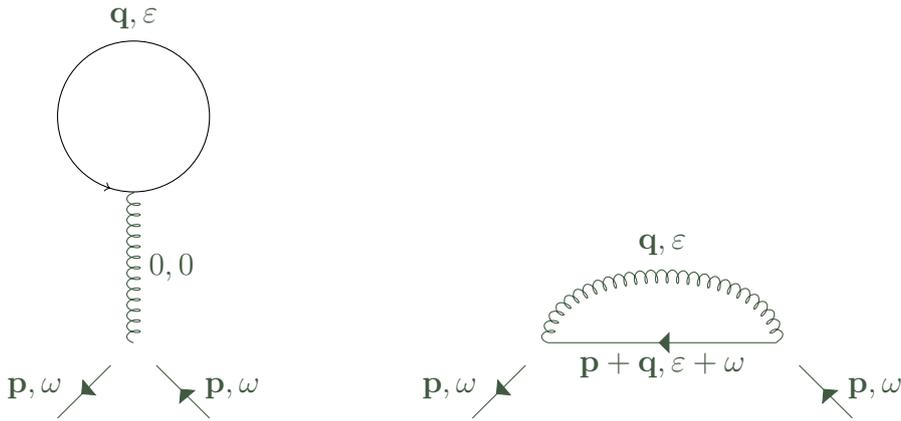


Figure 1: Hartree- and Fock contributions to the self-energy $\Sigma(\mathbf{p}, \omega)$. Phonon propagators are drawn as coiled lines. The disconnected lines are not part of the diagrams, they are drawn to show the external momentum and energy.

In the Hartree diagram, the phonon Green's function at $q = 0$ appears, which is exactly zero for acoustic phonons (formally, the regulator $i0$ in the denominator of the phonon Green's function is kept infinitesimally small but finite, while q is set exactly to zero). The phonon field at $q = 0$ does not correspond to any force acting on electrons.

Therefore, only the Fock diagram remains in the electron self-energy Σ :

$$\Sigma(\mathbf{p}, \varepsilon) = ig^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega}{2\pi} G(\varepsilon + \omega, \mathbf{p} + \mathbf{q}) D_0(\mathbf{q}, \omega) \quad (6)$$

$$= -ig^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{\varepsilon + \omega - \varepsilon_{\mathbf{p}+\mathbf{q}} - i0\text{sign}(\varepsilon_{\mathbf{p}+\mathbf{q}})} \frac{\omega_{\mathbf{q}}^2}{\omega^2 - \omega_{\mathbf{q}}^2 + i0} \quad (7)$$

$$= -\frac{1}{2}ig^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{\varepsilon + \omega - \varepsilon_{\mathbf{p}+\mathbf{q}} - i0\text{sign}(\varepsilon_{\mathbf{p}+\mathbf{q}})} \times \left(\frac{\omega_{\mathbf{q}}}{\omega - \omega_{\mathbf{q}} + i0} - \frac{\omega_{\mathbf{q}}}{\omega + \omega_{\mathbf{q}} - i0} \right). \quad (8)$$

for the last equality we used partial fraction decomposition

$$\frac{1}{\omega^2 - \omega_{\mathbf{q}}^2 + i0} = \frac{1}{(\omega - \omega_{\mathbf{q}} + i0)(\omega + \omega_{\mathbf{q}} - i0)} \quad (9)$$

$$= \frac{1}{2\omega_{\mathbf{q}}(\omega - \omega_{\mathbf{q}} + i0)} - \frac{1}{2\omega_{\mathbf{q}}(\omega + \omega_{\mathbf{q}} - i0)}. \quad (10)$$

The energy integral consists now of two terms which are both of the form

$$\int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{1}{x - z_1} \frac{1}{x - z_2} \quad (11)$$

which was discussed in the lecture, Eq. (3.263). Applying this equation, we find

$$\Sigma(\mathbf{p}, \varepsilon) = \frac{1}{2}g^2 \int \frac{d^3q}{(2\pi)^3} \left\{ \frac{\omega_{\mathbf{q}}\Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega_{\mathbf{q}} - i0} + \frac{\omega_{\mathbf{q}}[1 - \Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})]}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}} + i0} \right\}. \quad (12)$$

- (b) Consider $\text{Im} \Sigma(\mathbf{p}, \varepsilon)$ for $\varepsilon \rightarrow 0$ and $p \approx p_F$. Start with an exact expression for the imaginary part of Σ . Assuming that $s \ll v_F$, justify the extension of limits for the integral over $\xi = \varepsilon_{\mathbf{p}-\mathbf{q}}$ to $\pm\infty$. Find the energy scaling of the quasiparticle decay rate at small ε in this approximation.

Solution: We use Eq. (3.270) from the lecture

$$\text{Im} \frac{1}{x \pm i0} = \mp\pi\delta(x). \quad (13)$$

Therefore, we get from the first term of Eq. (12) (“emission part”):

$$\text{Im}\Sigma^{(1)}(\mathbf{p}, \varepsilon) = \frac{\pi}{2}g^2 \int \frac{d^3q}{(2\pi)^3} \omega_{\mathbf{q}}\Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})\delta(\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega_{\mathbf{q}}). \quad (14)$$

The argument of the delta-function:

$$\varepsilon - \varepsilon_{\mathbf{q}+\mathbf{p}} + \omega_{\mathbf{q}} = \varepsilon - \frac{p^2}{2m} - \frac{q^2}{2m} - \frac{\mathbf{q}\mathbf{p}}{m} + s|\mathbf{q}| + \varepsilon_F \quad (15)$$

$$\stackrel{p \approx p_F}{=} \varepsilon - \frac{q^2}{2m} - \frac{qp_F \cos(\theta)}{m} + sq \quad (16)$$

where θ is the angle between \mathbf{p} and \mathbf{q} . We evaluate the delta-function to solve the angular integral

$$\cos(\theta) = \frac{m}{qp_F} \left[\varepsilon + sq - \frac{q^2}{2m} \right] \quad (17)$$

$$= \frac{\varepsilon}{qv_F} + \frac{s}{v_F} - \frac{q}{2p_F} \quad (18)$$

Note, that $s \ll v_F$, ε small and $q_D \ll p_F$ (q_D , the Debye-frequency, serves as a cutoff for the q -integral). Therefore,

$$\left| \frac{\varepsilon}{qv_F} + \frac{s}{v_F} - \frac{q}{2p_F} \right| \ll 1 \quad (19)$$

and we can evaluate the delta-function without further restrictions:

$$\text{Im}\Sigma^{(1)}(\mathbf{p}, \varepsilon) = \frac{\pi^2}{(2\pi)^3 v_F} g^2 \int_0^{q_D} dq \omega_{\mathbf{q}} \Theta \left(- \left[\frac{q^2}{2m} + qv_F \left[\frac{\varepsilon}{qv_F} + \frac{s}{v_F} - \frac{q}{2p_F} \right] \right] \right) \frac{q^2}{q} \quad (20)$$

$$= \frac{\pi^2}{(2\pi)^3 v_F} s g^2 \int_0^{q_D} dq q^2 \Theta(-[\varepsilon + sq]) \quad (21)$$

$$= \frac{\pi^2}{(2\pi)^3 v_F} s g^2 \int_0^{\infty} dq q^2 \Theta(-[\varepsilon + sq]) \quad (22)$$

$$= \begin{cases} \frac{\pi^2}{(2\pi)^3 v_F} s g^2 \int_0^{|\varepsilon|/s} dq q^2 & \varepsilon < 0 \\ 0 & \text{else} \end{cases} \quad (23)$$

in the last two equalities we used $|\varepsilon|/s < q_D$, with the assumption of small ε from the task.

Similarly, we can evaluate the second term from equation (12). The argument of the delta function is

$$\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}} = \varepsilon - \frac{q^2}{2m} - qv_F \cos(\theta) - sq \quad (24)$$

$$\Rightarrow \cos(\theta) = \frac{\varepsilon}{qv_F} - \frac{s}{v_F} - \frac{q}{2p_F} \quad (25)$$

again, this does not limit the angular integration and we obtain (minus sign from Eq. (13))

$$\text{Im}\Sigma^{(2)}(\mathbf{p}, \varepsilon) = -\frac{\pi^2}{(2\pi)^3 v_F} g^2 \int_0^{q_D} dq \omega_{\mathbf{q}} \Theta \left(\frac{q^2}{2m} + qv_F \left[\frac{\varepsilon}{qv_F} - \frac{s}{v_F} - \frac{q}{2p_F} \right] \right) \frac{q^2}{q} \quad (26)$$

$$= -\frac{\pi^2}{(2\pi)^3 v_F} g^2 \int_0^{q_D} dq \omega_{\mathbf{q}} \Theta(\varepsilon - sq) \frac{q^2}{q} \quad (27)$$

$$= -\frac{\pi^2}{(2\pi)^3 v_F} g^2 s \int_0^{\infty} dq q^2 \Theta(\varepsilon - sq) \quad (28)$$

$$= \begin{cases} -\frac{\pi^2}{(2\pi)^3 v_F} g^2 s \int_0^{\varepsilon/s} dq q^2 & \varepsilon > 0 \\ 0 & \text{else} \end{cases} \quad (29)$$

So in any case the upper cutoff is irrelevant and we can extend the upper integration boundary to infinity as the q integral is limited by the Θ -function. We obtain

$$\text{Im}\Sigma^{(2)}(\mathbf{p}, \varepsilon) = -\text{sign}(\varepsilon) \frac{\pi^2}{(2\pi)^3 v_F} g^2 s \int_0^{|\varepsilon|/s} dq q^2 \quad (30)$$

$$= -\text{sign}(\varepsilon) \frac{g^2 |\varepsilon|^3}{24\pi v_F s^2}. \quad (31)$$

- (c) Write down an expression for $\text{Re} \Sigma(\mathbf{p}, \varepsilon)$ as an integral over the transferred momentum \mathbf{q} . Calculate $\text{Re} \Sigma$ in the two limiting cases $\varepsilon \ll \omega_D$ and $\varepsilon \gg \omega_D$ for $p = p_F$.

Solution: Taking the real part of (12):

$$\begin{aligned} \text{Re} [\Sigma(\mathbf{p}, \varepsilon)] &= \text{Re} \frac{1}{2} g^2 \int \frac{d^3 q}{(2\pi)^3} \left\{ \frac{\omega_{\mathbf{q}} \Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega_{\mathbf{q}} - i0} + \frac{\omega_{\mathbf{q}} [1 - \Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})]}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}} + i0} \right\} \quad (32) \\ &= \text{Re} \frac{1}{2} g^2 \int_0^{q_D} \frac{dq q^2}{2\pi} \int_{-1}^1 \frac{d \cos(\theta)}{2\pi} \left\{ \frac{\omega_{\mathbf{q}} \Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega_{\mathbf{q}} - i0} + \frac{\omega_{\mathbf{q}} [1 - \Theta(-\varepsilon_{\mathbf{p}+\mathbf{q}})]}{\varepsilon - \varepsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}} + i0} \right\}. \quad (33) \end{aligned}$$

First, we evaluate the Theta-functions by computing bounds for the angular integral.

The first term from Eq. (33)

$$-\frac{q^2}{2m} - \frac{p_F q \cos(\theta)}{m} > 0 \quad (34)$$

$$\Rightarrow \cos(\theta) < -\frac{q}{2p_F} \quad (35)$$

together with the integral bounds we have $\cos(\theta) \in [-1, -q/(2p_F)]$. We get

$$\text{Re} \frac{1}{2} g^2 s \int_0^{q_D} \frac{dq q^2}{2\pi} \int_{-1}^{-q/(2p_F)} \frac{d \cos(\theta)}{2\pi} \frac{q}{\varepsilon - \frac{q^2}{2m} - qv_F \cos(\theta) + sq - i0} \quad (36)$$

$$= -\text{Re} \frac{1}{2} \frac{g^2 s}{v_F} \int_0^{q_D} \frac{dq q^2}{2\pi} \int_{v_F q}^{q^2/(2m)} \frac{dx}{2\pi} \frac{1}{\varepsilon - \frac{q^2}{2m} + x + sq - i0} \quad (37)$$

$$= -\frac{1}{4\pi} \frac{g^2 s}{v_F} \int_0^{q_D} \frac{dq q^2}{2\pi} \log \left[\frac{|\varepsilon + sq|}{|\varepsilon - q^2/(2m) + v_F q + sq|} \right] \quad (38)$$

In order to evaluate the integral we used

$$\text{Re} \lim_{\epsilon \rightarrow 0} \int_a^b dx \frac{1}{x + c \pm i\epsilon} = \text{Re} \lim_{\epsilon \rightarrow 0} \int_a^b dx \frac{x + c \mp i\epsilon}{(x + c)^2 + \epsilon^2} \quad (39)$$

$$= \log \left[\frac{|b + c|}{|a + c|} \right] \quad (40)$$

where $\epsilon > 0$ and $a, b, c \in \mathbb{R}$.

The second term: from Eq. (33)

$$\frac{q^2}{2m} + v_F q \cos(\theta) > 0 \quad (41)$$

$$\Rightarrow \cos(\theta) > -\frac{q}{2p_F} \quad (42)$$

Therefore

$$\operatorname{Re} \frac{1}{2} g^2 s \int_0^{q_D} \frac{dq q^2}{2\pi} \int_{-q/(2v_F)}^1 \frac{d \cos(\theta)}{2\pi} \frac{q}{\varepsilon - \frac{q^2}{2m} - qv_F \cos(\theta) - sq} \quad (43)$$

$$= \operatorname{Re} \frac{1}{2} \frac{g^2 s}{v_F} \int_0^{q_D} \frac{dq q^2}{2\pi} \int_{-v_F q}^{q^2/(2m)} \frac{dx}{2\pi} \frac{1}{\varepsilon - \frac{q^2}{2m} + x - sq} \quad (44)$$

$$= \frac{1}{4\pi} \frac{g^2 s}{v_F} \int_0^{q_D} \frac{dq q^2}{2\pi} \log \left[\frac{|\varepsilon - sq|}{|\varepsilon - q^2/(2m) - v_F q - sq|} \right] \quad (45)$$

We obtain

$$\operatorname{Re} [\Sigma(\mathbf{p}, \varepsilon)] = -\frac{g^2 s}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \left(\log \left[\frac{|\varepsilon - q^2/(2m) - v_F q - sq|}{|\varepsilon - q^2/(2m) + v_F q + sq|} \right] + \log \left[\frac{|\varepsilon + sq|}{|\varepsilon - sq|} \right] \right). \quad (46)$$

Considering the second term from Eq. (46), we have for $\varepsilon \gg \omega_D$

$$-\frac{g^2 s}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \log \left[\frac{|\varepsilon + sq|}{|\varepsilon - sq|} \right] = -\frac{g^2 s}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \begin{cases} \log \left[\frac{|\varepsilon + sq|}{|\varepsilon - sq|} \right] & \varepsilon > 0 \\ \log \left[\frac{-|\varepsilon + sq|}{-|\varepsilon - sq|} \right] & \varepsilon < 0 \end{cases} \quad (47)$$

$$= -\frac{g^2 s}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \begin{cases} \log \left[\frac{|\varepsilon + sq|}{|\varepsilon - sq|} \right] & \varepsilon > 0 \\ \log \left[\frac{|\varepsilon - sq|}{|\varepsilon + sq|} \right] & \varepsilon < 0 \end{cases} \quad (48)$$

$$= -\frac{g^2 s \cdot \operatorname{sign}(\varepsilon)}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \log \left[\frac{|\varepsilon| + sq}{|\varepsilon| - sq} \right] \quad (49)$$

$$\approx -\frac{g^2 s \cdot \operatorname{sign}(\varepsilon)}{(2\pi)^2 v_F \varepsilon} \int_0^{q_D} dq q^3 \quad (50)$$

$$= -\frac{g^2 s \cdot \operatorname{sign}(\varepsilon)}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \log \left[\frac{|\varepsilon| + sq}{|\varepsilon| - sq} \right] \quad (51)$$

$$\approx -\frac{g^2 s}{(2\pi)^2 v_F} \frac{q_D^4 s}{4\varepsilon} \quad (52)$$

For $\varepsilon \ll \omega_D$ we can solve the integral with mathematica and obtain after expansion in ε

$$-\frac{g^2 s}{2(2\pi)^2 v_F} \frac{q_D^2 \varepsilon}{s}. \quad (53)$$

Considering now the first term from Eq. (46), we use

$$q_D \ll q_F \quad (54)$$

$$\Leftrightarrow q_D^2/2m \ll v_F q_D \quad (55)$$

to linearize numerator and denominator

$$\operatorname{Re} [\Sigma^{(1)}(\mathbf{p}, \varepsilon)] \approx -\frac{g^2 s}{2(2\pi)^2 v_F} \int_0^{q_D} dq q^2 \log \left[\frac{|\varepsilon - \alpha q|}{|\varepsilon + \alpha q|} \right] \quad \alpha := s + v_F \quad (56)$$

We note, that in both cases ($\varepsilon \gg \omega_D$ and $\varepsilon \ll \omega_D$) $\varepsilon_F \gg \varepsilon$ is the largest energy scale. With this in mind we can solve the integral and expand for large α first, finding in both cases $\text{Re } \Sigma^{(1)}(\mathbf{p}, \varepsilon) \approx -\frac{g^2 s}{2(2\pi)^2 v_F} \frac{q_D^2 \varepsilon}{\alpha}$. This is small compared to the contributions from $\Sigma^{(2)}$ and we finally get

$$\text{Re } \Sigma(\mathbf{p}, \varepsilon) \approx \begin{cases} -\frac{g^2 s}{2(2\pi)^2 v_F} \frac{q_D^2 \varepsilon}{s} & \varepsilon \ll \omega_D \\ -\frac{g^2 s}{(2\pi)^2 v_F} \frac{q_D^4 s}{4\varepsilon} & \varepsilon \gg \omega_D \end{cases} \quad (57)$$

(d) Use $\text{Re } \Sigma(\mathbf{p}, \varepsilon)$ to determine the quasi-particle residue Z and effective mass m^* .

Solution: From above result we find (since we calculate the ε derivate at $\varepsilon = 0$ we take the $\varepsilon \ll \omega_D$ result):

$$\partial_\varepsilon \text{Re } \Sigma(p = p_F, \varepsilon \ll \omega_D)|_{\varepsilon=0} = -\frac{g^2 k_D^2}{8\pi^2 v_F}. \quad (58)$$

Therefore,

$$Z = \frac{1}{1 - \partial_\varepsilon \text{Re } \Sigma(\mathbf{p} = p_F, \varepsilon \ll \omega_D)|_{\varepsilon=0}} = \frac{1}{1 + \frac{g^2 k_D^2}{8\pi^2 v_F}}. \quad (59)$$

For the p dependence we generalize result (46) to $p \neq p_F$ (proceeding along the same lines as the previous calculation)

$$\text{Re } \Sigma(\mathbf{p}, \varepsilon) = -\frac{g^2 sm}{8\pi^2 p} \int_0^{k_D} dq q^2 \left\{ \log \left(\frac{|\varepsilon - \varepsilon_p - pq/m - q^2/(2m) - \omega_{\mathbf{q}}|}{|\varepsilon - \varepsilon_p + pq/m - q^2/(2m) + \omega_{\mathbf{q}}|} \right) + \log \left(\frac{|\varepsilon + \omega_{\mathbf{q}}|}{|\varepsilon - \omega_{\mathbf{q}}|} \right) \right\} \quad (60)$$

We find:

$$\Sigma(\mathbf{p}, \varepsilon = 0) = -\frac{g^2 sm}{8\pi^2 p} \int_0^{k_D} dq q^2 \ln \left| \frac{\varepsilon_p + pq/m + q^2/2m + \omega_{\mathbf{q}}}{-\varepsilon_p + pq/m - q^2/2m + \omega_{\mathbf{q}}} \right|. \quad (61)$$

This gives a finite contribution to the mass renormalization but produces higher power of $s/v_F \ll 1$. Neglecting this contribution, we arrive at

$$\frac{m^*}{m} \simeq Z^{-1} = 1 + \frac{g^2 k_D^2}{8\pi^2 v_F}. \quad (62)$$

The effective mass is, therefore, increased by the electron-phonon interaction (“polaron effect”): an electron gets dressed with a phonon cloud and drags it when moving.

2. Compressibility of a two-dimensional electronic system (5 + 5 + 10 + 5 = 25 points)

Compressibility describes the relative change of volume of a system in response to a change in pressure

$$K(T, P, N) = -\frac{1}{V(T, P, N)} \frac{\partial V(T, P, N)}{\partial P}. \quad (63)$$

- (a) Using the internal energy $E = N\varepsilon$ (ε is the average energy per particle), and $V\rho = N$ show that

$$K^{-1} = \rho^2 \frac{\partial^2}{\partial \rho^2} \rho \varepsilon(\rho) \quad (64)$$

at zero temperature.

Solution: We consider $E(T, V, N) := E(S(T, V, N), V, N)$. The internal energy is defined by

$$dE = T dS - P dV + \mu dN \quad (65)$$

so we obtain for the pressure

$$P(T = 0, V, N) = - \left[\underbrace{\frac{\partial E(S, V, N)}{\partial S}}_{=T=0} \Big|_{S=S(T, V, N)} \frac{\partial S(T = 0, V, N)}{\partial V} + \frac{\partial E(T = 0, V, N)}{\partial V} \right] \quad (66)$$

We use $V(T, P(T, V, N), N) = 1$ to “invert the derivative” in the definition of the compressibility (63):

$$\frac{\partial V(T, P, N)}{\partial P} \Big|_{P=P(T, V, N)} = \frac{1}{\frac{\partial P(T, V, N)}{\partial V}} \quad (67)$$

Plugging in Eq. (66) we find:

$$K^{-1}(T = 0, V, N) = -V \frac{\partial P(T = 0, V, N)}{\partial V} \quad (68)$$

$$= V \frac{\partial^2}{\partial V^2} E(T = 0, V, N) \quad (69)$$

$$= VN \frac{\partial^2}{\partial V^2} \varepsilon(T = 0, V, N) \quad (70)$$

In the last line we used the definition of the average energy per particle. Now we express the derivative by V through a derivative by ρ by applying the chain rule:

$$K^{-1}(T = 0, V, N) = NV \frac{\partial}{\partial V} \frac{\partial \varepsilon(T = 0, \rho, N)}{\partial \rho} \frac{\partial \rho}{\partial V} \quad (71)$$

$$= -NV \frac{\partial}{\partial V} \left[\frac{\partial \varepsilon(T = 0, \rho, N)}{\partial \rho} N/V^2 \right] \quad (72)$$

$$= 2N^2/V^2 \frac{\partial \varepsilon(T = 0, \rho, N)}{\partial \rho} + \frac{\partial^2 \varepsilon(T = 0, \rho, N)}{\partial \rho^2} (N/V)^3 \quad (73)$$

$$= 2\rho^2 \frac{\partial \varepsilon(T = 0, \rho, N)}{\partial \rho} + \rho^3 \frac{\partial^2 \varepsilon(T = 0, \rho, N)}{\partial \rho^2} \quad (74)$$

$$= \rho^2 \frac{\partial^2}{\partial \rho^2} \rho \varepsilon(T = 0, \rho, N). \quad (75)$$

- (b) Calculate the compressibility for a 2D non-interacting electron system at zero temperature.

Solution: For non-interacting particles, the average energy per particle reads at $T = 0$:

$$\varepsilon(T = 0, V, N) = 2 \frac{V}{N} \int \frac{d^2p}{(2\pi)^2} \epsilon(\mathbf{p}) \theta(p - p_F) \quad (76)$$

The factor of 2 comes from spin, p_F is the free Fermi-momentum. In terms of p_F , we find

$$\varepsilon(T = 0, V, N) = 2V/(4\pi mN) \int_0^{p_F} dp p^3 \quad (77)$$

$$= \frac{V p_F^4}{8\pi mN} \quad (78)$$

Determining p_F in terms of the density, we have

$$N(T = 0) = \frac{2V}{2\pi} \int_0^{p_F} dp p \quad (79)$$

$$= p_F^2 V / (2\pi) \quad (80)$$

$$\Rightarrow p_F^2(T = 0, \rho, N) = 2\pi\rho \quad (81)$$

Finally, we find for the average energy per particle

$$\varepsilon(T = 0, \rho, N) = \frac{\rho\pi}{2m} \quad (82)$$

Calculating the contribution to the compressibility from Eq. (63), we find

$$1/K_0(T = 0, V, N) = \rho^2\pi/m \quad (83)$$

$$K_0(T = 0, V, N) = \frac{m}{\pi\rho^2}. \quad (84)$$

- (c) Consider a two-dimensional electronic system at zero temperature in the presence of Coulomb interaction $U(r) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$, where ϵ_0 is the vacuum permittivity. Calculate the interaction-induced correction to the ground state energy from the Fock diagram.

Solution: The correction to the vacuum energy reads (see also sheet 4 solutions):

$$\langle 0|U|0\rangle = \sum_{\sigma,\sigma'} \int dr dr' U(r-r') \langle \text{FS} | \mathcal{T} \psi_{0,\sigma}(r) \psi_{0,\sigma'}(r',t) \psi_{0,\sigma'}^\dagger(r',t+0) \psi_{0,\sigma}^\dagger(r,t+0) | \text{FS} \rangle \quad (85)$$

(here and in the following we abbreviate \mathbf{r} by r and d^2r by dr).

We identify the Fock contribution:

$$U_{\text{Fock}} = i \sum_{\sigma,\sigma'} \delta_{\sigma,\sigma'} \int dr dr' G_0(r-r', -0) G_0(r'-r, -0) U(r-r') \quad (86)$$

$$= iV \int dr G_0(r, -0) G_0(-r, -0) U(r) \quad (87)$$

We switch to Fourier space:

$$U_{\text{Fock}} = i2V \int dr \int \frac{dp}{(2\pi)^2} \exp(ipr) \int \frac{dp'}{(2\pi)^2} G_0(p - p', -0) \times \quad (88)$$

$$\times \int \frac{dp''}{(2\pi)^2} U(p' - p'') G_0(p'', -0) \quad (89)$$

$$= i2V \int \frac{dp'}{(2\pi)^2} G_0(-p', -0) \int \frac{dp''}{(2\pi)^2} U(p' - p'') G_0(p'', -0) \quad (90)$$

The 2D Fourier transform of the Fourier transform is

$$V(q) = \frac{e^2}{2q\epsilon_0}. \quad (91)$$

Thus, we have

$$U_{\text{Fock}} = -\frac{Ve^2}{\epsilon_0} \int \frac{dp'}{(2\pi)^2} \frac{dp''}{(2\pi)^2} \theta(|p'| - p_F) \theta(|p''| - p_F) \frac{1}{|p' - p''|} \quad (92)$$

$$= -\frac{Ve^2}{\epsilon_0} \frac{1}{(2\pi)^3} \int_0^{p_F} d|p'| \int_0^{p_F} d|p''| \int_0^{2\pi} d\phi \frac{|p'| |p''|}{\sqrt{|p'|^2 + |p''|^2 - 2|p'| |p''| \cos(\phi)}} \quad (93)$$

$$= -\frac{Ve^2}{\epsilon_0 (2\pi)^3} p_F^3 \int_0^1 dx \int_0^1 dy \int_0^{2\pi} d\phi \frac{xy}{\sqrt{x^2 + y^2 - 2xy \cos(\phi)}} \quad (94)$$

$$= -C \frac{Ve^2}{\epsilon_0 (2\pi)^3} p_F^3 \quad (95)$$

Where C is a number, and we find $C \approx 2.667 \approx 8/3$ via numerical integration. We calculate the average energy correction per particle

$$\varepsilon_{\text{Fock}} = U_{\text{Fock}}/N \quad (96)$$

and use $p_F = \sqrt{2\pi\rho}$ to obtain

$$\varepsilon_{\text{Fock}} = -C \frac{\rho^{1/2} e^2}{\epsilon_0 (2\pi)^{3/2}}. \quad (97)$$

- (d) Taking into account the energy correction from the Fock diagram, calculate the compressibility of the system. You should obtain

$$K^{-1} \propto \left[1 - \frac{\sqrt{2}}{\pi} r_s \right] \quad (98)$$

where $r_s = 1/\sqrt{\pi\rho a_0^2}$ is the dimensionless radius of the average volume containing one unit of charge, and $a_0 = 4\pi\epsilon_0\hbar^2/e^2m$ is the Bohr radius and m is the electron mass.

Solution: The average energy including the Fock-correction reads

$$\varepsilon(T = 0, \rho) = \frac{\rho\pi}{2m} - C \frac{\rho^{1/2} e^2}{\epsilon_0 (2\pi)^{3/2}}. \quad (99)$$

and we obtain for the compressibility

$$K^{-1}(T = 0, \rho) = \pi\rho^2/m - \frac{3}{8} \frac{Ce^2\rho^{3/2}}{\sqrt{2}\pi^{3/2}\epsilon_0} \quad (100)$$

$$= \pi\rho^2/m \left[1 - \frac{me^2}{\sqrt{2}\pi^{5/2}\rho^{1/2}\epsilon_0} \right] \quad (101)$$

$$= \pi\rho^2/m \left[1 - \frac{2\sqrt{2}}{\pi} r_s \right] \quad (102)$$

$$= \frac{1}{\pi a_0^4 r_s^4 m} \left[1 - \frac{2\sqrt{2}}{\pi} r_s \right]. \quad (103)$$

3. Bonus: Spin susceptibility of a non-interacting electron system (10 + 10 = 20 bonus points)

Consider a system of non-interacting electrons. The magnetic field $\mathbf{B}(\mathbf{r}, t)$ couples to the electron spin via the term

$$H' = -g\mu_B \int d\mathbf{r} \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{S}(\mathbf{r}), \quad (104)$$

where g is the electron g -factor, μ_B is the Bohr magneton, and the spin operator is $\mathbf{S}(\mathbf{r}) = \frac{\hbar}{2} \Psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \Psi(\mathbf{r})$. Here the field operators for different spins are collected into a single vector operator

$$\Psi(\mathbf{r})^\dagger = (\psi_\uparrow^\dagger(\mathbf{r}), \psi_\downarrow^\dagger(\mathbf{r})). \quad (105)$$

and $\boldsymbol{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is a vector of Pauli matrices.

- (a) Find a formal expression for the induced spin density $\langle \mathbf{S}(\mathbf{r}, t) \rangle$ as a linear response to the applied magnetic field \mathbf{B} . What is the diagram associated with the expression? Express your result as a momentum integral in energy representation.

Solution: From the lecture we know, that the linear response $\delta B(t)$ to a perturbation $H' = AF(t)$ is found as

$$\delta B(t) = \int_{-\infty}^{\infty} dt' \mathcal{D}_{BA}^R(t, t') F(t') \quad (106)$$

where

$$\mathcal{D}_{BA}^R(t, t') = -i\theta(t - t') \langle \phi_0 | [B(t), A(t')] | \phi_0 \rangle. \quad (107)$$

This retarded linear response function can be calculated from the corresponding time-ordered correlator.

Applying this to our task we have

$$\delta \langle S_i(\mathbf{r}, t) \rangle = -g\mu_B \int dt' \int d^3r' [\mathcal{D}_{SS}^R]_{i,j}(\mathbf{r}, \mathbf{r}', t, t') B_j(\mathbf{r}', t') \quad (108)$$

$$[\mathcal{D}_{SS}^R]_{i,j}(\mathbf{r}, \mathbf{r}', t, t') := -i\theta(t - t') \langle \phi_0 | [S_i(\mathbf{r}, t), S_j(\mathbf{r}', t')] | \phi_0 \rangle. \quad (109)$$

as we are calculating the response of the spin $S_j(\mathbf{r})$ to the external magnetic field, which couples via Eq. (104) to the system (see also lecture notes on linear response.) Therefore, we would like to calculate

$$\mathcal{D}_{i,j}(\mathbf{r}, \mathbf{r}'; t, t') := -i \langle \phi_0 | \mathcal{T} S_i(\mathbf{r}, t) S_j(\mathbf{r}', t') | \phi_0 \rangle. \quad (110)$$

Here, the time evolution is governed by the free hamiltonian and $\langle \phi_0 |$ is the unperturbed vacuum, as the effect of the perturbation was linearized. The retarded \mathcal{D} is obtained from the time ordered one (lecture Eq. (3.305)). We find

$$\mathcal{D}_{i,j}(\mathbf{r}, \mathbf{r}'; t, t') = -\frac{i}{4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} \langle 0 | \mathcal{T} \psi_{\sigma_1}^\dagger(\mathbf{r}, t) [\sigma_i]_{\sigma_1, \sigma_2} \psi_{\sigma_2}(\mathbf{r}, t) \psi_{\sigma_3}^\dagger(\mathbf{r}', t') [\sigma_j]_{\sigma_3, \sigma_4} \psi_{\sigma_4}(\mathbf{r}', t') | 0 \rangle \quad (111)$$

$$= -\frac{i}{4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} [\sigma_i]_{\sigma_1, \sigma_2} [\sigma_j]_{\sigma_3, \sigma_4} \langle 0 | \mathcal{T} \psi_{\sigma_1}^\dagger(\mathbf{r}, t) \psi_{\sigma_2}(\mathbf{r}, t) \psi_{\sigma_3}^\dagger(\mathbf{r}', t') \psi_{\sigma_4}(\mathbf{r}', t') | 0 \rangle \quad (112)$$

We use Wick's theorem to decompose the expectation value:

$$\mathcal{D}_{i,j}(\mathbf{r}, \mathbf{r}'; t, t') = \frac{i}{4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} [\sigma_i]_{\sigma_1, \sigma_2} [\sigma_j]_{\sigma_3, \sigma_4} [\delta_{\sigma_1, \sigma_2} \delta_{\sigma_3, \sigma_4} G_0^2(0, 0) \quad (113)$$

$$- \delta_{\sigma_1, \sigma_4} \delta_{\sigma_2, \sigma_3} G_0(\mathbf{r} - \mathbf{r}', t - t') G_0(\mathbf{r}' - \mathbf{r}, t' - t)] \quad (114)$$

$$= -\frac{i}{4} \sum_{\sigma_1, \sigma_2} [\sigma_i]_{\sigma_1, \sigma_2} [\sigma_j]_{\sigma_2, \sigma_1} G_0(\mathbf{r} - \mathbf{r}', t - t') G_0(\mathbf{r}' - \mathbf{r}, t' - t) \quad (115)$$

$$= -\frac{i}{4} \text{Tr}(\sigma_i \sigma_j) G_0(\mathbf{r} - \mathbf{r}', t - t') G_0(\mathbf{r}' - \mathbf{r}, t' - t) \quad (116)$$

$$= -\frac{i}{4} \text{Tr}(\sigma_i \sigma_j) G_0(\mathbf{r} - \mathbf{r}', t - t') G_0(\mathbf{r}' - \mathbf{r}, t' - t) \quad (117)$$

$$= -\frac{i}{2} \delta_{i,j} G_0(\mathbf{r} - \mathbf{r}', t - t') G_0(\mathbf{r}' - \mathbf{r}, t' - t) \quad (118)$$

This corresponds to the Fock vacuum diagram. The Hartree diagram vanishes, as $\text{Tr}(\sigma_j) = 0$. In Fourier-space, we find

$$\delta \langle S_i(\mathbf{r}, t) \rangle = -g\mu_B \int \frac{d\omega}{2\pi} \frac{d^3q}{(2\pi)^3} \exp[i(\omega t + \mathbf{q}\mathbf{r})] \chi_{i,j}^R(\mathbf{q}, \omega) B_j(\mathbf{q}, \omega) \quad (119)$$

$$\delta \langle S_i(\mathbf{q}, \omega) \rangle = -g\mu_B \chi_{i,j}^R(\mathbf{q}, \omega) B_j(\mathbf{q}, \omega) \quad (120)$$

For $\omega > 0$ $\chi_{i,j}^R(\omega) = \chi_{i,j}(\omega)$ with

$$\chi_{i,j}(\mathbf{q}, \omega) = -\frac{i}{2} \delta_{i,j} \int \frac{d\omega'}{2\pi} \frac{d^3q'}{(2\pi)^3} G_0(\mathbf{q} + \mathbf{q}', \omega + \omega') G_0(\mathbf{q}', \omega') \quad (121)$$

$$= \mathcal{FT} [\mathcal{D}_{i,j}(\mathbf{r}, t)](\mathbf{q}, \omega) \quad (122)$$

- (b) Assume that the system has Coulomb interaction. Calculate the interacting spin susceptibility by taking into account the RPA diagrams as in the lectures (Sec. 3.14). What do you find?

Solution: To take into account Coulomb interaction, we reconsider the expression for $\mathcal{D}_{i,j}(\mathbf{r}, \mathbf{r}'; t, t')$

$$\mathcal{D}_{i,j}(\mathbf{r}, \mathbf{r}'; t, t') := -i \langle \phi_0 | \mathcal{T} S_i(\mathbf{r}, t) S_j(\mathbf{r}', t') | \phi_0 \rangle. \quad (123)$$

The time evolution of the spin operators is now governed by the interacting hamiltonian (without the magnetic field, which is still treated to linear order as a perturbation) and $|\phi_0\rangle$ is the interacting vacuum. We insert the definition of the spin operators as before:

$$\mathcal{D}_{i,j}(\mathbf{r}, t) = -\frac{i}{4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} [\sigma_i]_{\sigma_1, \sigma_2} [\sigma_j]_{\sigma_3, \sigma_4} \langle \phi_0 | \mathcal{T} \psi_{\sigma_1}^\dagger(\mathbf{r}, t) \psi_{\sigma_2}(\mathbf{r}, t) \psi_{\sigma_3}^\dagger(0, 0) \psi_{\sigma_4}(0, 0) | \phi_0 \rangle \quad (124)$$

This is very similar to the polarization operator considered in the lecture. We can perform the RPA expansion analogously, using the diagrammatic approach. The zeroth-order term (polarization bubble) corresponds to the case without interaction, which we considered in the first subtask.

The lowest order RPA correction has the following structure:

$$\mathcal{D}_{i,j}^{\text{RPA } 1}(\mathbf{r}, t) \propto \int d^3 r_1 d^3 r_2 dt_1 dt_2 \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} \times \quad (125)$$

$$\times [\sigma_i]_{\sigma_1, \sigma_2} [\sigma_j]_{\sigma_3, \sigma_4} \delta_{\sigma_1, \sigma_2} \delta_{\sigma_3, \sigma_4} G_0(\mathbf{r} - \mathbf{r}_1, t - t_1) G_0(\mathbf{r}_1 - \mathbf{r}, t_1 - t) \times \quad (126)$$

$$\times U(\mathbf{r}_1, \mathbf{r}_2) G_0(\mathbf{r}_2, t_2) G_0(-\mathbf{r}_2, -t_2). \quad (127)$$

As $\text{Tr}(\sigma_i) = 0$, this diagram gives zero due to the spin sum. For the same reason, all diagrams from the RPA series vanish, as there are always bubbles forming traces over the Pauli matrices.

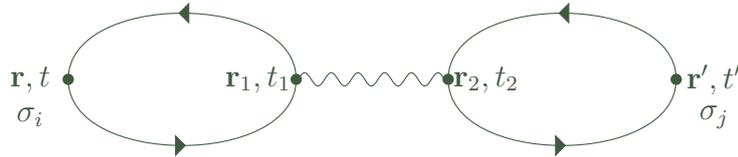


Figure 2: First interaction RPA term. This and all higher order RPA diagrams vanish, as the expressions contain traces of Pauli matrices.

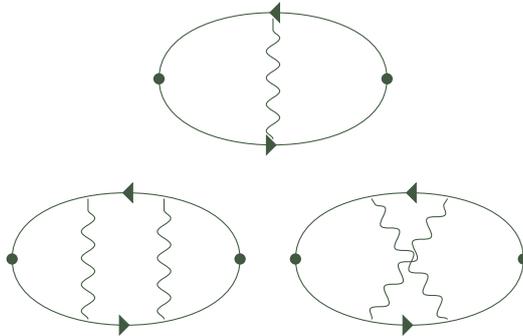


Figure 3: Non-RPA diagrams contributing to the spin susceptibility. Diagrams with different all different numbers of non-crossing lines are summed to obtain the “direct channel”.

It turns out that this is the wrong diagram series to sum in order to find the spin susceptibility in this system, as it does not take into account the effect of the interaction correctly. When using the Wick's theorem on the expectation value in the presence of interactions (124), there are different ways to sum series of diagrams (like the RPA series), which are called "channels":

- Direct channel
- Exchange channel
- Cooper channel

The direct channel gives the RPA series, the exchange channel gives particle-hole ladder series, and the cooper channel gives the particle-particle ladder series. When calculating the RPA result, we neglect those other infinite series of diagrams (see Fig. 3 for examples of diagrams that are not included in the direct channel), which is in this case not justified. The series that gives in this case the most relevant interaction contribution to the spin susceptibility is the particle-hole ladder series.