Karlsruher Institut für Technologie Institute for Condensed Matter Theory
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Condensed Matter Theory II: Many-Body Theory (TKM II) SoSe 2023

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Homework assignment 10
Deadline: 23 June 2023

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1. Effective action for electron-phonon system $(5 + 10 + 2 + 8 = 25 \text{ points})$

Consider electrons interacting with phonons. The system is described by the Hamilton operator $\hat{H} = \hat{H}_{\text{el}} + \hat{H}_{\text{ph}} + \hat{H}_{\text{el-ph}}$, where

$$\hat{H}_{\text{el}} = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}}\, a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \,, \qquad \hat{H}_{\text{ph}} = \sum_{\mathbf{q}} \omega_q\, b^\dagger_{\mathbf{q}} b_{\mathbf{q}} \,, \tag{1}$$

describe free electrons and phonons, and

$$\hat{H}_{\text{el-ph}} = g \sum_{\mathbf{p},\mathbf{q}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}+\mathbf{q}}\, i\sqrt{\omega_q}\,(b_{\mathbf{q}} - b^\dagger_{-\mathbf{q}}) \tag{2}$$

describes the electron-phonon interaction. In this task, we express the partition function of the system, as well as Green's functions, as functional integrals.

(a) Express the partition function of the system as a functional integral over fermionic and bosonic fields.

Solution: The definition of the partition function is

$$Z = \text{Tr}[\exp(-\beta(H - \mu N))]. \tag{3}$$

Here, we have to trace over all electronic and all phononic states. As a basis, we use the coherent states in analogy to the lecture

$$Z = \int \mathcal{D}(\phi^*, \phi) \exp\left(-\sum_l \phi_l^* \phi_l\right) \int \mathcal{D}(\eta^*, \eta) \exp\left(-\sum_k \eta_k^* \eta_k\right) \times \tag{4}$$

$$\times \langle \phi, -\eta | \exp(-\beta(H - \mu N)) | \phi, \eta \rangle \,. \tag{5}$$

Here ϕ are the bosonic- and η the fermionic states. As the chemical potential of the phonons is zero we have $\mu N \to \mu N_{\text{el}}$. Calculating the expectation value in analogy to the lectures, we find

$$Z = \int_{\eta^{(*)}(\beta) = -\eta^{(*)}(0)} \mathcal{D}(\eta, \eta^*) \int_{\phi^{(*)}(\beta) = \phi^{(*)}(0)} \mathcal{D}(\phi, \phi^*) \exp(-S[\eta, \eta^*, \phi, \phi^*]) \tag{6}$$

with the action

$$S[\eta, \eta^*, \phi, \phi^*] = \int_0^\beta \mathrm{d}\tau \left[\sum_k \eta_k^*(\tau)(\partial_\tau - \mu)\eta_k(\tau) + \sum_l \phi_l^*(\tau)\partial_\tau \phi_l(\tau) + H(\eta^*(\tau), \eta(\tau), \phi^*(\tau), \phi(\tau))\right] \tag{7}$$

As the Hamiltonian is given in momentum representation, we use momentum to label the single particle states. Explicitly,

$$H(\eta^*(\tau),\eta(\tau),\phi^*(\tau),\phi(\tau)) = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \eta^*_{\mathbf{p}}(\tau)\eta_{\mathbf{p}}(\tau) + \sum_{\mathbf{q}} \omega_q \phi^*_{\mathbf{q}}(\tau)\phi_{\mathbf{q}}(\tau) + \tag{8}$$

$$+ g\sum_{\mathbf{p},\mathbf{q}} \eta^*_{\mathbf{p}}(\tau)\eta_{\mathbf{p}+\mathbf{q}}(\tau)\mathrm{i}\sqrt{\omega_q}(\phi_{\mathbf{q}}(\tau) - \phi^*_{-\mathbf{q}}(\tau)). \tag{9}$$

Note that any unitary transformation of the fields (for example $\phi(\mathbf{r},\tau) \to \phi(\mathbf{q},\tau)$) leaves the integration measure $(\mathcal{D}\phi)$ unchanged after the corresponding substitution; as the modulus of the determinant of a unitary matrix (and thus of the Jacobian) is 1.

(b) Integrate out the bosonic field configurations in the partition function to derive an effective action for fermions

Solution: The action is quadratic in the bosonic fields ϕ, ϕ^*. Therefore, we can use Eq. (6.50) from the lecture notes to "integrate them out" (solve the integrals over ϕ, ϕ^*):

$$I := \int \mathcal{D}(\phi,\phi^*) \exp\left(- \int_0^\beta \mathrm{d}\tau \sum_l \phi^*_l(\tau)(\partial_\tau + \omega_q)\phi_l(\tau) + g\sum_{\mathbf{q}} \rho_{\mathbf{q}}(\tau)\mathrm{i}\sqrt{\omega_q}(\phi_{\mathbf{q}}(\tau) - \phi^*_{-\mathbf{q}}(\tau))\right) \tag{10}$$

where we introduced $\rho_{\mathbf{q}}(\tau) := \sum_{\mathbf{p}} \eta^*_{\mathbf{p}}(\tau)\eta_{\mathbf{p}+\mathbf{q}}(\tau)$. To deal with the derivative, we express the fields through their Matsubara Fourier transforms:

$$\int_0^\beta \mathrm{d}\tau\, \phi^*_l(\tau)(\partial_\tau + \omega_q)\phi_l(\tau) = \frac{1}{\beta}\sum_{\omega_n} \phi^*_l(\omega_n)(-\mathrm{i}\omega_n + \omega_q)\phi_l(\omega_n) \tag{11}$$

$$\int_0^\beta \mathrm{d}\tau\, \rho_{\mathbf{q}}(\tau)\phi_{\mathbf{q}}(\tau) = \frac{1}{\beta}\sum_{\omega_n} \rho_{\mathbf{q}}(-\omega_n)\phi_{\mathbf{q}}(\omega_n) \tag{12}$$

$$\int_0^\beta \mathrm{d}\tau\, \rho_{\mathbf{q}}(\tau)\phi^*_{-\mathbf{q}}(\tau) = \frac{1}{\beta}\sum_{\omega_n} \rho_{\mathbf{q}}(\omega_n)\phi^*_{-\mathbf{q}}(\omega_n) \tag{13}$$

All introduced Matsubara frequencies are bosonic.
We also change the integration measure to integrate over all $\phi_{\mathbf{q}}(\omega_n), \ldots$ instead of all $\phi_{\mathbf{q}}(\tau), \ldots$. The integral reads now (using the same symbol for the integration measure)

$$I = \int \mathcal{D}(\phi,\phi^*) \exp\left(-\frac{1}{\beta}\sum_{\omega_n,\mathbf{q}} \left[\phi^*_{\mathbf{q}}(\omega_n)(-\mathrm{i}\omega_n + \omega_q)\phi_{\mathbf{q}}(\omega_n) + g\rho_{\mathbf{q}}(\omega_n)\mathrm{i}\sqrt{\omega_q}(\phi_{\mathbf{q}}(-\omega_n) - \phi^*_{-\mathbf{q}}(\omega_n))\right]\right) \tag{14}$$

Applying (6.50) (A is diagonal, with entries (using (6.56) from the lecture) $A^{-1}_{\mathbf{q},\omega_n} = -\beta(-\mathrm{i}\omega_n + \omega_{\mathbf{q}})^{-1}$, $J_1^\dagger(\mathbf{q},\omega_n) = -\beta^{-1}\mathrm{i}g\sqrt{\omega_q}\rho_{\mathbf{q}}(-\omega_n)$, $J_2(\mathbf{q},\omega_n) = \beta^{-1}\mathrm{i}g\sqrt{\omega_q}\rho_{-\mathbf{q}}(\omega_n)$) we find

$$I = C\exp\left(-\frac{g^2}{\beta}\sum_{\mathbf{q}}\sum_{\omega_n} \frac{\omega_q \rho_{\mathbf{q}}(-\omega_n)\rho_{-\mathbf{q}}(\omega_n)}{-\mathrm{i}\omega_n + \omega_q}\right) \tag{15}$$

where C is a constant. We obtain for the effective action for the fermions

$$S_{\mathrm{eff}}[\eta,\eta^*] = \sum_{\mathbf{q}} \left[\sum_{\nu_n} \eta^*_{\mathbf{q}}(\nu_n)(\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu)\eta_{\mathbf{q}}(\nu_n) - \sum_{\omega_n} \frac{g^2}{\beta} \frac{\omega_q \rho_{\mathbf{q}}(-\omega_n)\rho_{-\mathbf{q}}(\omega_n)}{-\mathrm{i}\omega_n + \omega_q} \right] + \log(C) \tag{16}$$

$$\rho_{\mathbf{q}}(\omega_n) = \sum_{\sigma} \int \mathrm{d}^3 p \, \frac{1}{\beta} \sum_{\nu_m} \eta^*_{\mathbf{p}}(\nu_m)\eta_{\mathbf{p}+\mathbf{q}}(\nu_m + \omega_n). \tag{17}$$

ν_m is a fermionic Matsubara frequency.

(c) Derive the free electron Green's function from the partition function for non-interacting electrons. Introduce source fields in the action and take derivatives of the partition function with respect to them.

Solution: The partition function of the non-interacting electrons is

$$Z_{\mathrm{el}} = \int \mathcal{D}(\eta,\eta^*) \exp\left(- \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}(\tau)(\epsilon_{\mathbf{q}} + \partial_\tau - \mu)\eta_{\mathbf{q}}(\tau) \right). \tag{18}$$

To obtain the Green's function, we introduce "source fields" $J^{(1)}(\mathbf{q},\tau)$, $J^{(2)}(\mathbf{q},\tau)$ (similar to the derivation of Wick's theorem from sheet 9) and define

$$Z_{\mathrm{el}}[J^{(1)}, J^{(2)}] := \int \mathcal{D}(\eta,\eta^*) \exp\left(- \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}(\tau)(\epsilon_{\mathbf{q}} + \partial_\tau - \mu)\eta_{\mathbf{q}}(\tau) \right) \times \tag{19}$$

$$\times \exp\left(\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \left(\eta^*_{\mathbf{q}}(\tau) J^{(1)}(\mathbf{q},\tau) + \eta_{\mathbf{q}}(\tau) J^{(2)}(\mathbf{q},\tau) \right) \right) \tag{20}$$

with $Z_{\mathrm{el}} = Z_{\mathrm{el}}[J^{(1)} = 0, J^{(2)} = 0]$. We can now see, that

$$G^{(0)}(\mathbf{q}_1,\tau_1;\mathbf{q}_2,\tau_2) = -\langle \mathcal{T}_\tau a_{\mathbf{q}_1}(\tau_1)\bar{a}_{\mathbf{q}_2}(\tau_2)\rangle \tag{21}$$

$$= -\frac{1}{Z_{\mathrm{el}}} \int_{\eta(0)=-\eta(\beta)} \mathcal{D}(\eta,\eta^*)\eta_{\mathbf{q}_1}(\tau_1)\eta^*_{\mathbf{q}_2}(\tau_2) \times \tag{22}$$

$$\times \exp\left(- \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}(\tau)(\epsilon_{\mathbf{q}} + \partial_\tau - \mu)\eta_{\mathbf{q}}(\tau) \right) \tag{23}$$

$$= -\frac{1}{Z_{\mathrm{el}}[J^{(1)} = 0, J^{(2)} = 0]} \left. \frac{\partial^2 Z_{\mathrm{el}}[J^{(1)}, J^{(2)}]}{\partial J^{(2)}(\mathbf{q}_1,\tau_1)\partial J^{(1)}(\mathbf{q}_2,\tau_2)} \right|_{J^{(1)}=0, J^{(2)}=0}. \tag{24}$$

Here and in the following we use the symbol $G^{(0)}$ for the free electronic Green's function.

Using Eq. (6.80) of the lecture notes, we can evaluate $Z_{\text{el}}[J^{(1)}, J^{(2)}]$:

$$Z_{\text{el}}[J^{(1)}, J^{(2)}] = \int \mathcal{D}(\eta, \eta^*) \exp\left(- \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}(\tau)(\epsilon_{\mathbf{q}} + \partial_\tau - \mu)\eta_{\mathbf{q}}(\tau) \right) \times \tag{25}$$

$$\times \exp\left(\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{q}} \left(\eta^*_{\mathbf{q}}(\tau) J^{(1)}(\mathbf{q}, \tau) + \eta_{\mathbf{q}}(\tau) J^{(2)}(\mathbf{q}, \tau) \right) \right) \tag{26}$$

$$= \int \mathcal{D}(\eta, \eta^*) \exp\left(- \sum_{\nu_n} \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}(\nu_n)(\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu)\eta_{\mathbf{q}}(\nu_n) \right) \times \tag{27}$$

$$\times \exp\left(\sum_{\nu_n} \sum_{\mathbf{q}} \left(\eta^*_{\mathbf{q}}(\nu_n) J^{(1)}(\mathbf{q}, \nu_n) + \eta_{\mathbf{q}}(\nu_n) J^{(2)}(\mathbf{q}, \nu_n) \right) \right) \tag{28}$$

$$= C \exp\left(\sum_{\mathbf{q}} \sum_{\nu_n} \frac{J^{(1)}(\mathbf{q}, \nu_n) J^{(2)}(\mathbf{q}, \nu_n)}{\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu} \right) \tag{29}$$

$$= C \exp\left(\sum_{\mathbf{q}} \sum_{\nu_n} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \exp(\mathrm{i}\nu_n(\tau_1 - \tau_2)) \frac{J^{(2)}(\mathbf{q}, \tau_1) J^{(1)}(\mathbf{q}, \tau_2)}{\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu} \right) \tag{30}$$

where C is a constant. Thus

$$G^{(0)}(\mathbf{q}_1, \tau_1; \mathbf{q}_2, \tau_2) = - \sum_{\nu_n} \exp(\mathrm{i}\nu_n(\tau_1 - \tau_2)) \frac{\delta(\mathbf{q}_1 - \mathbf{q}_2)}{\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu}. \tag{31}$$

As expected we obtain the familiar Green's function of free electrons.

(d) Expand the partition function to first order in g^2 and derive an expression for the lowest-order correction to the fermionic Green's function induced by the electron-phonon interaction.

Solution: We have

$$Z = \int \mathcal{D}(\eta, \eta^*) \exp(-S_{\text{eff}}) \tag{32}$$

$$S_{\text{eff}}[\eta, \eta^*] = \sum_{\mathbf{q}} \left[\sum_{\nu_n} \eta^*_{\mathbf{q}}(\nu_n)(\epsilon_{\mathbf{q}} - \mathrm{i}\nu_n - \mu)\eta_{\mathbf{q}}(\nu_n) - \frac{g^2}{\beta} \sum_{\omega_n} \frac{\omega_q \rho_{\mathbf{q}}(-\omega_n)\rho_{-\mathbf{q}}(\omega_n)}{-\mathrm{i}\omega_n + \omega_q} \right] + \log(C) \tag{33}$$

$$:= S_{\text{el}} + S_{\text{int}} \tag{34}$$

g only appears in the interaction. We thus get

$$Z \approx \int \mathcal{D}(\eta, \eta^*) \exp(-S_{\text{el}})(1 - S_{\text{int}}) \tag{35}$$

$$:= Z^{(0)} + Z^{(2)} \tag{36}$$

We ignore the constant, as it cancels in the Green's function. The electronic Green's function is approximately:

$$G^{(2)}(\mathbf{q}_1, \tau_1; \mathbf{q}_2, \tau_2) \approx - \frac{1}{Z^{(0)} + Z^{(2)}} \int \mathcal{D}(\eta, \eta^*) \eta_{\mathbf{p}_1}(\tau_1) \eta^*_{\mathbf{p}_2}(\tau_2) \exp(-S_{\text{el}}) \left(1 - S_{\text{int}}\right) \tag{37}$$

Expanding to second order in g consistently:

$$G^{(2)}(\mathbf{q}_1,\tau_1;\mathbf{q}_2,\tau_2) = -\frac{1}{Z^{(0)}}\left(\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\eta_{\mathbf{p}_1}(\tau_1)\eta^*_{\mathbf{p}_2}(\tau_2)\left[1-S_{\mathrm{int}}\right]-\right. \tag{38}$$

$$\left.-\frac{Z^{(2)}}{Z^{(0)}}\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\eta_{\mathbf{p}_1}(\tau_1)\eta^*_{\mathbf{p}_2}(\tau_2)\right) \tag{39}$$

$$= G^{(0)}(\mathbf{q}_1,\tau_1;\mathbf{q}_2,\tau_2)+\frac{1}{Z^{(0)}}\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\eta_{\mathbf{p}_1}(\tau_1)\eta^*_{\mathbf{p}_2}(\tau_2)S_{\mathrm{int}}- \tag{40}$$

$$-Z^{(2)}G^{(0)}(\mathbf{q}_1,\tau_1;\mathbf{q}_2,\tau_2) \tag{41}$$

For the second equality we identified the free electronic Green's function $G^{(0)}$ we calculated before.
We calculate the remaining expectation values using Wick's theorem.

$$Z^{(2)} = \int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})S_{\mathrm{int}} \tag{42}$$

$$= -\frac{g^2}{\beta}\int \mathrm{d}^3q\sum_{\omega_n}\frac{\omega_q}{-\mathrm{i}\omega_n+\omega_q}\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\rho_{\mathbf{q}}(-\omega_n)\rho_{-\mathbf{q}}(\omega_n) \tag{43}$$

$$\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\rho_{\mathbf{q}}(-\omega_n)\rho_{-\mathbf{q}}(\omega_n) = \tag{44}$$

$$= \frac{1}{\beta^2}\sum_{\nu_m,\nu_n}\int \mathrm{d}^3p\int \mathrm{d}^3p'\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\eta^*_{\mathbf{p}}(\nu_n)\eta_{\mathbf{p}+\mathbf{q}}(\nu_n+\omega_m)\eta^*_{\mathbf{p}'}(\nu_m)\eta_{\mathbf{p}'-\mathbf{q}}(\nu_m-\omega_m) \tag{45}$$

$$= Z^{(0)}\frac{1}{\beta^2}\sum_{\nu_m,\nu_n}\int \mathrm{d}^3p\int \mathrm{d}^3p'\,\langle\eta^*_{\mathbf{p}}(\nu_n)\eta_{\mathbf{p}+\mathbf{q}}(\nu_n+\omega_m)\eta^*_{\mathbf{p}'}(\nu_m)\eta_{\mathbf{p}'-\mathbf{q}}(\nu_m-\omega_m)\rangle \tag{46}$$

where the expectation value is calculated with respect to the free fermionic action. Thus, the result after applying Wick's theorem is a sum of products of free electron Green's functions corresponding to all combinations of pairwise contractions. We do not write them down, because they cancel against the corresponding terms from the Wick-decomposition of the second second order term

$$\frac{1}{Z^{(0)}}\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\mathrm{el}})\eta_{\mathbf{p}_1}(\tau_1)\eta^*_{\mathbf{p}_2}(\tau_2)S_{\mathrm{int}}. \tag{47}$$

This is just as expected; disconnected terms cancel in the expansion. We calculate the remaining connected terms:

$$\frac{1}{Z^{(0)}}\int \mathcal{D}(\eta,\eta^*)\exp(-S_{\rm el})\eta_{\mathbf{p}_1}(\tau_1)\eta^*_{\mathbf{p}_2}(\tau_2)S_{\rm int} = \tag{48}$$

$$= -\frac{g^2}{\beta^3}\sum_{\nu_l,\nu_o}\exp(\mathrm{i}\nu_l\tau_1)\exp(-\mathrm{i}\nu_o\tau_2)\int \mathrm{d}^3q\sum_{\omega_n}\frac{\omega_q}{-\mathrm{i}\omega_n+\omega_q}\sum_{\nu_m,\nu_n}\int \mathrm{d}^3p\int \mathrm{d}^3p'\times \tag{49}$$

$$\times\,\langle \eta^*_{\mathbf{p}}(\nu_n)\eta_{\mathbf{p}+\mathbf{q}}(\nu_n+\omega_n)\eta^*_{\mathbf{p}'}(\nu_m)\eta_{\mathbf{p}'-\mathbf{q}}(\nu_m-\omega_n)\eta_{\mathbf{p}_1}(\nu_l)\eta^*_{\mathbf{p}_2}(\nu_o)\rangle \tag{50}$$

$$= -\frac{g^2}{\beta^3}\delta(\mathbf{p}_2-\mathbf{p}_1)\sum_{\nu_l,\nu_o}\delta_{\nu_l,\nu_o}\exp(\mathrm{i}\nu_l\tau_1)\exp(-\mathrm{i}\nu_o\tau_2)G^{(0)}(\mathbf{p}_2,\nu_o)G^{(0)}(\mathbf{p}_1,\nu_l)\times \tag{51}$$

$$\times\int \mathrm{d}^3q\sum_{\omega_n}\frac{\omega_q}{-\mathrm{i}\omega_n+\omega_q}\sum_{\nu_n}\int \mathrm{d}^3p\,(\mathrm{disc}- \tag{52}$$

$$-\,\delta(\mathbf{q})\delta_{\nu_n,0}G^{(0)}(\mathbf{p},\nu_n)+G^{(0)}(\mathbf{p}_1-\mathbf{q},\nu_l-\omega_n)+G(\mathbf{p}_1+\mathbf{q},\nu_l+\omega_n)-G^{(0)}(\mathbf{p},\nu_n)\delta(\mathbf{q})\delta_{\nu_n,0}) \tag{53}$$

$$= -\frac{g^2}{\beta^3}\delta(\mathbf{p}_2-\mathbf{p}_1)\sum_{\nu_l,\nu_o}\delta_{\nu_l,\nu_o}\exp(\mathrm{i}\nu_l\tau_1)\exp(-\mathrm{i}\nu_o\tau_2)G^{(0)}(\mathbf{p}_2,\nu_o)G^{(0)}(\mathbf{p}_1,\nu_l)\times \tag{54}$$

$$\times\int \mathrm{d}^3q\sum_{\omega_n}\frac{\omega_q^2}{\omega_n^2+\omega_q^2}\sum_{\nu_n}\int \mathrm{d}^3p\,\left(\mathrm{disc}-\delta(\mathbf{q})\delta_{\nu_n,0}G^{(0)}(\mathbf{p},\nu_n)+G^{(0)}(\mathbf{p}_1-\mathbf{q},\nu_l-\omega_n)\right) \tag{55}$$

Identifying the free phononic Green's function, we obtain

$$G^{(2)}(\mathbf{p}_1,\tau_1;\mathbf{p}_2,\tau_2) = \frac{g^2}{\beta^3}\delta(\mathbf{p}_2-\mathbf{p}_1)\sum_{\nu_l,\nu_o}\delta_{\nu_l,\nu_o}\exp(\mathrm{i}\nu_l(\tau_1-\tau_2))[G^{(0)}]^2(\mathbf{p}_1,\nu_l)\times \tag{56}$$

$$\times\int \mathrm{d}^3q\,\mathrm{d}^3p\sum_{\omega_n,\nu_n}G^{(0)}_{\rm ph}(\mathbf{q},\omega_n)\left(\delta(\mathbf{q})\delta_{\nu_n,0}G^{(0)}(\mathbf{p},\nu_n)+G^{(0)}(\mathbf{p}_1-\mathbf{q},\nu_l-\omega_n)\right). \tag{57}$$

2. Hubbard-Stratonovich transformation (1 + 7 + 7 + 2 + 3 + 5 = 25 points)

Assume that we have a general electron-electron interaction

$$H^{\rm int}(\psi^*,\psi) = \frac{1}{2}\sum_{abcd}V_{ad,bc}\psi^*_a\psi^*_b\psi_c\psi_d, \tag{58}$$

where a,b,c,d refer to *e.g.* spin σ and space-time coordinates $(\mathbf{r},\tau)$ or $(\mathbf{p},\omega_n)$. Within the path integral, we can introduce some suitable set of bilinear operators $\rho_n=\psi^*_a\psi_d$ and $\rho_m=\psi^*_b\psi_c$ to write the interaction as

$$H^{\rm int}(\psi^*,\psi) = \frac{1}{2}\sum_{nm}\rho_nV_{nm}\rho_m. \tag{59}$$

It is then possible to introduce a new (real) bosonic field ϕ, and express the interaction as

$$\exp\left(-\frac{1}{2}\sum_{nm}\rho_mV_{mn}\rho_n\right) = \mathcal{N}\int \mathcal{D}\phi\exp\left(-\frac{1}{2}\sum_{nm}\phi_mV^{-1}_{mn}\phi_n-\sum_m i\phi_m\rho_m\right), \tag{60}$$

where the prefactor $\mathcal{N}$ does not contain any fields and does not affect the dynamics. This is similar to using Eq. (6.55) in reverse. However, we have introduced an extra imaginary unit to obtain the negative sign on the left-hand side. This is necessary in case of repulsive interaction ($V_{nm} > 0$). For an attractive interaction we can use Eq. (6.55) as it stands.

The equation (60) is known as the Hubbard-Stratonovich transformation, and it allows us to express any electron-electron interaction as an interaction between an electron and a Gaussian bosonic field ϕ. The transformation is exact; new action is completely equivalent to the original one, but does not contain a quartic electronic term anymore. The price we pay is that there is an extra field with its own dynamics. The power of the Hubbard-Stratonovich transformation comes from the fact that it allows us to make approximations systematically.

Let us study the fermionic action for electrons interacting through the Coulomb potential, and use the Hubbard-Stratonovich transformation to derive the effective RPA interaction between the electrons.

(a) To begin, write down the action for electrons interacting via the Coulomb potential.

Solution: See also Altland-Simons book about this task (parts of the solutions are based on the corresponding discussion in this book). According to lecture Eq. (6.100), the action functional for fermions has the form

$$S[\psi, \psi^*] = \int_0^\beta \mathrm{d}\tau \left[\sum_k \psi^*(\tau)(\partial_\tau - \mu)\psi_k(\tau) + H(\psi^*(\tau), \psi(\tau)) \right] \tag{61}$$

$$H(\psi^*(\tau), \psi(\tau)) := H(\{\psi_k(\tau)\}, \{\psi_k^*(\tau)\}) \tag{62}$$

We label single-particle states by position and spin:

$$k = (\mathbf{r}, \sigma) \tag{63}$$

The Hamilton reads

$$H = \sum_\sigma \int \mathrm{d}^3p \left[\frac{\mathbf{p}^2}{2m} a^\dagger_{\mathbf{p},\sigma} a_{\mathbf{p},\sigma} \right] + \frac{1}{2} \sum_{\sigma,\sigma'} \int \mathrm{d}^3r\, \mathrm{d}^3r'\, \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \tag{64}$$

$$= -\sum_\sigma \int \mathrm{d}^3r \left[\psi^\dagger_\sigma(\mathbf{r}) \frac{\nabla^2}{2m} \psi_\sigma(\mathbf{r}) \right] + \frac{1}{2} \sum_{\sigma,\sigma'} \int \mathrm{d}^3r\, \mathrm{d}^3r'\, \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \tag{65}$$

where $U(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$. As H is normal ordered, the function $H(\{\psi_k(\tau)\}, \{\psi_k^*(\tau)\})$ is found by replacing the operators $\psi^\dagger$ and ψ by complex variables ψ^* and ψ. We thus find the action

$$S[\psi, \psi^*] = \sum_\sigma \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r\, \psi^*_\sigma(\mathbf{r},\tau) \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r},\tau) + \tag{66}$$

$$+ \sum_{\sigma,\sigma'} \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi^*_\sigma(\mathbf{r},\tau)\psi^*_{\sigma'}(\mathbf{r}',\tau)U(\mathbf{r}-\mathbf{r}')\psi_{\sigma'}(\mathbf{r}',\tau)\psi_\sigma(\mathbf{r},\tau). \tag{67}$$

(b) For the Coulomb interaction, make a Hubbard-Stratonovich transformation by introducing a bosonic field ϕ that couples to the electron density

$$\rho(\mathbf{q},\tau) = \sum_{\mathbf{p},\sigma} \psi^*_\sigma(\mathbf{p},\tau)\psi_\sigma(\mathbf{p}+\mathbf{q},\tau). \tag{68}$$

Solution: We start by writing the interaction part of the action in Fourier space:

$$S_{\text{int}} := \frac{1}{2}\sum_{\sigma,\sigma'}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi^*_\sigma(\mathbf{r},\tau)\psi^*_{\sigma'}(\mathbf{r}',\tau)U(\mathbf{r}-\mathbf{r}')\psi_{\sigma'}(\mathbf{r}',\tau)\psi_\sigma(\mathbf{r},\tau) \tag{69}$$

$$= \frac{1}{2}\sum_{\sigma,\sigma'}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \psi^*_{\sigma'}(\mathbf{r}',\tau)\psi_{\sigma'}(\mathbf{r}',\tau)U(\mathbf{r}-\mathbf{r}')\psi^*_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau) \tag{70}$$

$$= \frac{1}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r \int \mathrm{d}^3r' \int \mathrm{d}^3p' \int \mathrm{d}^3p \exp(\mathrm{i}\mathbf{p}\mathbf{r})\exp(\mathrm{i}\mathbf{p}'\mathbf{r}')\times \tag{71}$$

$$\times\, \rho(\mathbf{p},\tau)U(\mathbf{r}-\mathbf{r}')\rho(\mathbf{p}',\tau) \tag{72}$$

$$= \frac{1}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r' \int \mathrm{d}^3p' \int \mathrm{d}^3p \exp(\mathrm{i}(\mathbf{p}+\mathbf{p}')\mathbf{r}')\rho(\mathbf{p},\tau)\frac{4\pi e^2}{\mathbf{p}^2}\rho(\mathbf{p}',\tau) \tag{73}$$

$$= \frac{1}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3p\, \rho(\mathbf{p},\tau)\frac{4\pi e^2}{\mathbf{p}^2}\rho(-\mathbf{p},\tau) \tag{74}$$

We can now perform the Hubbard-Stratonovich transformation as described. The "matrix elements" of the potential are $V((\mathbf{p},\tau),(\mathbf{p}',\tau')) = \delta(\mathbf{p}+\mathbf{p}')\delta(\tau-\tau')\frac{4\pi e^2}{\mathbf{p}^2}$. Using the definition of the inverse function (6.56) from the lecture, we find that $V^{-1}((\mathbf{p},\tau),(\mathbf{p}',\tau')) = \delta(\mathbf{p}+\mathbf{p}')\delta(\tau-\tau')\frac{\mathbf{p}^2}{4\pi e^2}$. We thus have

$$\exp\left(-\frac{1}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3p\, \rho(\mathbf{p},\tau)\frac{4\pi e^2}{\mathbf{p}^2}\rho(-\mathbf{p},\tau)\right) = \tag{75}$$

$$= \mathcal{N}\int \mathcal{D}\phi \exp\left(-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3p \left[\frac{1}{2}\phi(\mathbf{p},\tau)\frac{\mathbf{p}^2}{4\pi e^2}\phi(-\mathbf{p},\tau) + \mathrm{i}\phi(\mathbf{p},\tau)\rho(\mathbf{p},\tau)\right]\right) \tag{76}$$

(c) After the Hubbard-Stratonovich transformation, the electronic action is quadratic. Integrate out the fermions using Eq. (6.80) and obtain an effective action $S_{\text{eff}}[\phi]$ that only includes the field ϕ as a variable.

Solution: The part of the action containing electron fields reads

$$S_{\text{ferm}} = \sum_\sigma \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3r\, \psi^*_\sigma(\mathbf{r},\tau)\left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi_\sigma(\mathbf{r},\tau) + \tag{77}$$

$$+ \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3p\, \mathrm{i}\phi(\mathbf{p},\tau)\rho(\mathbf{p},\tau) \tag{78}$$

We use

$$\int \mathrm{d}^3p\, \phi(\mathbf{p},\tau)\rho(\mathbf{p},\tau) = \int \mathrm{d}^3r'\, \phi(\mathbf{r}',\tau)\rho(\mathbf{r}',\tau) \tag{79}$$

where

$$\rho(\mathbf{r}',\tau) = \sum_\sigma \psi^*_\sigma(\mathbf{r}',\tau)\psi_\sigma(\mathbf{r}',\tau) \tag{80}$$

to write this action as

$$S_{\text{ferm}} = \sum_{\sigma} \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}^3r\, \psi^*_\sigma(\mathbf{r},\tau) \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu + \mathrm{i}\phi(\mathbf{r},\tau)\right) \psi_\sigma(\mathbf{r},\tau) \tag{81}$$

$$= \int \mathrm{d}^3q\, \mathrm{d}^3q' \sum_{\nu_n,\nu_m} \times \tag{82}$$

$$\times\, \psi^*_\sigma(\mathbf{q},\nu_n) \left[\left(-\mathrm{i}\nu_m + \frac{\mathbf{q}^2}{2m} - \mu\right) \delta_{\nu_n,\nu_m} \delta(\mathbf{q}-\mathbf{q}') + \mathrm{i}\phi(\mathbf{q}-\mathbf{q}',\nu_n-\nu_m)\right] \psi_\sigma(\mathbf{q},\nu_m) \tag{83}$$

ν_n, ν_m are fermionic Matsubara frequencies. Now we use (6.80) from the lecture notes and obtain a contribution for the effective action

$$\int \mathcal{D}(\psi,\psi^*) \exp(-S_{\text{ferm}}) = \det\left[\left(-\mathrm{i}\nu_m + \frac{\mathbf{q}^2}{2m} - \mu\right) \delta_{\nu_n,\nu_m} \delta(\mathbf{q}-\mathbf{q}') + \mathrm{i}\phi(\mathbf{q}-\mathbf{q}',\nu_n-\nu_m)\right]. \tag{84}$$

We obtain the effective action for the Hubbard-Stratonovich field

$$S_{\text{eff}}[\phi] = \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}^3p \left[\frac{1}{2}\phi(\mathbf{p},\tau)\frac{\mathbf{p}^2}{4\pi e^2}\phi(-\mathbf{p},\tau)\right] - \log(\det[A]) \tag{85}$$

$$A_{n,m}(\mathbf{q},\mathbf{q}') := \left(-\mathrm{i}\nu_m + \frac{\mathbf{q}^2}{2m} - \mu\right) \delta_{\nu_n,\nu_m} \delta(\mathbf{q}-\mathbf{q}') + \mathrm{i}\phi(\mathbf{q}-\mathbf{q}',\nu_n-\nu_m) \tag{86}$$

using the identity (6.122) from the lecture, this can be rewritten as

$$S_{\text{eff}}[\phi] = \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}^3p \left[\frac{1}{2}\phi(\mathbf{p},\tau)\frac{\mathbf{p}^2}{4\pi e^2}\phi(-\mathbf{p},\tau)\right] - \mathrm{Tr}(\log[A]) \tag{87}$$

$$= \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}^3p \left[\frac{1}{2}\phi(\mathbf{p},\tau)\frac{\mathbf{p}^2}{4\pi e^2}\phi(-\mathbf{p},\tau)\right] - \sum_{\nu_n} \int \mathrm{d}^3q \log[A]\,(\mathbf{q},\nu_n;\mathbf{q},\nu_n). \tag{88}$$

(d) The dominant contribution to the functional integral comes from the vicinity of the minimum of the action $S_{\text{eff}}[\phi]$. Find the minimum by taking a functional derivative

$$\frac{\delta S_{\text{eff}}[\phi]}{\delta\phi} = 0. \tag{89}$$

The minimum corresponds to the mean-field value of the field ϕ.

Solution: To take the functional derivative, we use Eq. (6.128) from the lecture: Matrix A depends on parameters $\{\phi(\mathbf{q},\omega_n)\}$ and according to this equation we can evaluate the derivative with respect to a parameter as

$$\partial_z\, \mathrm{Tr}(f(A)) = \mathrm{Tr}[f'(A)\partial_z A] \tag{90}$$

We find

$$\frac{\partial S_{\text{eff}}[\phi]}{\partial\phi(\mathbf{q},\omega_l)} = \left(\left[\frac{\mathbf{q}^2}{4\pi e^2}\phi(-\mathbf{q},\omega_l)\right] - \right. \tag{91}$$

$$\left. -\mathrm{i} \sum_{\nu_n,\nu_m} \int \mathrm{d}^3p \int \mathrm{d}^3p'\, [A^{-1}](\nu_n,\mathbf{p};\nu_m,\mathbf{p}')\delta(\mathbf{q}-(\mathbf{p}'-\mathbf{p}))\delta_{\omega_l,\nu_m-\nu_n}\right) \tag{92}$$

$$= \left(\left[\frac{\mathbf{q}^2}{4\pi e^2}\phi(-\mathbf{q},\omega_l)\right] - \mathrm{i}\sum_{\nu_n} \int \mathrm{d}^3p\, [A^{-1}](\nu_n,\mathbf{p};\nu_n-\omega_l,\mathbf{p}-\mathbf{q})\right) \tag{93}$$

We make an Ansatz of a constant (in space-time space) solution:

$$\phi_0(\mathbf{q}, \omega_m) := C\delta(\mathbf{q})\delta_{\omega_m,0} \tag{94}$$

This diagonalizes A:

$$A_{n,m}(\mathbf{q}, \mathbf{q}') = \delta(\mathbf{q} - \mathbf{q}')\delta_{\nu_n,\nu_m}\left(-\mathrm{i}\nu_n + \frac{\mathbf{q}^2}{2m} - \mu + \mathrm{i}C\right) \tag{95}$$

The inverse is thus given by

$$\left[A^{-1}\right](\nu_n, \mathbf{q}; \nu_m, \mathbf{q}') = \frac{\delta_{\nu_n,\nu_m}\delta(\mathbf{q} - \mathbf{q}')}{-\mathrm{i}\nu_n + \frac{\mathbf{q}^2}{2m} - \mu + \mathrm{i}C}. \tag{96}$$

We see, that the second term of Eq. (93) vanishes for any C for $\omega_l \neq 0$ or $\mathbf{q} \neq 0$. The same hods true for the first term. $\mathbf{q} = 0$ is irrelevant for the mean field solution (see Altland). Therefore, the action is indeed stationary for any constant (in $(\mathbf{r}, \tau)$) field. Requiring charge neutrality, we set $C = 0$. Our mean field solution is thus

$$\phi_0(\mathbf{r}, \tau) = 0. \tag{97}$$

(e) The low-energy dynamics of the field are given by the fluctuations of the field ϕ around its mean-field value. Expand the action to quadratic order in ϕ and identify the polarization operator and the screened Coulomb interaction U_{eff}^{-1}.

Solution: We denote the fluctuations by $\phi(\mathbf{r}, \tau)$. The first term of the action is already quadratic in ϕ. To expand the term with the logarithm, we proceed along the lines of lecture Eqs. (6.142 - 6.144). First, we separate our matrix in a mean field part and the fluctuation field ϕ (everything should be understood in terms of the matrix (86) here)

$$A = A_0 + \mathrm{i}\phi \tag{98}$$

then

$$\operatorname{tr}(\log(A_0 + \mathrm{i}\phi)) = \operatorname{Tr}\big(\log\big(A_0\left[1 + A_0^{-1}\mathrm{i}\phi\right]\big)\big) \tag{99}$$

$$\approx \operatorname{Tr}\log(A_0) - \frac{1}{2}\operatorname{Tr}\big(A_0^{-1}\phi A_0^{-1}\phi\big) \tag{100}$$

From the last task we see

$$A_0^{-1} = G_0 \tag{101}$$

where G_0 is the Green's function of a free electron.
We find

$$S_{\text{eff}}[\phi] \approx \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3p \left[\frac{1}{2}\phi(\mathbf{p}, \tau)\frac{\mathbf{p}^2}{4\pi e^2}\phi(-\mathbf{p}, \tau)\right] + \operatorname{Tr}(\log(A_0)) - \frac{1}{2}\operatorname{Tr}\big(A_0^{-1}\phi A_0^{-1}\phi\big) \tag{102}$$

The second term can be identified with the partition sum of the free electron gas (see Altland-Simons). The third term, again using the definition (86) of matrix A:

$$\frac{1}{2}\operatorname{Tr}\big(A_0^{-1}\phi A_0^{-1}\phi\big) = \frac{1}{2}\sum_{i,j,k,l}[G_0]_{i,j}\phi_{j,k}[G_0]_{k,l}\phi_{l,i} \tag{103}$$

$$= \frac{1}{2}\sum_{i,k}[G_0]_i\phi_{i,k}[G_0]_k\phi_{k,i} \tag{104}$$

$$= \frac{1}{2}\sum_{\nu_n,\nu_m}\int \mathrm{d}^3p\,\mathrm{d}^3p'\,G_0(\mathbf{p},\nu_n)\phi(\mathbf{p}-\mathbf{p}',\nu_n-\nu_m)G_0(\mathbf{p}',\nu_m)\phi(\mathbf{p}'-\mathbf{p},\nu_m-\nu_n) \tag{105}$$

$$= \frac{1}{2}\sum_{\nu_n,\nu_m}\int \mathrm{d}^3p\,\mathrm{d}^3p'\,G_0(\mathbf{p}+\mathbf{p}',\nu_n+\nu_m)\phi(\mathbf{p},\nu_n)G_0(\mathbf{p}',\nu_m)\phi(-\mathbf{p},-\nu_n) \tag{106}$$

$$:= \frac{1}{2}\int \mathrm{d}^3p\sum_{\nu_n}\phi(\mathbf{p},\nu_n)\Pi(\mathbf{p},\nu_n)\phi(-\mathbf{p},-\nu_n) \tag{107}$$

In the last step we identified the polarization operator $\Pi(\mathbf{p},\nu_n)$. Rewriting the effective interaction, we have

$$S_{\text{eff}}[\phi] \approx \sum_{\nu_n}\int \mathrm{d}^3p\left[\frac{1}{2}\phi(\mathbf{p},\nu_n)U_{\text{eff}}^{-1}(\mathbf{p},\nu_n)\phi(-\mathbf{p},-\nu_n)\right] + \operatorname{Tr}(\log(A_0)) \tag{108}$$

$$U_{\text{eff}}^{-1}(\mathbf{p},\nu_n) := \left(\frac{\mathbf{p}^2}{4\pi e^2} - \Pi(\mathbf{p},\nu_n)\right) \tag{109}$$

Where the effective interaction potential corresponds to the screened Coulomb interaction.

(f) Using the quadratic approximation for the effective action written in terms of the Hubbard-Stratonovich fields, express the RPA free energy of the interacting electron gas in terms of the polarization operator.

Solution: As we expanded the interaction to second order in ϕ, we can explicitly solve the now gaussian path integral of the partition function in this expansion. This solution to quadratic order corresponds to the RPA approximation.

$$F_{\text{RPA}} = -T\log(Z_{\text{RPA}}) = -T\log(Z_0) + T\int \mathrm{d}^3q\sum_{\nu_n}\log\left(1+\frac{4\pi e^2}{q^2}\Pi(\mathbf{q},\nu_n)\right)^{1/2} \tag{110}$$