

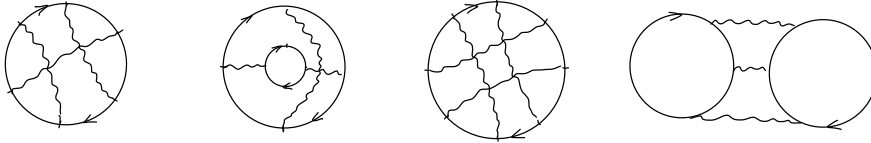
Homework 3, 620 Many body

November 20, 2023

- 1) Draw all connected topologically distinct (unlabeled) Feynman diagrams for the self-energy up to the second order with expansion on the Hartree state. Exclude tadpoles, which are accounted for by expanding on the Hartree state with redefined single particle potential.

Assume that the system is translationally invariant, use momentum and frequency basis to write complete expression for the value of these diagrams. Use the Coulomb interaction v_q and single-particle propagator $G_{\mathbf{k}}^0(i\omega_n)$ in your expressions.

- 2) Calculate the symmetry factors for the following Feynman diagrams, which contribute to $\log Z$ expansion.



- 3) Use the Kleinart's trick to show that the following integral

$$I(g) = \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2 - \frac{1}{4}gx^4} \quad (1)$$

can be well approximated with the few lowest order terms in perturbation theory.

The exact result of the integral is

$$I^{exact}(g) = \frac{e^{\frac{1}{8g}}}{2\sqrt{\pi g}} BesselK\left(\frac{1}{4}, \frac{1}{8g}\right)$$

We start by expanding in powers of ξ around arbitrary frequency Ω , which gives

$$\begin{aligned} I(g, \Omega) &= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}\Omega^2 x^2 - \xi(\frac{1}{4}gx^4 - \frac{1}{2}x^2(\Omega^2 - 1))} \\ &= \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}\Omega^2 x^2} \sum_{n=0}^{\infty} \frac{(-\xi)^n}{n!} \left(\frac{1}{4}gx^4 - \frac{1}{2}x^2(\Omega^2 - 1)\right)^n \end{aligned} \quad (2)$$

For $\xi = 1$ the original action has not been changed. ξ here just keeps track of perturbative order, and is set to 1 once the expansion is evaluated.

- Show that $I^{(0)}(g, \Omega) = \frac{1}{\Omega}$, which does not have optimum in terms of parameter Ω .
- Show that at order ξ^1 the value of the integral is

$$I^{(1)}(g, \Omega) = -\frac{3}{4} \frac{g}{\Omega^2} - \frac{1}{2\Omega^3} + \frac{3}{2\Omega}.$$

- Show that the principal of minimal sensitivity requires $\Omega^2 = \frac{1}{2}(1 \pm \sqrt{1+10g})$.
- Show that $I(g)$ at the first order can be approximated by

$$I^{(1)}(g) = \frac{3g + \frac{1}{2} + \frac{1}{2}\sqrt{1+10g}}{(\frac{1}{2}(1 + \sqrt{1+10g}))^{5/2}} \quad (3)$$

- Check numerically the difference between $I^{(1)}(g) - I^{exact}(g)$.
- Check analytically the leading order expansion at large g . Note that the exact result has expansion $I^{exact} = 1.023g^{-1/4}$. What is the exponent and coefficient for $I^{(1)}(g)$?

The rest of the questions in this problem are optional.

It turns out that at order ξ^2 there is no optimum. However, all odd terms have optimum, and at order ξ^3 we again get a good approximation for $I(g)$. Check numerically, and analytically at large g , that the difference between $I^{(3)}$ and I^{exact} is smaller than between $I^{(1)} - I^{exact}$. What is the coefficient a for $I^{(3)}(g) = ag^{-1/4}$ expansion at large g ?

- 4) The Uniform Electron Gas is translationally invariant homogeneous system of interacting electrons, which is kept in-place by uniformly distributed positive background charge. The action for the model is

$$S[\psi] = \sum_{\mathbf{k}, \sigma} \int_0^\beta d\tau \psi_{\mathbf{k}\sigma}^\dagger(\tau) \left(\frac{\partial}{\partial \tau} - \mu + \varepsilon_{\mathbf{k}} \right) \psi_{\mathbf{k}\sigma}(\tau) + \frac{1}{2V} \sum_{\sigma, \sigma', \mathbf{k}, \mathbf{k}', \mathbf{q} \neq 0} v_{\mathbf{q}} \int_0^\beta d\tau \psi_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger(\tau) \psi_{\mathbf{k}'-\mathbf{q}, \sigma'}^\dagger(\tau) \psi_{\mathbf{k}', \sigma'}(\tau) \psi_{\mathbf{k}, \sigma}(\tau) \quad (4)$$

Here $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ and $v_{\mathbf{q}} = \frac{e_0^2}{\varepsilon_0 q^2}$ is the Coulomb repulsion. The uniform density n_0 is equal to the number of electrons per unit volume, i.e., $n_0 = N_e/V$ for charge neutrality. The density n_0 is usually expressed in terms of distance parameter r_s , which is the typical radius between two electrons, and is defined by $1/n_0 = 4\pi r_s^3/3$. Furthermore, the Coulomb repulsion and the single-particle energy can be conveniently expressed in Rydberg units ($13.6 \text{ eV} = \hbar^2/(2ma_0^2)$, a_0 Bohr radius), in which $v_{\mathbf{q}} = 8\pi/q^2$ and $\varepsilon_{\mathbf{k}} = k^2$, and all momentums are measured in $1/a_0$.

- Show that the Fermi momentum $k_F = (9\pi/4)^{1/3}/r_s$, where $E_F = k_F^2$ in these units.

- Show that the kinetic energy per density is $E_{kin}/(Vn_0) = \varepsilon_{kin} = \frac{3}{5}k_F^2$ or $\varepsilon_{kin} = 2.2099/r_s^2$.
- Calculate the exchange (Fock) self-energy diagram and show it has the form

$$\Sigma_{\mathbf{k}}^x = -\frac{2k_F}{\pi} S\left(\frac{k}{k_F}\right) \quad (5)$$

where

$$S(x) = 1 + \frac{1-y^2}{2y} \log \left| \frac{1+y}{1-y} \right| \quad (6)$$

Note that $S(x)$ can be obtained by the following integral

$$S(x) = \frac{1}{x} \int_0^1 du u \log \left| \frac{u+x}{u-x} \right| \quad (7)$$

- Derive the expression for the effective mass of the system, which is defined in the following way

$$G_{\mathbf{k} \approx k_F}(\omega \approx 0) = \frac{Z_k}{\omega - \frac{k^2 - k_F^2}{2m^*}} \quad (8)$$

Start from the definition of the Green's function $G_{\mathbf{k}}(\omega) = 1/(\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega))$ and Taylor's expression of the self-energy

$$\Sigma_{\mathbf{k} \approx k_F}(\omega \approx 0) = \Sigma_{k_F}(0) + \frac{\partial \Sigma_{k_F}(0)}{\partial \omega} \omega + \frac{\partial \Sigma_{k_F}(0)}{\partial k} (k - k_F) \quad (9)$$

and define $Z_k^{-1} = 1 - \frac{\partial \Sigma_{k_F}(0)}{\partial \omega}$ and take into account the validity of the Luttinger's theorem (the volume of the Fermi surface can not change by interaction). Show that under these assumptions, the effective mass of the quasiparticle is

$$\frac{m}{m^*} = Z_k \left(1 + \frac{m}{k_F} \frac{\partial \Sigma_{k_F}(0)}{\partial k} \right) \quad (10)$$

- Use the exchange self-energy and show that within Hartee-Fock approximation the effective mass is vanishing. Is there any quasiparticle left at the Fermi level in this theory? What does that mean for the stability of the metal in this approximation? What is the cause of (possible) instability?
- What is the form of the spectral function $A_k(\omega)$ near $k = k_F$ and $\omega = 0$?
- Calculate the contribution to the total energy of the exchange self-energy, which is defined by

$$\Delta E_{tot} = \frac{T}{2} \sum_{\mathbf{k}, \sigma, i\omega_n} G_{\mathbf{k}}(i\omega_n) \Sigma_{\mathbf{k}}(i\omega_n) \quad (11)$$

Show that $\Delta E_{tot}/(n_0V) = -0.91633/r_s$ is Rydberg units.

Note that the correction to the kinetic energy, which goes as $1/r_s^2$ is large when r_s is large, i.e., when the density is small (dilute limit).

- Evaluate the higher order correction for self-energy of the RPA form, which is composed of the following Feynman diagrams

$$\Sigma_{\mathbf{k}}(i\omega) = \text{[Diagram 1]} + \text{[Diagram 2]} + \text{[Diagram 3]} + \dots$$

Show that the self-energy can be evaluated to

$$\Sigma_{\mathbf{k}}(i\omega_n) = -\frac{1}{\beta} \sum_{\mathbf{q}, i\Omega_m} v_q^2 G_{\mathbf{k}+\mathbf{q}}^0(i\omega_n + i\Omega_m) \frac{P_q(i\Omega_m)}{1 - v_q P_q(i\Omega_m)} \quad (12)$$

where

$$P_q(i\Omega_m) = \frac{1}{\beta} \sum_{i\omega_n, \mathbf{k}, s} G_{\mathbf{k}}^0(i\omega_n) G_{\mathbf{k}+\mathbf{q}}^0(i\omega_n + i\Omega_m) \quad (13)$$

- Show that the Polarization function $P_q(i\Omega_m)$ on the real axis ($i\Omega_m \rightarrow \Omega + i\delta$) takes the following form

$$P_q(\Omega + i\delta) = -\frac{k_F}{4\pi^2} \left(\mathcal{P} \left(\frac{\Omega}{k_F^2} + i\delta, \frac{q}{k_F} \right) + \mathcal{P} \left(-\frac{\Omega}{k_F^2} - i\delta, \frac{q}{k_F} \right) \right) \quad (14)$$

where

$$\mathcal{P}(x, y) = \frac{1}{2} - \left[\frac{(x + y^2)^2 - 4y^2}{8y^3} \right] [\log(x + y^2 + 2y) - \log(x + y^2 - 2y)] \quad (15)$$

- RPA contribution to the total energy is again

$$\Delta E_{tot} = \frac{T}{2} \sum_{\mathbf{k}, s, i\omega_n} G_{\mathbf{k}}^0(i\omega_n) \Sigma_{\mathbf{k}}(i\omega_n) \quad (16)$$

Show that within this RPA approximation the total energy takes the form

$$\Delta E_{tot} = -\frac{V}{2} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\Omega}{\pi} n(\Omega) \text{Im} \left\{ \frac{v_q^2 P_q(\Omega + i\delta)^2}{1 - v_q P_q(\Omega + i\delta)} \right\} \quad (17)$$

The analytic expression for this total energy contribution can not expressed in a closed form, however, an asymptotic expression for small r_s has the form $\Delta E_{tot}/n_0 \approx -0.142 + 0.0622 \log(r_s)$, which signals that the total energy is not an analytic function of r_s or density, hence perturbation theory in powers of v_q is bound to fail. Analytic solution of this problem is still not available, and only numerical estimates by QMC can be found in literature. Note that this total energy density is at the heart of the Density Functional Theory.