Karlsruher Institut für Technologie Institute for Condensed Matter Theory
Institute for Quantum Materials and Technologies

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

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Homework assignment 7
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1. Plasmon dispersion in the hydrodynamic approximation ($5 + 13 + 2 = 20$ points)

Let us calculate the plasmon dispersion for a Fermi gas in the hydrodynamic limit. Use the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

for the mass density $\rho(\mathbf{r}, t) = mn(\mathbf{r}, t)$, where $\mathbf{u}(\mathbf{r}, t)$ is the velocity distribution, m is the electron mass and n is the electron number density. The force acting on the electron distribution is given by the Euler equation

$$\partial_t(\rho \mathbf{u}) = -en\mathbf{E} - \boldsymbol{\nabla} P. \tag{2}$$

where $\mathbf{E}$ is the electric field and P is the internal pressure of the Fermi gas.

(a) Due to Pauli repulsion, the pressure of a Fermi gas does not vanish at zero temperature. Use a suitable thermodynamic relation and calculate the pressure of a 3D Fermi gas with a parabolic dispersion as a function of the electron density n at zero temperature.

Solution: Thermodynamically, pressure is defined as the volume derivative at fixed temperature and particle number

$$P = -\left.\frac{\partial F}{\partial V}\right|_{T=0,N} = -\left.\frac{\partial U}{\partial V}\right|_{T=0,N}. \tag{3}$$

The particle number and the internal energy of a 3D Fermi gas is

$$N = V \sum_\sigma \int_{|\mathbf{p}|<p_\mathrm{F}} \frac{\mathrm{d}\mathbf{p}}{(2\pi)^3} = V \frac{p_\mathrm{F}^3}{3\pi^2} \tag{4}$$

$$U = V \sum_\sigma \int_{|\mathbf{p}|<p_\mathrm{F}} \frac{\mathrm{d}\mathbf{p}}{(2\pi)^3} \frac{p^2}{2m} = V \frac{p_F^5}{10\pi^2 m} \tag{5}$$

The internal energy in terms of N is

$$U = \frac{V}{10\pi^2 m} \left(\frac{3\pi^2 N}{V}\right)^{5/3} = \frac{(3\pi^2 N)^{5/3} V^{-2/3}}{10\pi^2 m} \tag{6}$$

The pressure is

$$P = \frac{(3\pi^2)^{2/3}}{5m} \left(\frac{N}{V}\right)^{5/3}. \tag{7}$$

(b) Assume an external electric field $\mathbf{E}_{\text{ext}}(\mathbf{r},t) = \mathbf{E}_0 e^{i(\omega t - \mathbf{q}\cdot\mathbf{r})}$ acting on the system. Calculate the linear response of the electron density $\delta n(\mathbf{q},\omega)$ to the external field. At low frequency and long-wavelength limit, the induced electric field can be calculated from the electric scalar potential ϕ_{ind} which is determined by the Poisson equation

$$\nabla^2 \phi_{\text{ind}} = 4\pi e \delta n, \tag{8}$$

where $e > 0$. The total electric field is $\mathbf{E} = \mathbf{E}_{\text{ind}} + \mathbf{E}_{\text{ext}}$, where $\mathbf{E}_{\text{ind}}$ is the induced field given by Eq. (8). At long-wavelength limit the pressure can be calculated by locally using the relation derived in subtask (a).

Solution: The external electric field induces a change in the electron density $n(\mathbf{r},t)$. There are three effects in Eq. (2) which affect the dynamics of the electrons: the inertia of the electrons, the induced electric field due to inhomogeneous charge distribution, and the pressure gradients due to inhomogeous particle distribution.

We linearize the equations around the equilibrium density n_0. In linear response, the perturbation δn will occur at the same frequency and wavevector as the perturbing field:

$$n(\mathbf{r},t) \approx n_0 + \delta n \; e^{i(\omega t - \mathbf{q}\cdot\mathbf{r})}. \tag{9}$$

The velocity field $\mathbf{u}$ vanishes at zeroth order:

$$\mathbf{u}(\mathbf{r},t) \approx \delta\mathbf{u} \; e^{i(\omega t - \mathbf{q}\cdot\mathbf{r})}. \tag{10}$$

We are interested in the long-wavelength, low-frequency limit, so that we define a local pressure which we can calculate from the relation of part (a) using the local electron density. The variation of pressure and the pressure gradient are

$$P(\mathbf{q},\omega) \approx \frac{(3\pi n_0)^{2/3}}{3m} \delta n. \tag{11}$$

The induced electric field is obtained by solving the Poisson equation:

$$\mathbf{E}_{\text{ind}}(\mathbf{q},\omega) = -\mathrm{i}\mathbf{q}\phi_{\text{ind}} = -\frac{4\pi e \mathrm{i}\mathbf{q}}{q^2}\delta n. \tag{12}$$

Now the Euler equation can be written as

$$(\mathrm{i}\omega m n_0)\delta\mathbf{u} = -e n_0 \left(\mathbf{E}_0 - \frac{4\pi e \mathrm{i}\mathbf{q}}{q^2}\delta n \right) + \mathrm{i}\mathbf{q}\frac{(3\pi n_0)^{2/3}}{3m}\delta n. \tag{13}$$

We can eliminate $\mathbf{q}\cdot\delta\mathbf{u}$ in favor of δn by using the continuity equation, which tells us that

$$\omega \delta n = n_0 \mathbf{q}\cdot\delta\mathbf{u}. \tag{14}$$

Taking the dot product with $\mathbf{q}$ from both sides of Eq. (13) and using the continuity equation, we find

$$\left(m\omega^2 - 4\pi e^2 n_0 - q^2 \frac{(3\pi n_0)^{2/3}}{3m} \right) \delta n = \mathrm{i} e n_0 \mathbf{q}\cdot\mathbf{E}_0. \tag{15}$$

Solving for δn gives

$$\delta n = \frac{\mathrm{i} e n_0 \mathbf{q}\cdot\mathbf{E}_0}{m\omega^2 - 4\pi e^2 n_0 - q^2 \frac{(3\pi n_0)^{2/3}}{3m}} \tag{16}$$

(c) Determine the plasmon dispersion $\omega = \omega_{\mathrm{p}}(\mathbf{q})$.

Solution: Above we find the response function $\delta n = \boldsymbol{\chi} \cdot \mathbf{E}_0$. Study the poles of the response function to determine the dispersion.

The dispersion is given by

$$\begin{aligned} \omega^2 &= \frac{4\pi e^2 n_0}{m} + \frac{(3\pi n_0)^{2/3}}{3m^2} q^2 \\ &= \frac{4\pi e^2 \nu v_{\mathrm{F}}^2}{3} + \frac{1}{3\pi^{2/3}} v_{\mathrm{F}}^2 q^2. \end{aligned} \tag{17}$$

2. Plasmon dispersion relation from RPA (10 points)

In the lectures, the following expression was derived for the polarization bubble $\Pi(q, \omega)$ at zero temperature in three dimensions:

$$\Pi(q, \omega) = \nu \left[1 - \frac{s}{2} \ln \frac{s+1}{s-1} \right] \tag{18}$$

$$s = \frac{\omega + \mathrm{i}0 \operatorname{sign}(\omega)}{q v_{\mathrm{F}}} \tag{19}$$

where ν is the density of states at the Fermi surface and v_{F} is the Fermi velocity.

In the lectures, the plasmon frequency $\omega_{\mathrm{p}}(q = 0)$ was calculated. Determine the plasmonic dispersion relation $\omega_{\mathrm{p}}(q)$ in the limit of small q.

Solution: Assume $\omega > 0$. We make an expansion in the limit $q \to 0$ (which corresponds to $s \to \infty$):

$$\Pi(q = \frac{\omega + \mathrm{i}0}{s v_{\mathrm{F}}}, \omega) = \nu \left[1 - \frac{s}{2} \ln \frac{s+1}{s-1} \right] \approx -\frac{1}{3s^2} - \frac{1}{5s^4}. \tag{20}$$

The plasma mode corresponds to a pole in the effective interaction

$$U_{\text{eff}}(q, \omega) = \frac{U(q)}{1 + U(q)\Pi(q, \omega)} = \frac{U(q)}{\epsilon(q, \omega)} \tag{21}$$

We search for the pole

$$\begin{aligned} \epsilon(q, \omega) = 1 + U(q)\Pi(q, \omega) &= 1 + \frac{4\pi e^2 \nu}{q^2} \left[-\frac{q^2 v_{\mathrm{F}}^2}{3(\omega + \mathrm{i}0)^2} - \frac{q^4 v_{\mathrm{F}}^4}{5(\omega + \mathrm{i}0)^4} \right] \\ &= 1 - 4\pi e^2 \nu \frac{q^2 v_{\mathrm{F}}^2}{3(\omega + \mathrm{i}0)^2} - 4\pi e^2 \nu \frac{q^2 v_{\mathrm{F}}^4}{5(\omega + \mathrm{i}0)^4} \end{aligned} \tag{22}$$

Setting $\epsilon(q, \omega) = 0$, we find the equation (neglecting the imaginary parts, which are not that important here)

$$15\omega^4 - 20\pi e^2 \nu v_{\mathrm{F}}^2 \omega^2 - 12\pi e^2 \nu q^2 v_{\mathrm{F}}^4 = 0, \tag{23}$$

which can be straightforwardly solved for ω^2. Expanding the solution in q, we find

$$\omega^2 \approx \frac{4\pi e^2 \nu v_{\mathrm{F}}^2}{3} + \frac{3}{5} v_{\mathrm{F}}^2 q^2. \tag{24}$$

3. Matsubara Sums $(4 + 4 + 4 + 4 + 4 = 20$ points$)$

(a) Find the poles and residues of the Fermi and Bose distribution functions

$$n_{\mathrm{F}}(z) = \frac{1}{\exp(z\beta)+1} \tag{25}$$

$$n_{\mathrm{B}}(z) = \frac{1}{\exp(z\beta)-1} \tag{26}$$

assuming complex arguments $z \in \mathbb{C}$.

Solution: There is a pole in $n_\epsilon(z) = [\exp(z\beta)+\epsilon]^{-1}$ when $\exp(z\beta) = -\epsilon$. Writing $z = i\omega$,

$$\exp(i\omega\beta) = -\epsilon = \begin{cases} +1 & \text{Bosons} \\ -1 & \text{Fermions} \end{cases} \tag{27}$$

we find

$$\omega = \omega_n = \begin{cases} 2n\pi/\beta, & \text{Bosons} \\ (2n+1)\pi/\beta, & \text{Fermions} \end{cases} \tag{28}$$

The residues are given by

$$\begin{aligned} \mathrm{Res}_{z=i\omega_n}[n_\epsilon(z)] &= \lim_{z\to i\omega_n}(z-i\omega_n)n_\epsilon(z) = \lim_{z\to i\omega_n}\frac{z-i\omega_n}{\exp(\beta z)+\epsilon} \\ &= \lim_{z\to i\omega_n}\frac{z-i\omega_n}{\cancel{\exp(i\beta\omega_n)}+\beta\exp(i\beta\omega_n)(z-i\omega_n)+\cancel{\epsilon}} \\ &= -\frac{1}{\beta\epsilon} = \begin{cases} +\frac{1}{\beta}, & \text{Bosons} \\ -\frac{1}{\beta}, & \text{Fermions} \end{cases} \end{aligned} \tag{29}$$

(b) Consider an integral of the form

$$I := \oint_{\mathcal{C}} \mathrm{d}z\, n_{\mathrm{B/F}}(z)h(z) \tag{30}$$

where $n_{\mathrm{B/F}}$ is the Bose / Fermi function, and $\oint_{\mathcal{C}}\mathrm{d}z$ an integral over a complex contour $\mathcal{C}$ which encloses all poles of $n_{\mathrm{B/F}}$ but no poles of $h(z)$.

Use the residue theorem to express I as a sum. Use your result to express a generic *Matsubara sum*

$$S := \frac{1}{\beta}\sum_{\omega_n} h(\mathrm{i}\omega_n) \tag{31}$$

in terms of a complex contour integral.

Solution: Using the results from part (a), we find

$$\begin{aligned} I &= \oint_{\mathcal{C}} \mathrm{d}z\, n_\epsilon(z)h(z) = 2\pi i \sum_{z_n\in\Omega} \mathrm{Res}_{z=z_n}[n_\epsilon(z)]h(i\omega_n) \\ &= 2\pi i(-\epsilon)\frac{1}{\beta}\sum_{\omega_n} h(i\omega_n). \end{aligned} \tag{32}$$

Turning the procedure the other way, we may write any Matsubara sum as a contour integral

$$S = \frac{1}{\beta}\sum_{\omega_n} h(i\omega_n) = (-\epsilon)\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z)h(z), \tag{33}$$

where $\mathcal{C}$ is any contour that encloses all the $z = i\omega_n$ in a counter-clockwise fashion. $h(z)$ must also be analytic for all z within the contour.

(c) Calculate the Matsubara sum

$$S(\tau) := \frac{1}{\beta}\sum_{\omega_n} g(\mathrm{i}\omega_n)\exp(\mathrm{i}\omega_n\tau) \qquad 0 \leq \tau < \beta \tag{34}$$

where $g(z)$ is holomorphic everywhere in $\mathbb{C}$ but on a countable number of points z_j. Further it holds $g(z)\lim_{|z|\to\infty} = 0$.
Calculate the sum $S(\tau)$ for both bosonic and for fermionic Matsubara frequencies by choosing an appropriate contour $\mathcal{C}$. You can assume that $g(z)$ is of the form

$$g(z) = \prod_j \frac{1}{z - z_j}. \tag{35}$$

Solution: Using the result from (b), we express the sum as a contour integral

$$S(\tau) = (-\epsilon)\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau} - (-\epsilon)\sum_j \oint_{\mathcal{D}_j} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau}, \tag{36}$$

where the contour $\mathcal{C}$ is a large circle with radius $R \to \infty$ enclosing all of complex plane, and $\mathcal{D}_j$ are small circles around the poles of $g(z)$. By the assumption, the integral over the large circle vanishes, and we are left with the second term, which can be evaluated using the Residue theorem.
We find

$$S(\tau) = \epsilon \sum_j n_\epsilon(z_j)\mathrm{Res}_{z=z_j}[g(z)]e^{z_j\tau} \tag{37}$$

where the residues of $g(z)$ are

$$\mathrm{Res}_{z=z_j}[g(z)] = \prod_{i\neq j} \frac{1}{z_j - z_i}. \tag{38}$$

(d) Calculate the Matsubara sums

$$S_1 = \frac{1}{\beta}\sum_{\omega_n} G_0(\mathbf{k}, \mathrm{i}\omega_n)\exp(\mathrm{i}\omega_n\tau) \tag{39}$$

$$S_2 = \frac{1}{\beta}\sum_{\omega_n} G_0(\mathbf{k}, \mathrm{i}\omega_n) G_0(\mathbf{k}+\mathbf{q}, \mathrm{i}\omega_n + \mathrm{i}\nu_m) \tag{40}$$

where

$$G_0(\mathbf{k}, \mathrm{i}\omega_m) = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}}}, \qquad \xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \tag{41}$$

$$\omega_n = \frac{(2n+1)\pi}{\beta}, \qquad \nu_m = \frac{2m\pi}{\beta}. \tag{42}$$

Solution: Let us start with the first sum which is the Fourier expansion of a Green's function $G_0(\mathbf{k}, -\tau)$ with $0 < \tau < \beta$. G_0 has a single pole on the real axis at $z_1 = \xi_{\mathbf{k}}$ with residue 1. Part (c) gives us

$$S_1 = \frac{1}{\beta}\sum_{\omega_n} G_0(\mathbf{k}, \mathrm{i}\omega_n)\exp(\mathrm{i}\omega_n\tau) = n_{\mathrm{F}}(z_1)e^{z_1\tau} = n_{\mathrm{F}}(\xi_{\mathbf{k}})e^{\xi_{\mathbf{k}}\tau}, \tag{43}$$

Which is consistent with the definition of the thermal Green's function

$$G_0(\mathbf{k}, -\tau) = -\langle \mathcal{T} c_{\mathbf{k}}(-\tau) c_{\mathbf{k}}^\dagger(0)\rangle = \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}\rangle e^{\xi_{\mathbf{k}}\tau}.$$

In the next sum we have explicitly

$$G_0(\mathbf{k}, z) G_0(\mathbf{k}+\mathbf{q}, z + \mathrm{i}\nu_m) = \frac{1}{z-\xi_{\mathbf{k}}} \frac{1}{z + \mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}}} \tag{44}$$

which has two poles, one at $z_1 = \xi_{\mathbf{k}}$ with residue $1/(\mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}} + \xi_{\mathbf{k}})$, and another at $z_2 = \xi_{\mathbf{k}+\mathbf{q}} - \mathrm{i}\nu_m$ with residue $-1/(\mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}} + \xi_{\mathbf{k}})$. Using part (c) with $\tau \to 0$ gives

$$\begin{aligned} S_2 &= \frac{n_{\mathrm{F}}(\xi_{\mathbf{k}})}{\mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}} + \xi_{\mathbf{k}}} - \frac{n_{\mathrm{F}}(\xi_{\mathbf{k}+\mathbf{q}} - \mathrm{i}\nu_m)}{\mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}} + \xi_{\mathbf{k}}} \\ &= \frac{n_{\mathrm{F}}(\xi_{\mathbf{k}}) - n_{\mathrm{F}}(\xi_{\mathbf{k}+\mathbf{q}})}{\mathrm{i}\nu_m - \xi_{\mathbf{k}+\mathbf{q}} + \xi_{\mathbf{k}}}, \end{aligned} \tag{45}$$

where we used for the Fermi function the fact that $\exp(\beta z + i\beta\nu_m) = \exp(\beta z + 2\pi n \mathrm{i}) = \exp(\beta z)$ for a bosonic Matsubara frequency ν_m.

(e) Consider sum (34) again. Assume, that $g(z)$ is analytic everywhere, but on the real axis. Choose an appropriate contour to express $S(\tau)$ as an integral

$$S(\tau) = \epsilon \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} n_{\mathrm{B/F}}(\omega) a(\omega) \exp(\omega\tau) \qquad 0 < \tau < \beta \tag{46}$$

where $\epsilon = -1$ for bosons, $\epsilon = 1$ for fermions, $a(\omega) = \mathrm{i}(g(\omega + \mathrm{i}\delta) - g(\omega - \mathrm{i}\delta))$.

Solution: We now choose the contour that consists of two infinite semicircles: $\mathcal{C}_+$ in the upper half-plane and $\mathcal{C}_-$ in the lower half-plane. These two contours taken together enclose all the Matsubara points. For fermionic frequencies, we have

$$S(\tau) = (-\epsilon)\left(\oint_{\mathcal{C}_+} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau} + \oint_{\mathcal{C}_-} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau}\right). \tag{47}$$

In the case of bosonic Matsubara frequencies, we have to single out the point $\omega_n = 0$:

$$S(\tau) = Tg(0) + (-\epsilon)\left(\oint_{\mathcal{C}_+} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau} + \oint_{\mathcal{C}_-} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau}\right) \tag{48}$$

The arcs of the semicircles vanish because $n_\epsilon(z) e^{z\tau}$ decays $|z| \to \infty$. Only the parts just above and below the real axis remain.

$$(-\epsilon)\left(\int_{-\infty+\mathrm{i}\delta}^{\infty+\mathrm{i}\delta} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau} + \int_{\infty-i\delta}^{-\infty-i\delta} \frac{\mathrm{d}z}{2\pi i} n_\epsilon(z) g(z) e^{z\tau}\right) \tag{49}$$

$$= (-\epsilon)\left(\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} n_\epsilon(\omega) g(\omega + \mathrm{i}\delta) e^{\omega\tau} - \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} n_\epsilon(\omega) g(\omega - \mathrm{i}\delta) e^{\omega\tau}\right) \tag{50}$$

$$= \epsilon \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} n_\epsilon(\omega) i \left[g(\omega + \mathrm{i}\delta) - g(\omega - \mathrm{i}\delta)\right] e^{\omega\tau} \tag{51}$$

$$= \epsilon \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} n_\epsilon(\omega) a(\omega) e^{\omega\tau} \tag{52}$$

This equation is useful *e.g.*, when we want to express the electron density as

$$n(\mathbf{x}) = \frac{1}{\beta}\sum_{\omega_n} G(i\omega_n, \mathbf{x}) = \int \frac{\mathrm{d}\omega}{2\pi} n_{\mathrm{F}}(\omega)[G^R(\omega, \mathbf{x}) - G^A(\omega, \mathbf{x})]. \tag{53}$$

We find that the density of states at position $\mathbf{x}$ is given by

$$N(\omega, \mathbf{x}) = G^R(\omega, \mathbf{x}) - G^A(\omega, \mathbf{x}). \tag{54}$$