Institut für Theoretische Festkörperphysik
Karlsruher Institut für Technologie

Prof. Dr. M. Garst
Dr. J. Masell
Dr. S. Sorn

Condensed Matter Theory 1 — Exercise 12

Winter term 2023/24

https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2024/02/01*

1. The Lindhard function in one and two spatial dimensions

In the lecture, the static susceptibility $\chi_0(\boldsymbol{q})$ of an electron gas at $T = 0$

$$\chi_0(\boldsymbol{q}) = 2e^2 \int \frac{d^dk}{(2\pi)^d} \frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}} \equiv -e^2 \nu_d F_d\left(\frac{q}{2k_F}\right) \quad \text{and} \quad F_d(0) = 1 \ . \tag{1}$$

was discussed for spatial dimension $d = 3$, where ν_d is the density of states at the Fermi level and F_d is the Lindhard function.
Evaluate the susceptibility in spatial dimensions $d = 1$ and $d = 2$ and determine the corresponding Lindhard functions analytically. Sketch the functions $F_d(x)$ for $d = 1, 2, 3$ in the range $0 \leq x \leq 2$ and discuss the behavior at $x = 1$.

2. Dynamic susceptibility

The *dynamic* susceptibility reads

$$\chi_0(\boldsymbol{q}, \omega) = 2e^2 \int \frac{d^dk}{(2\pi)^d} \frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} + i0^+} \ , \tag{2}$$

which reduces to Eq. (1) for $\omega = 0$. Consider in the following a three-dimensional model, $d = 3$, of free electrons at $T = 0$.

a) When the frequency in Eq. (2) is *on-shell*, i.e., when the denominator in the integrand vanishes, the resulting spectrum describes the continuum of particle-hole excitations, $\hbar\omega_{\text{ph}}(\boldsymbol{k}, \boldsymbol{q}) = \epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}$. Sketch the continuum $\omega_{\text{ph}}(\boldsymbol{k}, \boldsymbol{q})$ as a function of $|\boldsymbol{q}|$ for a fixed $\boldsymbol{k}$ with $|\boldsymbol{k}| = k_F$, i.e., determine the boundaries of the continuum within the $(\omega, |\boldsymbol{q}|)$ plane. The continuum arises because the angle between $\boldsymbol{q}$ and $\boldsymbol{k}$ can take all possible values.

b) Consider the limit of small $\boldsymbol{q}$. In this limit, you can perform a Taylor expansion of both the numerator and denominator of the integrand of Eq. (2) up to linear order in $\boldsymbol{q}$. Show that in this limit the integral simplifies to

$$\chi_0(\boldsymbol{q}, \omega) \approx e^2 \nu \int_{-1}^{1} \frac{dx}{2} \frac{x}{\frac{\omega}{qv_F} - x + i0^+} \ , \tag{3}$$

where v_F is the Fermi velocity and ν is the density of states at the Fermi level. Evaluate the remaining integral.

c) Consider now additionally the limit of small frequencies, $\frac{\omega}{qv_F} \ll 1$. Show that up to linear order in $\frac{\omega}{qv_F}$, the susceptibility takes the form

$$\chi_0(\boldsymbol{q},\omega) \approx -e^2\nu\left(1 + i\frac{\pi}{2}\frac{\omega}{qv_F}\right) . \tag{4}$$

The real part is the Thomas-Fermi result from the lecture and the imaginary part is known as Landau damping, i.e., damping due to the excitations of particle-hole pairs. Indicate in the plot of **a)** the parameter regime which is considered here.

d) Consider now the limit of large frequencies $\frac{\omega}{qv_F} \gg 1$. Expand $\chi_0(\boldsymbol{q},\omega)$ up to fourth order in $\frac{qv_F}{\omega}$. Using this result, determine the dispersion of plasmons $\omega_p(q)$ for small q by solving $\varepsilon(\boldsymbol{q},\omega) = 0$ where the dielectric function is given by $\varepsilon(\boldsymbol{q},\omega) = 1 - \frac{4\pi}{q^2}\chi_0(\boldsymbol{q},\omega)$. Show that it takes the form

$$\omega_p(q) \approx \omega_p\left(1 + \frac{9}{10}\frac{q^2}{k_{TF}^2}\right) , \tag{5}$$

where k_{TF} is the Thomas-Fermi wave vector with $k_{TF}^2 = 4\pi e^2\nu$ and $\omega_p^2 = 4\pi n e^2/m$. Indicate in the plot of **a)** the parameter regime which is considered here and add a sketch of $\omega_p(q)$.

3. Hartree-Fock approximation in graphene

The tight-binding Hamiltonian of two-dimensional graphene has been discussed on sheet 8. There, it was derived that the band structure touches at the Dirac points $\boldsymbol{K}$ and $\boldsymbol{K'}$ and that a linear order expansion around these points yields the effective Hamiltonian

$$\mathcal{H}_{\boldsymbol{K}+\boldsymbol{k}} \approx \hbar v_F(k_y\sigma^x - k_x\sigma^y) \tag{6}$$

for $0 \leq k < \Lambda$ where Λ is a momentum cut-off scale. The eigenenergies of this Hamiltonian are given by $\varepsilon_{\mathbf{k}}^{\pm} = \pm\hbar v_F|\boldsymbol{k}|$ where $\boldsymbol{k}^T = (k_x, k_y)$. We consider the groundstate where all states with negative energies $\varepsilon_{\mathbf{k}}^{-}$ are occupied and all states with positive energies $\varepsilon_{\mathbf{k}}^{+}$ are unoccupied. The goal of this exercise is to use the Hartree-Fock approximation to derive the correction to $\varepsilon_{\mathbf{k}}^{\pm}$ caused by Coulomb interaction.

a) Convince yourself that a rotation transformation on the Pauli matrices can be used to cast the Hamiltonian into the form

$$\mathcal{H} = \hbar v_F(k_x\sigma^x + k_y\sigma^y) , \tag{7}$$

which we will for convenience use as a modified starting point in the following. Rewrite $\boldsymbol{k}$ in two-dimensional polar coordinates and determine the eigenvectors of $\mathcal{H}$. Show that the real-space eigenstates with eigenvalues $\varepsilon_{\boldsymbol{k}_i}^{\sigma}$ take the form

$$\boldsymbol{\phi}_{i,\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{2V}}e^{i\boldsymbol{k}_i\cdot\boldsymbol{r}}\begin{pmatrix}\sigma \\ e^{i\varphi_i}\end{pmatrix} , \tag{8}$$

where $\sigma = \pm 1$ and i labels the state with wave vector $\boldsymbol{k}_i$ whose direction in the two-dimensional plane is described by the angle φ_i, e.g. $k_{i,x} = k_i\cos(\varphi_i)$.

b) The eigenfunctions (8) also solve the Hartree-Fock equations for the present problem. Similar to free electrons, the Hartree term yields a uniform density which cancels against the uniform positive charge density background. The correction $\delta\varepsilon^{\sigma}_{\boldsymbol{k}_i}$ to the eigenenergies is then given by the Fock term which reads

$$\delta\varepsilon^{\sigma}_{\boldsymbol{k}_i}\, \boldsymbol{\phi}_{i,\sigma}(\boldsymbol{r}) = -e^2 \int d^2r' \sum_j \frac{\boldsymbol{\phi}^{\dagger}_{j,-1}(\boldsymbol{r}') \cdot \boldsymbol{\phi}_{i,\sigma}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \boldsymbol{\phi}_{j,-1}(\boldsymbol{r}) \ . \tag{9}$$

Extract the energy correction by projecting this Schrödinger equation onto $\boldsymbol{\phi}^{\dagger}_{i,\sigma}(\boldsymbol{r})$, i.e., multiply with this function and integrate over $\boldsymbol{r}$. You can then shift $\boldsymbol{r}$ by $\boldsymbol{r}'$. Perform the Fourier transform of $1/r$ in *two* spatial dimensions by utilizing the Fourier transform in *three* spatial dimensions and restrict it to $z = 0$. Use the result from Eq. (8) to show that the energy correction takes the form

$$\delta\varepsilon^{\sigma}_{\boldsymbol{k}} = -\frac{e^2}{4\pi} \int d^2k' \, \frac{1 - \sigma\cos(\varphi - \varphi')}{|\boldsymbol{k}-\boldsymbol{k}'|} \ , \tag{10}$$

where φ and φ' are the angles parametrizing $\boldsymbol{k}$ and $\boldsymbol{k}'$, respectively.

c) Verify that the integrand in Eq. (10) is trivial for $k' \to 0$ but diverges for $k' \to \infty$. To capture the dominant divergent behavior, expand the integral to leading order in $1/k'$. Show that the Coulomb interaction in Hartree-Fock approximation leads to a correction

$$v_F(\boldsymbol{k}) = v_F \left(1 + \frac{e^2}{4\hbar v_F} \ln \frac{\Lambda}{|k|} \right) \tag{11}$$

of the Fermi velocity.

This logarithmic divergence was also confirmed experimentally by D.C. Elias et.al, Nature Physics 7, 701 (2011).