Theoretische Festkörperphysik – Herbstsemester 2010 **Exercise series 10**
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RPA: Dielectric function, screening, Friedel oscillations

Motivation Divergences in a perturbation theory have a very distinct meaning: Consider, for instance, a so-called ultraviolet divergence, where a diagram in perturbation theory diverges due to the integral over large momenta k. Such a divergence has usually a physical cutoff, such as the electron bandwidth D, which limits the integration to some maximal k. The diagrams in the perturbation theory then typically are on the order of $\ln D$ or D^α with $\alpha > 0$. This means that in higher order diagrams consisting of repetitions of this first diverging diagram the divergences become even larger, such as $(\ln D)^n$ or $D^{n\alpha}$.

In most cases this does not tell us that the system behaves pathologically. It tells us that the naive perturbation theory must not be used. The summation over *all* these divergent diagrams (or sometimes already over the most divergent diagrams only) then miraculously often produces again an entirely regular result, meaning that the elementary excitations in the system are not simple one- or few-particle excitations, but modes that involve a macroscopic part of the collective of electrons.

We have seen in a past exercise series that the polarization function Π_0^c has precisely such a divergence (of the logarithmic type) at $q = 2k_F$. If we want to study perturbations that involve this polarization function, we must therefore sum over infinite series of Π_0^c. The Random Phase Approximation (RPA) precisely does this for the renormalization of the Coulomb vertex. The result is an entirely regular effective Coulomb interaction, in which even the divergence at $q = 0$ is suppressed. This has important physical consequences, which are investigated in part in the following exercises.

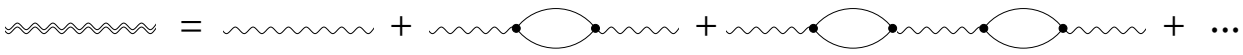
Validity of the RPA: The natural dimensionless parameter characterizing an interacting electron gas is r_s, the mean electronic separation expressed in units of the Bohr radius $a_0 = \frac{\hbar^2}{me^2}$ (with e the electron charge and m its effective mass). In terms of electrons per unit volume n_e, r_s is defined by $n_e = \frac{1}{\frac{4\pi}{3}(r_s a_0)^3}$. Roughly r_s measures the ratio of potential over kinetic energy. Strictly speaking, RPA is only valid for $r_s \ll 1$, i.e. in the high electron density limit, where the kinetic energy largely dominates over the interaction energy. Most of our available materials, however, have a much larger r_s: For instance, for alkali metals $r_s \sim 2$ to 6; similar values are obtained for semiconductor heterostructures, going up to $r_s \sim 8$ in ultra-clean semiconductor heterostructures that can be fabricated nowadays. Nonetheless, RPA gives often still quite reasonable results. For this reason, RPA is often one of the first approaches one makes to investigate the effect of electron-electron interactions in a system. It is then mostly followed by one of the gazillion improvements made to this theory.

Exercise 1: Effective Coulomb potential in RPA approximation (3 points) In Exercise Series 8 you have calculated the dipolar function $\Pi^c(\bar{q})$,

$$\begin{aligned}
\mathrm{Re}\Pi_0^c(\bar{q}) &= -\nu(\epsilon_F)\left[\frac{1}{2} + \frac{f(x,x_0)+f(x,-x_0)}{8x}\right], \\
\mathrm{Im}\Pi_0^c(\bar{q}) &= \begin{cases} \nu(\epsilon_F)\left|\frac{\pi}{8x}\left[1-\left(\frac{x_0}{x}-x\right)^2\right]\right| & \text{for } |x^2-x| < x_0 < x^2+x, \\ \nu(\epsilon_F)\frac{\pi}{2}\left|\frac{x_0}{x}\right| & \text{for } 0 < x_0 < |x-x^2|, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned} \tag{1}$$

with $\bar{q} = (\mathbf{q}, \omega), x = \frac{|\mathbf{q}|}{2k_F}, x_0 = \frac{\omega}{2\epsilon_F}$.

The RPA is a renormalization of the bare Coulomb interaction: One takes into account that two electrons in a metal can interact indirectly by exciting particle-hole pairs. Assuming that there is no further process than any possible sequence of such excited particle-hole pairs defines the RPA. The following diagrams then yield the effective Coulomb interaction:



Write down the Dyson equation for the renormalized potential $V_{\text{eff}}(\bar{q})$ and solve it explicitly using the bare Coulomb interaction $V(q) = \frac{e^2}{\epsilon_0 q^2}$, and the polarization function $\Pi_0^c(\bar{q})$.

Writing $V_{\text{eff}}(\bar{q}) = V(q)/\epsilon(\bar{q})$, we define the **dielectric function** $\epsilon(\bar{q})$ (in units of ϵ_0), which modifies the vacuum value of ϵ_0.

Exercise 2: Static screening (2 points) A charge Q placed at position $\mathbf{r} = 0$ in empty space creates a Coulomb potential decaying as $1/r$. However, if the charge is introduced into a metal the surrounding conduction electrons can move towards it (if $Q > 0$) or away from it (if $Q < 0$), such that at long distances charge neutrality is restored (recall that there is a background of positively charged ions). The effective potential seen at long distances therefore decreases faster than $1/r$. This is known as **screening**.

To evaluate the screening effect of the Coulomb interaction within the RPA picture, we consider the static limit $\omega = 0$. Observe that in this limit we have

$$\Pi_0^c(\mathbf{q}, 0) = -\sum_\sigma \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \mathcal{P} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}} \overset{q\to 0}{\longrightarrow} -\sum_\sigma \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \mathcal{P} \frac{\partial f_{\mathbf{k}}}{\partial \epsilon_{\mathbf{k}}} \overset{T\to 0}{\longrightarrow} -\nu(\epsilon_F), \tag{2}$$

where $f_{\mathbf{k}} = f(\epsilon_{\mathbf{k}})$ is the Fermi function. Show that in the classical limit $T \gg \epsilon_F/k_B$ we have $f(\epsilon) = \mathrm{e}^{-(\epsilon-\mu)/k_B T}$, and so

$$\Pi_0^c(\mathbf{q}, 0) \overset{q\to 0}{\longrightarrow} -\frac{n_e}{k_B T} \tag{3}$$

with n_e the electron density. Show that this then implies for the dielectric function

$$\epsilon(\mathbf{q}, 0) = 1 + \frac{k_s^2}{q^2}, \tag{4}$$

where $k_s = \kappa_{TF}$ at $T = 0$ and $k_s = \kappa_{DH}$ at $T \gg \epsilon_F/k_B$, with $\kappa_{TF}^2 = \frac{4k_F}{\pi a_0}$ the "Thomas-Fermi" screening wavevector[1] and $\kappa_{DH} = \frac{4\pi n_e}{k_B T}$ the "Debye-Hückel" screening wavevector[2].

Using these approximations, estimate the long-distance behavior of the potential $V_{\text{eff}}(r)$ for $r \gg 1/k_s$ (look where the poles are in the Fourier transformation $q \to r$). Explain why k_s is called the "screening wavevector".

Exercise 3: Friedel oscillations (4 points) Consider again the static limit $\omega = 0$ at temperature $T = 0$, in which the dielectric function becomes

$$\epsilon(\mathbf{q}, 0) = 1 + \frac{\kappa_{TF}^2}{q^2} \left[\frac{1}{2} - \frac{1}{4x}(1 - x^2) \ln \left| \frac{1-x}{1+x} \right| \right] \equiv 1 + \frac{\kappa_{TF}^2}{q^2} g(q) \tag{5}$$

[1]The Thomas-Fermi approximation describes the screening of charges by a locally free electron gas.

[2]The Debye or Debye-Hückel theory describes the screening of charges by a hot plasma. (Its has been derived originally to characterize electrolytes though.)

with the Thomas-Fermi wavevector from above. We calculate (formally, don't try to actually do the calculation) now as above $V_{\rm eff}(r)$ but use the full expression for $g(q)$,

$$V_{\rm eff}(\mathbf{q},\omega=0)=\frac{e^2}{\epsilon_0}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\frac{\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}}}{q^2+\kappa_{TF}^2 g(q)}. \tag{6}$$

Observe that $g(q)$ diverges logarithmically at $q=2k_F$. From this, show that for long-distances ($r\gg 1/2k_F$) of $V_{\rm eff}(r)\sim\cos(2k_Fr)/r^3$. [1 point]

These oscillations are known as **Friedel oscillations** [after H. Friedel, *Adv. Phys.* **3**, 446 (1954)]. Their decay is algebraic and so much slower than the exponential decay you should have obtained in the previous exercise. Give an interpretation why it is so much different, i.e. what precisely is the physical cause of the slower decay. (Hint: Obviously, the main role is played by the Fermi surface whose influence, via the $2k_F$ contribution, was neglected before. What type of physical fluctuation process is expressed by $\Pi_0^c(2k_F,0)$ and is responsible for the singular behavior? Why is it important that, at $T=0$, the Fermi surface is sharp, i.e., the Fermi function is just a step?) [For the curious: see W. Kohn, *Phys. Rev. Lett.* **2**, 393 (1959).] Based on the Debye-Hückel result above speculate then what happens at $T>0$. [3 points]

Note that $V_{\rm eff}(r)$ can become *negative* at some distances. This means that a purely repulsive interaction can effectively (through the presence of the other electrons – the Fermi surface – see the hint above...) become *attractive* for electrons over these distances. Remarkably, this can lead to bound states of two electrons similar to Cooper pairs and to the onset of superconductivity at very very very low temperatures. This known as the Kohn-Luttinger mechanism for superconductivity [see W. Kohn and J. H. Luttinger, *Phys. Rev. Lett.* **15**, 524 (1965)].

Exercise 4: High frequency limit, collective modes, plasmons (1 point) The shape of $V_{\rm eff}(\bar{q})$, and in particular its maxima (or divergences) tells us furthermore, which type of excitation dominates the response of the interacting electron system at various wave vectors and frequencies. Looking at the zeros of the dielectric function $\epsilon(\bar{q})$ as a function of complex frequency ω gives us therefore information on the dispersion and damping of collective excitations in the system.

We here focus on the limit of large ω and small $q=|\mathbf{q}|$, which allows us to expand Π_0^c in powers of x/x_0. Show that we then have

$$\mathrm{Re}\Pi_0^c(q)=\nu(\epsilon_F)\left[\frac{1}{3}\left(\frac{x}{x_0}\right)^2+\frac{1}{5}\left(\frac{x}{x_0}\right)^4+\ldots\right] \tag{7}$$

and that the condition $\mathrm{Re}\,\epsilon(q)=0$ leads to the condition

$$\omega=\omega_p+\alpha\frac{q^2}{m}, \tag{8}$$

where $\omega_p^2=\frac{n_e e^2}{m\epsilon_0}$ is the **plasma frequency** with n_e the electron density and m the effective mass, and where $\alpha=\frac{3\epsilon_F}{5\omega_p}=\frac{0.64}{\sqrt{r_s}}$

The plasma oscillations at zero wave vector $\mathbf{q}=0$ represent sloshing of the electron liquid at a fixed frequency ω_p. The dispersion that appears in the RPA treatment of the dielectric function describes plasmon quasiparticles.