**Universität Bonn** 9.5.2011
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# Advanced Theoretical Condensed Matter Physics — SS11

## Exercise 4

(Please return your solutions before Tue 17.5.2011)

### 3.1. Screening in an electron gas I: Lindhard function

We will consider the response of a weakly interacting electron gas to a static impurity with electric charge $q_0$. The static electric potential induced by the impurity is

$$\phi_{el}(\mathbf{r},t) = \frac{q_0}{r}. \tag{1}$$

and couples to the electron density of the gas via the relation

$$V_t = -e_0 \int d^d r\, \phi_{el}(\mathbf{r},t)\, n(\mathbf{r},t). \tag{2}$$

The interaction of electron gas and impurity will change the electron distribution in the vicinity of the impurity. We know that within linear response theory, the change is given by

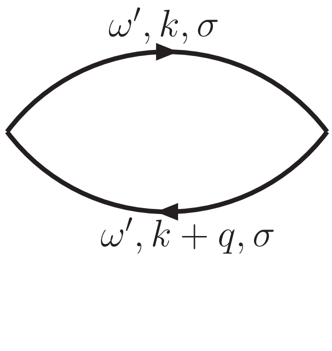
$$\begin{aligned}\Delta n(\mathbf{r},t) &= -e_0 \int_{-\infty}^{\infty} dt' \int d^d r' \phi_{el}(\mathbf{r}',t')\, \chi(\mathbf{r}-\mathbf{r}',t-t') \\ &= -e_0 \int \frac{d^d q}{(2\pi)^d}\, \mathrm{e}^{-\mathrm{i}\mathbf{qr}} \hat{\phi}_{el}(\mathbf{q})\, \hat{\chi}(\mathbf{q},\omega=0),\end{aligned}$$

where $\chi(\mathbf{r}-\mathbf{r}',t-t') = -\mathrm{i}\Theta(t-t')\langle [n(\mathbf{r},t), n(\mathbf{r}',t')]_-\rangle_0$ is called the *response function* of the system to the electron density change caused by the interaction, $\hat{\chi}(\mathbf{q},\omega)$ is its Fourier transform and $\hat{\phi}_{el}(\mathbf{q})$ the Fourier transform of the Coulomb potential. (The system is translationally invariant and therefore $\chi$ depends only on $\mathbf{r}-\mathbf{r}'$.)

a) To calculate the response function we have to evaluate the Fourier transform of the time ordered function

$$\chi_{\mathrm{M}}(\tau-\tau',\mathbf{r}-\mathbf{r}') = -\sum_{\sigma,\sigma'} \langle T_\tau \psi^\dagger_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau)\psi^\dagger_{\sigma'}(\mathbf{r}',\tau')\psi_{\sigma'}(\mathbf{r}',\tau')\rangle,$$

which is in absence of interaction is given by the polarization bubble

$\Pi(\mathbf{q}) =$ 

Carry out the Matsubara sum required and show that it yields

$$\Pi(\mathbf{q}) = 2\sum_{\mathbf{k}} \frac{f(\epsilon(\mathbf{k}+\mathbf{q})-\mu) - f(\epsilon(\mathbf{k})-\mu)}{\epsilon(\mathbf{k}+\mathbf{q})-\epsilon(\mathbf{k})} \tag{3}$$

$$\overset{T\to 0}{=} 2\int \frac{d^d k}{(2\pi)^d} \frac{\Theta(\mu-\epsilon(\mathbf{k}+\mathbf{q}/2)) - \Theta(\mu-\epsilon(\mathbf{k}-\mathbf{q}/2))}{\epsilon(\mathbf{k}+\mathbf{q}/2)-\epsilon(\mathbf{k}-\mathbf{q}/2)}. \tag{4}$$

b) The main contribution arises from small momentum transfer. Therefore, assume $\epsilon(\mathbf{k}) = k^2/2m$ and neglect all terms of order $\mathcal{O}(q^2)$ in the denominator of the integrand. Show

$$\Pi(\mathbf{q}) \approx \frac{2m}{\pi\, q} \int \frac{d^{d-1}k_\perp}{(2\pi)^{d-1}} \int_{k_+}^{k_-} \frac{dk_\parallel}{k_\parallel} \qquad \text{with: } k_\pm = \sqrt{k_\mathrm{F}^2 - k_\perp^2} \pm \frac{q}{2}. \tag{5}$$

Hint: Use a coordinate system such that $\mathbf{k} = (\mathbf{k}_\perp, k_\parallel)$, where $k_\parallel$ denotes the component of $\mathbf{k}$ pointing in the direction of $\mathbf{q}$.

c) Finally, derive the *Lindhard function* in $d = 1, 3$ dimensions

$$\Pi(\mathbf{q}) = \begin{cases} \frac{m}{\pi k_\mathrm{F}} \frac{1}{q/2k_\mathrm{F}} \ln\left|\frac{1-q/2k_\mathrm{F}}{1+q/2k_\mathrm{F}}\right| & , \quad d=1 \\ -\frac{m\,k_\mathrm{F}}{2\pi^2}\left(1 + \frac{1-(q/2k_\mathrm{F})^2}{q/k_\mathrm{F}} \ln\left|\frac{1+q/2k_\mathrm{F}}{1-q/2k_\mathrm{F}}\right|\right) & , \quad d=3 \end{cases}, \tag{6}$$

which is plotted below.

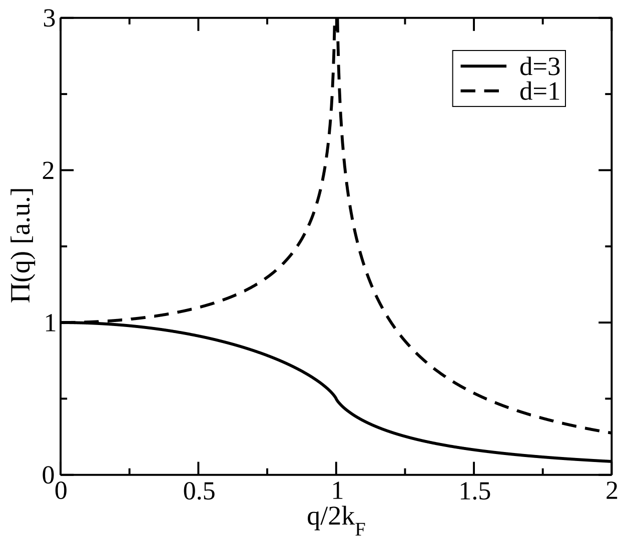



Figure 1: The Lindhard function in $d = 1, 3$ dimensions.

## 3.2. Screening in an electron gas II: Thomas-Fermi approximation and Friedel oscillations

We will continue with our calculation of the response of an electron gas to a static impurity with charge $q_0 = e_0$ in three dimensions. In 3.1 we derived the expression for the induced change of the charge density

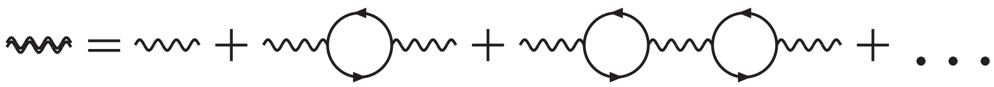
$$\Delta n(\mathbf{r}, t) \quad = \quad -e_0 \int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathbf{iqr}}\, \hat{\phi}_{el}(\mathbf{q})\, \Pi(\mathbf{q}). \tag{7}$$

a) Show that according to Eq. (7), with the bare Coulomb interaction $\hat{\phi}_{\mathrm{el}}(\mathbf{q})$, the induced charge

$$\Delta Q \quad = \quad -e_0 \int d^3r\, \Delta n(\mathbf{r}, t)$$

is infinite!

b) To obtain a physically meaningful result we must take into account the screening of the Coulomb interaction by the electron gas. For that purpose, we will re-sum the leading contributions (*random phase approximation*) to get an effective interaction



corresponding to

$$\hat{\phi}_{\mathrm{eff}}(\mathbf{q}) \quad = \quad \hat{\phi}_{el}(\mathbf{q}) \,+\, \hat{\phi}_{el}(\mathbf{q}) e_0 \Pi(\mathbf{q}) \hat{\phi}_{el}(\mathbf{q}) \,+\, \hat{\phi}_{el}(\mathbf{q}) e_0 \Pi(\mathbf{q}) \hat{\phi}_{el}(\mathbf{q}) e_0 \Pi(\mathbf{q}) \hat{\phi}_{el}(\mathbf{q}) \,+\, \ldots$$

Replace in Eq. (7) the bare Coulomb interaction by the effective one and show that it yields

$$\Delta n(\mathbf{r}, t) \quad = \quad -\int \frac{d^3q}{(2\pi)^3}\, \mathrm{e}^{-\mathbf{iqr}} \left( \frac{1}{\kappa(\mathbf{q})} - 1 \right), \tag{8}$$

with

$$\kappa(\mathbf{q}) \quad = \quad 1 + \frac{q_{\mathrm{TF}}^2}{q^2}\, g(q/k_{\mathrm{F}}) \quad , \qquad \begin{aligned} q_{\mathrm{TF}} &= \sqrt{\tfrac{4e_0^2 m}{\pi} k_{\mathrm{F}}} \\ g(x) &= \left( \tfrac{1}{2} + \tfrac{1-(x/2)^2}{2x} \ln \left| \tfrac{1+\frac{x}{2}}{1-\frac{x}{2}} \right| \right) . \end{aligned}$$

c) Show that the induced charge now becomes

$$\Delta Q \quad = \quad -e_0,$$

which shows that the additional charge at the origin becomes completely screened at large distances.

d) To get a rough estimate on the asymptotic behaviour of $\Delta n(\mathbf{r}, t)$ for $r \to \infty$, we set $g(q/k_\mathrm{F}) \approx g(0)$ (*Thomas-Fermi approximation*). Show that this yields

$$\Delta n(\mathbf{r}, t) \stackrel{r\to\infty}{\approx} -\frac{q_\mathrm{TF}^2}{4\pi} \frac{\mathrm{e}^{-q_\mathrm{TF} r}}{r}.$$

e) A careful evaluation of Eq. (8) shows that the correct result is

$$\Delta n(\mathbf{r}, t) \stackrel{r\to\infty}{\approx} -\frac{4e_0}{\pi} \frac{q_\mathrm{TF}^2/k_\mathrm{F}^2}{(8 + q_\mathrm{TF}^2/k_\mathrm{F}^2)^2} \frac{\cos(2k_\mathrm{F} r)}{r^3}.$$

The long-range oscillations with wavelength $\pi/k_\mathrm{F}$ are called *Friedel oscillations* and arise from the presence of a sharp Fermi surface. To obtain them one has to take into account the singularity of $g(x)$, $g'(x) \approx -\delta(x-2)$. Using the asymptotics of $g(x)$ we approximate

$$\Delta n(\mathbf{r}, t) = -\int \frac{d^3q}{(2\pi)^3} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{r}} \left(\frac{1}{\kappa(\mathbf{q})} - 1\right) \simeq q_\mathrm{TF}^2 \int \frac{d^3q}{(2\pi)^3} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{r}} \frac{g(q/k_\mathrm{F})}{q^2 + q_\mathrm{TF}^2}.$$

Use integration by parts and approximate

$$F(x) = \int_0^x dy \, \frac{y}{y^2 + r^2 q_\mathrm{TF}^2} \sin(y) \quad \Rightarrow \quad F(2k_\mathrm{F} r) \simeq -\frac{\cos(2k_\mathrm{F} r)}{r}$$

to obtain the Friedel oscillations of the density modulation.