Solid State Theory
Solution 8

Problem 8.1 Lindhard function

At $T = 0$ the Fermi-Dirac distribution function $n_{0,\vec{k}}$ reduces to $\theta(\epsilon_\mathrm{F} - \epsilon_{\vec{k}})$. As usual, we go from the discrete summation to a d-dimensional integral. Then, the static Lindhard function is given by

$$\chi_0(\vec{q}) \equiv \chi_0(\vec{q}, \omega = 0) = \frac{1}{\Omega}\sum_{\vec{k}} \frac{n_{0,\vec{k}+\vec{q}} - n_{0,\vec{k}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - i\hbar\eta} = \frac{1}{(2\pi)^d}\int \mathrm{d}^d k \frac{\theta(\epsilon_\mathrm{F} - \epsilon_{\vec{k}+\vec{q}}) - \theta(\epsilon_\mathrm{F} - \epsilon_{\vec{k}})}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - i\hbar\eta} \tag{1}$$

with the Fermi energy ϵ_F and the Heaviside step function

$$\theta(x) = \begin{cases} 1\,, & x \geq 0 \\ 0\,, & x < 0 \end{cases}. \tag{2}$$

Next we split the integral and perform a change of variables in the first integral ($\vec{k} \to \vec{k} - \vec{q}$) such that

$$\chi_0(\vec{q}) = -\frac{1}{(2\pi)^d}\int \mathrm{d}^d k\ \theta(\epsilon_\mathrm{F} - \epsilon_{\vec{k}}) \left(\frac{1}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - i\hbar\eta} - \frac{1}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - i\hbar\eta} \right). \tag{3}$$

The dispersion relation for free electrons is given by $\epsilon_{\vec{k}} = \hbar^2 \vec{k}^2/2m$. We can therefore define the Fermi wave vector $k_\mathrm{F} = \sqrt{2m\epsilon_\mathrm{F}/\hbar}$ and the integration can be simplified further to

$$\chi_0(\vec{q}) = -\frac{1}{(2\pi)^d}\frac{2m}{\hbar^2}\int\limits_{|\vec{k}|<k_\mathrm{F}} \mathrm{d}^d k\ \left(\frac{1}{\vec{q}(\vec{q}+2\vec{k}) - i\hbar'\eta} + \frac{1}{\vec{q}(\vec{q}-2\vec{k}) + i\hbar'\eta} \right). \tag{4}$$

where we introduced the abbreviation $\hbar' = 2m/\hbar$.
Now we can split the Lindhard function into its real and imaginary part using the relation

$$\lim_{\eta\to 0}(z - i\eta)^{-1} = \mathcal{P}\left(\frac{1}{z}\right) + i\pi\delta(z)\,. \tag{5}$$

This leads to

$$\mathrm{Re}(\chi_0(\vec{q})) = -\frac{1}{(2\pi)^d}\frac{2m}{\hbar^2}\int\limits_{|\vec{k}|<k_\mathrm{F}} \mathrm{d}^d k\ \mathcal{P}\left(\frac{1}{\vec{q}(\vec{q}+2\vec{k})} + \frac{1}{\vec{q}(\vec{q}-2\vec{k})} \right), \tag{6a}$$

$$\mathrm{Im}(\chi_0(\vec{q})) = -\frac{\pi}{(2\pi)^d}\frac{2m}{\hbar^2}\int\limits_{|\vec{k}|<k_\mathrm{F}} \mathrm{d}^d k\ \left[\delta(\vec{q}(\vec{q}+2\vec{k})) - \delta(\vec{q}(\vec{q}-2\vec{k}))\right]. \tag{6b}$$

We see that when considering two points $\vec{k}_1 = -\vec{k}_2$, the integrand for the imaginary part is the same but with an opposite sign. As the integration volume is symmetric under inversion, both points will contribute to the integral and therefore cancel. This leads to a vanishing imaginary part for all dimensions. We are therefore now only interested in the real part of the Lindhard function.

(a) In the 1 dimensional case the respective integral is then simply given by

$$\mathrm{Re}(\chi_0^{1\mathrm{d}}(q)) = -\frac{1}{2\pi}\frac{2m}{\hbar^2}\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k \mathcal{P}\left(\frac{1}{q(q+2k)} + \frac{1}{q(q-2k)}\right). \tag{7}$$

We remark that the singular point in the integral for $|q| < 2k_\mathrm{F}$ is 'cured' by η. This means that we are actually calculating the Cauchy principal value, which leads to a well-defined integral.

For instance, let's consider the integral

$$\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\mathrm{d}k}{q+2k} \tag{8}$$

for $|q| < 2k_\mathrm{F}$. There is a singularity at $k = -q/2$ such that the integral is not well defined from a 'mathematical' point of view. However, the principal value

$$\mathcal{P}\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\mathrm{d}k}{q+2k} = \lim_{\delta\to 0}\left(\int\limits_{-k_\mathrm{F}}^{-q/2-\delta} \frac{\mathrm{d}k}{q+2k} + \int\limits_{-q/2+\delta}^{k_\mathrm{F}} \frac{\mathrm{d}k}{q+2k}\right) \tag{9}$$

is well defined because there are no singularities within the integrals. We calculate then

$$\begin{aligned}\mathcal{P}\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\mathrm{d}k}{q+2k} &= \lim_{\delta\to 0}\left(\frac{1}{2}\log|q+2k|\Big|_{-k_\mathrm{F}}^{-q/2-\delta} + \frac{1}{2}\log|q+2k|\Big|_{-q/2+\delta}^{k_\mathrm{F}}\right) \\ &= \lim_{\delta\to 0}\left(\frac{1}{2}\log\left|\frac{q+2k_\mathrm{F}}{q-2k_\mathrm{F}}\right| + \frac{1}{2}\log\left|\frac{-\delta}{\delta}\right|\right) = \frac{1}{2}\log\left|\frac{q+2k_\mathrm{F}}{q-2k_\mathrm{F}}\right|.\end{aligned} \tag{10}$$

Therefore we can work with the integrals as if there were no singular points

$$\begin{aligned}\mathrm{Re}(\chi_0^{1\mathrm{d}}(q)) &= -\frac{m}{\pi\hbar^2 q}\mathcal{P}\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k\left(\frac{1}{q+2k} + \frac{1}{q-2k}\right) = -\frac{m}{\pi\hbar^2 q}\left(\frac{1}{2}\log\left|\frac{q+2k}{q-2k}\right|\right)\Bigg|_{-k_\mathrm{F}}^{k_\mathrm{F}} \\ &= -\frac{m}{\pi\hbar^2 q}\log\left|\frac{q+2k_\mathrm{F}}{q-2k_\mathrm{F}}\right|.\end{aligned} \tag{11}$$

This function is shown in Fig. 1 (left).

(b) In the three dimensional case we may assume $\vec{q} = q\,\vec{e}_z$ since the system is isotropic. The integral then reduces to

$$\chi_0^{3\mathrm{d}}(\vec{q}) = -\frac{1}{(2\pi)^3}\frac{2m}{\hbar^2}\int\limits_{|\vec{k}|<k_\mathrm{F}} \mathrm{d}^3k\left(\frac{1}{q(q+2k_z) - i\hbar'\eta} + \frac{1}{q(q-2k_z) + i\hbar'\eta}\right). \tag{12}$$

After a change to cylindrical coordinates ($k_x = r\cos(\phi), k_y = r\sin(\phi), k_z = k_z$ with $k^2 = r^2 + k_z^2 < k_\mathrm{F}^2$) we get

$$-\frac{m}{4\pi^3\hbar^2}\int\limits_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k_z \int\limits_0^{\sqrt{k_\mathrm{F}^2-k_z^2}} \mathrm{d}r\; r\int\limits_0^{2\pi} \mathrm{d}\phi\left(\frac{1}{q(q+2k_z) - i\hbar'\eta} + \frac{1}{q(q-2k_z) + i\hbar'\eta}\right). \tag{13}$$

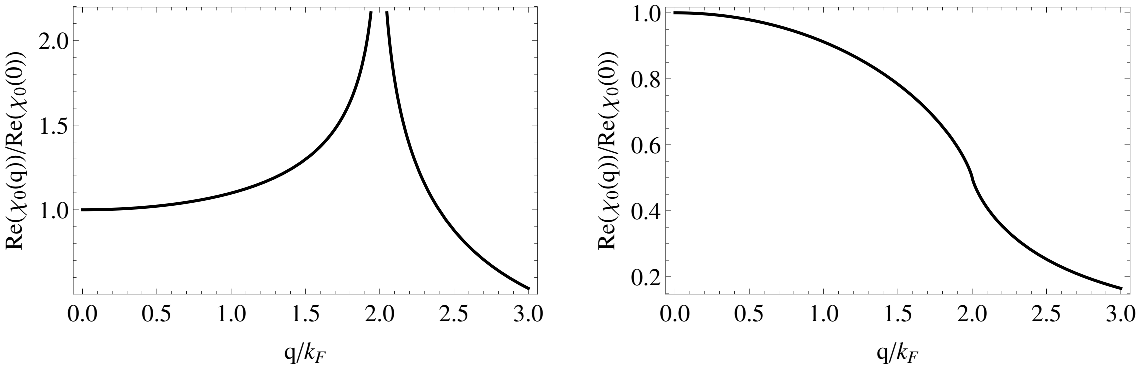

Figure 1: Plots of $\mathrm{Re}(\chi_0(q))$ for a 1-dimensional (left) and 3-dimensional system (right). The exact graph is difficult to interpret, but the divergence at $q = 2k_\mathrm{F}$ in the 1D system is clearly visible. We will see later that this is responsible for (among others) the Peierl's instability in 1D systems.

The integration over r and ϕ is straightforward and we find similar to (a) the real part of $\chi_0(\vec{q})$

$$\mathrm{Re}(\chi_0^{\mathrm{3d}}(\vec{q})) = -\frac{m}{2\pi^2\hbar^2 q}\mathcal{P}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k_z \frac{k_\mathrm{F}^2 - k_z^2}{2}\left(\frac{1}{q+2k_z} + \frac{1}{q-2k_z}\right). \tag{14}$$

After performing the integral we obtain

$$\mathrm{Re}(\chi_0^{\mathrm{3d}}(\vec{q})) = -\frac{mk_\mathrm{F}}{4\pi^2\hbar^2}\left[1 - \frac{q}{4k_\mathrm{F}}\left(1 - \frac{4k_\mathrm{F}^2}{q^2}\right)\log\left|\frac{q+2k_\mathrm{F}}{q-2k_\mathrm{F}}\right|\right]. \tag{15}$$

This function is shown in Fig. 1 (right).