Solid State Theory
Solution Sheet 9

Exercise 9.1

We write the summation as a integral and use cylindrical coordinates along the k_x direction

$$S(\omega, \boldsymbol{q}) = \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_0^{\infty} dr\ r \int_{-\infty}^{\infty} dk'_x\ n_{0,\boldsymbol{k}'}(1 - n_{0,\boldsymbol{k}'+\boldsymbol{q}})\ \delta(\epsilon_{\boldsymbol{k}'+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}} - \hbar\omega). \tag{1}$$

Since the system of free electrons is isotropic we can choose $\boldsymbol{q} = (q, 0, 0)$ where we assume $q > 0$. The factor $n_{0,\boldsymbol{k}'}(1 - n_{0,\boldsymbol{k}'+\boldsymbol{q}})$ strongly reduces the volume in k-space which contributes to the integral, see the shaded area in Fig. 1.

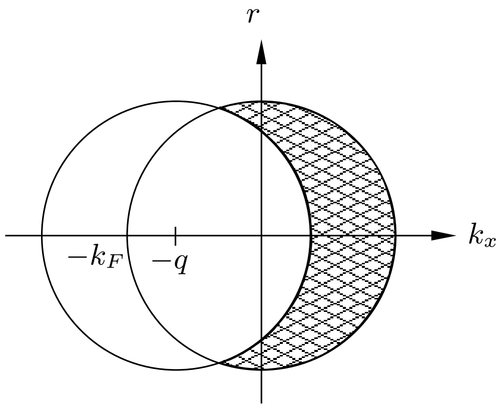

Figure 1: The region in k-space which contributes to the integral.

Then, we want to write the δ-term in a more transparent way. We start with

$$\begin{aligned}\epsilon_{\boldsymbol{k}'+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}'} &= \frac{\hbar^2}{2m}\left((\boldsymbol{k}' + \boldsymbol{q})^2 - \boldsymbol{k}'^2\right) = \frac{\hbar^2}{2m}\left((k'_x + q)^2 + r^2 - (k'^2_x + r^2)\right) \\ &= \frac{\hbar^2}{2m}\left(2k'_x q + q^2\right) \end{aligned} \tag{2}$$

and find then

$$\delta\left(\epsilon_{\boldsymbol{k}'+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}'} - \hbar\omega\right) = \delta\left(\frac{\hbar^2}{2m}\left(2k'_x q + q^2\right) - \hbar\omega\right) = \frac{m}{\hbar^2 q}\delta\left(k'_x - \bar{k}_x\right). \tag{3}$$

With the initial condition $0 \leqslant \hbar\omega \leqslant \hbar^2(2qk_F - q^2)/2m$ one can show that

$$\bar{k}_x = \frac{1}{2q\hbar}\left(2m\omega - \hbar q^2\right) \in [-q/2, k_F - q]. \tag{4}$$

Thus, it is sufficient to integrate only over this interval in k_x-direction. In radial direction we integrate from $r = \sqrt{k_F^2 - (k_x + q)^2}$ up to $r = \sqrt{k_F^2 - k_x^2}$ and the integration over ϕ is trivial. We obtain

$$S(\omega, \boldsymbol{q}) = \frac{2\pi}{(2\pi)^3} \int_{-q/2}^{k_F - q} dk'_x \int_{\sqrt{k_F^2 - (k_x+q)^2}}^{\sqrt{k_F^2 - k_x^2}} dr\ r\ \frac{m}{\hbar^2 q}\delta\left(k'_x - \bar{k}_x\right) \tag{5}$$

which results in

$$S(\omega, \boldsymbol{q}) = \frac{m^2\omega}{(2\pi)^2\hbar^3 q} = \underbrace{\frac{mk_F}{\pi^2\hbar^2}}_{N(\epsilon_F)} \frac{m\omega}{4qk_F\hbar} = \frac{N(\epsilon_F)}{4}\frac{\omega}{qv_F}. \tag{6}$$

Exercise 9.2 Uniaxial Compressibility

Since the spherical harmonic functions play an important role in this exercise, let us briefly recapitulate some facts:

- We will need the two functions

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \quad , \quad Y_{20} = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right). \tag{7}$$

- There are different conventions of the spherical harmonic functions and their orthogonality relation. In our convention of the functions, the orthogonality relation is

$$\int d\Omega\; Y^*_{lm}(\theta,\phi)Y_{l'm'}(\theta,\phi) = \delta_{ll'}\delta_{mm'} \tag{8}$$

  where the integral goes over the whole sphere and $d\Omega = d\theta d\phi\;\sin\theta$.

- If $\hat{\boldsymbol{k}}$ and $\hat{\boldsymbol{k}}'$ are the normalized vectors at (θ,ϕ) and (θ',ϕ') and Θ the angle between $\hat{\boldsymbol{k}}$ and $\hat{\boldsymbol{k}}'$, then there exists the following relation

$$P_l(\cos\Theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)Y^*_{lm}(\theta',\phi'). \tag{9}$$

Then, we first write the deformation of the Fermi surface as

$$k_F(\phi,\theta) = k_F^0 + \gamma k_F^0[3\cos^2\theta - 1] = k_F^0\left(1 + \alpha Y_{20}(\theta,\phi)\right) = k_F^0\left(1+\delta\right). \tag{10}$$

where $\alpha = 4\gamma\sqrt{\pi/5}$ and $\delta = \delta(\theta,\phi) = \alpha Y_{20}(\theta,\phi)$.

a) The change in volume enclosed by the Fermi surface is thus

$$\begin{aligned} V &= \int d\Omega \int_0^{k_F(\phi,\theta)} k^2 dk = \frac{(k_F^0)^3}{3}\int d\Omega\,(1+\delta)^3 \\ &= \frac{(k_F^0)^3}{3}\int d\Omega\Big(1 + \underbrace{3\alpha}_{\propto Y_{00}} Y_{20}(\theta,\phi) + \mathcal{O}(\gamma^2)\Big) = \frac{4\pi}{3}(k_F^0)^3 + \mathcal{O}(\gamma^2). \end{aligned} \tag{11}$$

where the vanishing of the first order term follows directly from the orthogonality of the spherical harmonics.

b) To calculate the uniaxial compressibility, we first need to calculate the difference of the energy functional accounting for the deformed Fermi surface up to second order. We start with the general expression

$$E - E_0 = \sum_{\boldsymbol{k},\sigma}\left(\epsilon_\sigma(\boldsymbol{k}) - \mu\right)\delta n_\sigma(\boldsymbol{k}) + \frac{1}{2V}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\sigma,\sigma'} f_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{k}')\delta n_\sigma(\boldsymbol{k})\delta n_{\sigma'}(\boldsymbol{k}') \tag{12}$$

and find that $\delta n_\sigma(\boldsymbol{k})$ is given by

$$\delta n_\sigma(\boldsymbol{k}) = \begin{cases} 1 & , k_F^0 \leqslant |\boldsymbol{k}| < k_F^0\,(1+\delta) \text{ and } \delta > 0 \\ -1 & , k_F^0\,(1+\delta) \leqslant |\boldsymbol{k}| < k_F^0 \text{ and } \delta < 0 \\ 0 & , \text{else} \end{cases} . \tag{13}$$

By replacing the summation over $\boldsymbol{k}$ by an integral, we can therefore write

$$\begin{aligned} E - E_0 &= \frac{V}{(2\pi)^3}\sum_\sigma \int d\Omega \int_{k_F^0}^{k_F^0(1+\delta)} dk\; k^2\,(\epsilon_\sigma(\boldsymbol{k}) - \mu) \\ &+ \frac{1}{2}\frac{V}{(2\pi)^6}\sum_{\sigma,\sigma'}\int d\Omega d\Omega' \int_{k_F^0}^{k_F^0(1+\delta)} dk \int_{k_F^0}^{k_F^0(1+\delta')} dk'\; k^2 k'^2 f_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{k}') \end{aligned} \tag{14}$$

where we wrote $\delta' = \delta(\theta', \phi')$.

Let us concentrate on the first term.

We introduce the dimensionless variable $x = k/k_F^0$ and linearize

$$\epsilon_\sigma(\boldsymbol{k}) - \mu \approx \frac{k_F^0\hbar^2}{m^*}(k - k_F^0) = \frac{(k_F^0)^2\hbar^2}{m^*}(x-1) \tag{15}$$

such that we are able to perform firstly the k-integration and secondly, the integration over the sphere

$$\begin{aligned} &\frac{V}{(2\pi)^3}\sum_\sigma \int d\Omega\; (k_F^0)^3 \int_1^{1+\delta} dx\; x^2 \frac{(k_F^0)^2\hbar^2}{m^*}(x-1) \\ &\quad = \frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\frac{1}{2}\sum_\sigma \int d\Omega\; \Big(\delta^2(\phi,\theta) + \mathcal{O}(\alpha^3)\Big) \\ &\quad = \frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\alpha^2 + \mathcal{O}(\alpha^3) \end{aligned} \tag{16}$$

where we used the orthogonality relation.

For the second term we use analogously to the lecture notes

$$\begin{aligned} f_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{k}') &\approx f_{\sigma\sigma'}(\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}') = \sum_l \left(f_l^s + \sigma\sigma' f_l^a\right) P_l(\cos\Theta) \\ &= \sum_l (f_l^s + \sigma\sigma' f_l^a)\frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^*(\theta,\phi)Y_{lm}(\theta',\phi'). \end{aligned} \tag{17}$$

The integration in k and k' (x and x') is easily computed such that the second term is

$$\frac{V}{2(2\pi)^6}\sum_{l,m}\sum_{\sigma\sigma'}(f_l^s + \sigma\sigma' f_l^a)\frac{4\pi(k_F^0)^6}{2l+1}\int d\Omega d\Omega'\; \frac{x^3}{3}\bigg|_1^{1+\delta}\; \frac{x^3}{3}\bigg|_1^{1+\delta'}\; Y_{lm}^*(\phi,\theta)Y_{lm}(\phi',\theta'). \tag{18}$$

We keep terms only up to order α^2 and sum over σ and σ' which cancels f_l^a out:

$$\frac{V}{2(2\pi)^6}\sum_{l,m}(4f_l^s)\frac{4\pi(k_F^0)^6}{2l+1}\int d\Omega d\Omega'\; \left[\delta(\phi,\theta)\delta(\phi',\theta') + \mathcal{O}(\alpha^3)\right] Y_{lm}^*(\phi,\theta)Y_{lm}(\phi',\theta'). \tag{19}$$

With

$$\int d\Omega \; \delta(\phi,\theta) Y_{lm}(\theta,\phi) = \alpha \; \delta_{2,l}\delta_{0,m} \tag{20}$$

we obtain for the second term

$$\frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\underbrace{\frac{m^* k_F^0}{\pi^2\hbar^2}}_{N(\epsilon_F)}\frac{f_2^s}{5}\alpha^2 + \mathcal{O}(\alpha^3) = \frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\frac{F_2^s}{5}\alpha^2 + \mathcal{O}(\alpha^3). \tag{21}$$

Thus, neglecting higher order terms, the total change of energy is

$$E - E_0 = \frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\alpha^2\left(1 + \frac{F_2^s}{5}\right) = \frac{V}{(2\pi)^3}\frac{(k_F^0)^5\hbar^2}{m^*}\frac{16\pi\gamma^2}{5}\left(1 + \frac{F_2^s}{5}\right). \tag{22}$$

It is now straight forward to calculate the uniaxial compressibility

$$\kappa_u = \frac{1}{V}\frac{\partial^2 E}{\partial P_z^2} = \frac{1}{V}\frac{1}{P_0^2}\frac{\partial^2 E}{\partial \gamma^2} = \frac{8}{5\pi^2}\frac{E_F}{P_0^2}(k_F^0)^3(1 + \frac{F_2^s}{5}) = \frac{24}{5}n\frac{E_F}{P_0^2}(1 + \frac{F_2^s}{5}). \tag{23}$$

Here we have used $n = \frac{(k_F^0)^3}{3\pi^2}$.

Note: If the volume enclosed by the distorted Fermi surface is constant for any external disturbance, the adding of the chemical potential μ is only a shift in the energy and does not affect any response quantity (χ, κ, etc.). However, in our case the volume is fixed only up to first order in α and the response κ is given by the second derivative of the energy with respect to the parameter α. Thus, the adding of μ directly changes the final result κ. Fortunately, the change of the volume in order of α^2 also influences the integral over $\epsilon_\sigma(\boldsymbol{k})$ in the order of α^2.

A slightly more sophisticated calculation with a constant volume up to second order in α requires the distortion

$$k_F(\theta,\phi) = k_F^0\left(1 - \frac{\alpha^2}{4\pi}\right)(1 + \delta(\theta,\phi)) \tag{24}$$

where the additional α^2-term assures the consistency of the volume. Using this distortion one is able to show, that the 'illness' of the integral over $\epsilon_\sigma(\boldsymbol{k})$ is actually cured by substracting μ and that the final result is correct.