Karlsruhe Institute of Technology

Institute for Theoretical
Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Solutions 12
Tutorial: 02.02.2022

Category A

1. Dielectric function for the non-interacting electron gas $(15 + 10 = 25$ points)

In this problem, we propose to compute the dielectric function for the non-interacting electron gas, $\epsilon(\boldsymbol{q}, \omega)$. Consider a semi-classical electron gas with band mass m.

(a) Starting from the Boltzmann equation at equilibrium with the electric field $\boldsymbol{E} = \boldsymbol{E}_0 e^{i(\boldsymbol{qr}-\omega t)} = -\nabla_{\vec{r}}\varphi(\vec{r}, t)$, show that the induced current in Fourier space is

$$\mathbf{j}_{\text{ind}}(\mathbf{q}, \omega) = -\frac{e^2 k_F^3}{(2\pi)^2 m\omega}\left[\frac{2}{3} + \frac{2}{5}\left(\frac{k_F q}{m\omega}\right)^2\right]\mathbf{q}\varphi(\mathbf{q}, \omega)$$

for small $\mathbf{q}$.

Solution: We start from the Boltzmann equation $\frac{\mathrm{d}}{\mathrm{d}}f(\mathbf{k}, \mathbf{r}, t) = -I[f(\mathbf{k}, \mathbf{r}, t)]$ for the distribution function $f(\mathbf{k}, \mathbf{r}, t) = f_0(\mathbf{k}) + \tilde{f}(\mathbf{k}, \mathbf{r}, t)$. Here, f_0 is the equilibrium distribution and $\tilde{f} \propto E_0$ is a small correction induced by the field. In the linear response regime of sufficiently small E_0, we neglect $\frac{\partial \tilde{f}}{\partial \mathbf{k}}$ in the kinetic equation on $\tilde{f}$. Therefore, in τ-approximation for $I[f(\mathbf{k}, \mathbf{r}, t)]$), we have

$$\frac{\partial \tilde{f}}{\partial t} + \dot{\mathbf{r}}\frac{\partial \tilde{f}}{\partial \mathbf{r}} + \dot{\mathbf{k}}\frac{\partial f_0}{\partial \mathbf{k}} = -\frac{\tilde{f}}{\tau}.$$

Using the identities $\dot{\mathbf{r}} = \mathbf{v} = \mathbf{k}/m$ and $\dot{\mathbf{k}} = \mathbf{F} = -e\mathbf{E}$, and applying the Fourier transformation ($\frac{\partial}{\partial t} \to -i\omega$ and $\frac{\partial}{\partial \mathbf{r}} \to i\mathbf{q}$) in the equation, we find for the correction:

$$\tilde{f}(\mathbf{k}, \mathbf{q}, \omega) = \frac{e\varphi(\mathbf{q}, \omega)}{\mathbf{k}\cdot\mathbf{q}/m - (\omega + i\tau^{-1})}\mathbf{q}\cdot\frac{\partial f_0(\mathbf{k})}{\partial \mathbf{k}}$$

where we used $e\mathbf{E}(\mathbf{q}, \omega) = -i\mathbf{q}\varphi(\mathbf{q}, \omega)$. Substitute it into the induced current:

$$\begin{aligned}
\mathbf{j}_{\text{ind}}(\mathbf{q}, \omega) &= -e\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\mathbf{v}\tilde{f}(\mathbf{k}, \mathbf{q}, \omega) \\
&= -\frac{e^2\varphi(\mathbf{q}, \omega)}{m}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\mathbf{k}}{\mathbf{k}\cdot\mathbf{q}/m - \omega}\mathbf{q}\cdot\frac{\partial f_0(\mathbf{k})}{\partial \mathbf{k}}.
\end{aligned}$$

Using that $\frac{\partial f(\mathbf{k})}{\partial \mathbf{k}} = -\hat{e}_{\mathbf{k}}\delta(k - k_F)$ at $k_B T \ll \epsilon_F$ where $\hat{e}_{\mathbf{k}} = \mathbf{k}/k$ and $k = |\mathbf{k}|$, we switch the integral to spherical coordinates choosing z-axis parallel to $\mathbf{q}$ (the corresponding unit vector is $\hat{\mathbf{e}}_z = \frac{\mathbf{q}}{q}$):

$$\mathbf{j}_{\text{ind}}(\mathbf{q},\omega) = \frac{e^2\varphi(\mathbf{q},\omega)}{m}\int_0^\infty \frac{k^2 \mathrm{d}k}{(2\pi)^3}\int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi \frac{kq\cos\theta}{kq\cos\theta/m - \omega}\begin{pmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{pmatrix}\delta(k-k_F) =$$

$$= e^2\varphi(\mathbf{q},\omega)\begin{pmatrix}0\\0\\1\end{pmatrix}\frac{k_F^2}{(2\pi)^2}\int_0^\pi \frac{\sin\theta\cos^2\theta}{\cos\theta - \frac{\omega+i\tau^{-1}}{v_F q}}\mathrm{d}\theta = \qquad (v_F = \frac{k_F}{m} \text{ is the Fermi velocity})$$

$$= e^2\frac{k_F^2}{(2\pi)^2}\varphi(\mathbf{q},\omega)\hat{\mathbf{e}}_z\int_{-1}^{1}\frac{u^2}{u - \frac{\omega+i\tau^{-1}}{v_F q}}\mathrm{d}u =$$

$$= e^2\frac{k_F^2}{(2\pi)^2}\frac{\mathbf{q}}{q}\varphi(\mathbf{q},\omega)x\Big(2 - x\ln\frac{x+1}{x-1}\Big) \qquad (\text{here } x = \frac{\omega+i\tau^{-1}}{v_F q})$$

Consider the regime of homogeneous in space field, which means $q \to 0$, and assume finite ω. It means that $|x| \gg 1$. The logarithm is expanded in x^{-n} series as follows: $\ln\frac{x+1}{x-1} = \frac{2}{x} + \frac{2}{3x^3} + \frac{2}{5x^5} + \ldots$. Therefore we find in $q \to 0$ limit

$$\mathbf{j}_{\text{ind}}(\mathbf{q},\omega) = -e^2\frac{v_F k_F^2}{2\pi^2(\omega+i\tau^{-1})}\mathbf{q}\varphi(\mathbf{q},\omega)\Big(\frac{1}{3} + \frac{q^2 v_F^2}{5(\omega+i\tau^{-1})^2}\Big).$$

(b) Derive the relation

$$\mathbf{j}_{\text{ind}}(\mathbf{q},\omega) = -\frac{i\omega}{4\pi}[\epsilon(\mathbf{q},\omega)-1]\mathbf{E}(\mathbf{q},\omega) = -\frac{\omega}{4\pi}[\epsilon(\mathbf{q},\omega)-1]\mathbf{q}\varphi(\mathbf{q},\omega)$$

using the continuity equation for the induced current and density, $\omega\rho_{\text{ind}} = \mathbf{q}\cdot\mathbf{j}_{\text{ind}}$, the relation between ρ_{ind} and the polarisation $\mathbf{P}$, $\rho_{\text{ind}} = -i\mathbf{q}\cdot\mathbf{P}$, where $\mathbf{P} = \frac{\epsilon(\mathbf{q},\omega)-1}{4\pi}\mathbf{E}$. Then, identify the dielectric function $\epsilon(\mathbf{q},\omega)$.

Solution: Using the two last relations we have:

$$\rho_{\text{ind}} = -i\frac{\epsilon(\mathbf{q},\omega)-1}{4\pi}\mathbf{q}\cdot\mathbf{E}.$$

Injecting this expression in the continuity equation we have for any $\mathbf{q}$:

$$\mathbf{q}\cdot(\mathbf{j}_{\text{ind}} + i\omega\frac{\epsilon(\mathbf{q},\omega)-1}{4\pi}\mathbf{E}) = 0 \qquad \forall\mathbf{q}.$$

Therefore we deduce the expression of the question. Finally, neglecting τ^{-1} compared to ω, we have

$$\epsilon(\mathbf{q},\omega) \underset{qv_F \ll \omega}{\simeq} 1 - \frac{e^2 k_F^3}{\pi m\omega^2}\left(\frac{2}{3} + \frac{2}{5}\left(\frac{qk_F}{m\omega}\right)^2\right)$$

Category B

2. Debye-Waller factor (30 Points)

In the lecture the following expression for the structure factor of phonons for a monoatomic crystal was derived

$$S(\boldsymbol{q},\omega) = e^{-2W}\int \frac{dt}{2\pi}e^{i\omega t}\sum_{\boldsymbol{R}} e^{-i\boldsymbol{qR}}\exp\langle[\boldsymbol{qu}(0)][\boldsymbol{qu}(\boldsymbol{R},t)]\rangle,$$

where $\boldsymbol{u}(\boldsymbol{R},t)$ is the atomic displacement, $\boldsymbol{R}$ denotes the vectors of the Bravais lattice, and W is the Debye-Waller factor, given by the expression

$$W = \frac{1}{2}\langle[\boldsymbol{qu}(0)]^2\rangle.$$

(a) Show, that the Debye-Waller factor can be written as

$$W = \frac{V}{2}\int\frac{d^dk}{(2\pi)^d}\sum_s \frac{[\boldsymbol{q\epsilon}_s(\boldsymbol{k})]^2}{2M\omega_s(\boldsymbol{k})}\coth\frac{\omega_s(\boldsymbol{k})}{2T}.$$

Here V is the appropriate cell volume ans s denotes the phonon branch.

(b) Show that $e^{-2W}=0$ in one and two dimensions. What are the implications of this result for the possible existence of one- and two-dimensional crystalline ordering?
Hint Consider the behavior of the integrand for small k.

(c) Estimate the size of the Debye-Waller factor for a monoatomic three-dimensional crystal. Analyze your result for the limiting cases of temperatures low and high as compared to the Debye temperature.

(d) Evaluate the one-phonon contribution to the structure factor. Interpret the result in terms of absorbtion and emission of phonons.
Hint The one-phonon contribution corresponds to the linear term in the expansion of the last exponential in the above expression for the structure factor.

Solution:

(a) We calculate

$$\begin{aligned} W &= \frac{1}{2}\langle(\boldsymbol{qu})^2\rangle \\ &= \frac{1}{2N}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,s_1,s_2}\left\langle\left[\boldsymbol{q}\left(\boldsymbol{u}_{\boldsymbol{k}_1s_1}e^{i\boldsymbol{k}_1\boldsymbol{R}}+\boldsymbol{u}^\dagger_{\boldsymbol{k}_1s_1}e^{-i\boldsymbol{k}_1\boldsymbol{R}}\right)\right]\left[\boldsymbol{q}\left(\boldsymbol{u}_{\boldsymbol{k}_2s_2}e^{i\boldsymbol{k}_2\boldsymbol{R}}+\boldsymbol{u}^\dagger_{\boldsymbol{k}_2s_2}e^{-i\boldsymbol{k}_2\boldsymbol{R}}\right)\right]\right\rangle, \end{aligned}$$

in which

$$\boldsymbol{u}_{\boldsymbol{k}s} = \sqrt{\frac{1}{2M\omega_{\boldsymbol{k}s}}}\boldsymbol{\epsilon}_s(\boldsymbol{k})\hat{a}_{\boldsymbol{k}s}.$$

We calculate the mean $\langle\ldots\rangle$ for the same ground state, so only the diagonal terms contribute:

$$\left\langle\hat{a}^\dagger_{\boldsymbol{k}s}\hat{a}_{\boldsymbol{k}s}+\hat{a}_{\boldsymbol{k}s}\hat{a}^\dagger_{\boldsymbol{k}s}\right\rangle = 2n_{\boldsymbol{k}s}+1 = \coth\frac{\omega_{\boldsymbol{k}s}}{2T}.$$

We find that

$$W = \frac{1}{2N}\sum_{\boldsymbol{k},s}\frac{(\boldsymbol{q\epsilon}_s(\boldsymbol{k})))^2}{2M\omega_{\boldsymbol{k}s}}\coth\frac{\omega_{\boldsymbol{k}s}}{2T} \quad\Rightarrow\quad \frac{V}{2N}\int\frac{d^dk}{(2\pi)^d}\sum_s\frac{(\boldsymbol{q\epsilon}_s(\boldsymbol{k}))^2}{2M\omega_{\boldsymbol{k}s}}\coth\frac{\omega_{\boldsymbol{k}s}}{2T}.$$

(b) For acoustic phonons applies

$$\omega_{\boldsymbol{k}s} = c_s k.$$

For small k

$$\frac{1}{\omega_{\boldsymbol{k}s}} \coth \frac{\omega_{\boldsymbol{k}s}}{2T} \sim \frac{1}{k^2}.$$

Therefore the integral

$$\int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2}$$

diverges for $d \leq 2$.

(c) Three acoustic branches occur in a 3D monoatomic crystal: 1 longitudinal and 2 transverse. We choose the branch with

$$\boldsymbol{\epsilon}_s(\boldsymbol{k}) \parallel \boldsymbol{q} \qquad \Rightarrow \qquad (\boldsymbol{q}\boldsymbol{\epsilon}_s(\boldsymbol{k}))^2 = q^2.$$

Then we introduce the density of states of the phonons

$$\int \frac{d^3 k}{(2\pi)^3} \sum_s \to \int_0^{\omega_D} d\omega D(\omega), \qquad D(\omega) = \frac{3\omega^2}{2\pi^2 c^3},$$

and find

$$2W = \frac{V}{N} \int_0^{\omega_D} d\omega \frac{3\omega^2}{2\pi^2 c^3} \frac{q^2}{2M\omega} \coth \frac{\omega}{2T} = \frac{3q^2}{4M} \frac{V}{N\pi^2 c^3} \int_0^{\omega_D} d\omega \omega \coth \frac{\omega}{2T}.$$

At $T = 0$

$$\coth \frac{\omega}{2T} \to 1 \qquad \Rightarrow \qquad 2W = \frac{3q^2}{4M} \frac{1}{ck_D}.$$

At $T \gg \omega_D$

$$\coth \frac{\omega}{2T} \to \frac{2T}{\omega} \qquad \Rightarrow \qquad 2W = \frac{3q^2}{4M} \frac{4T}{c^2 k_D^2}.$$

(d) We expand the structure factor to the first order

$$\exp \langle (\boldsymbol{q} \cdot \boldsymbol{u}(0)) (\boldsymbol{q} \cdot \boldsymbol{u}(\boldsymbol{R})) \rangle \approx 1 + \langle (\boldsymbol{q} \cdot \boldsymbol{u}(0)) (\boldsymbol{q} \cdot \boldsymbol{u}(\boldsymbol{R})) \rangle .$$

Calculate the average value

$$\langle (\boldsymbol{q} \cdot \boldsymbol{u}(0)) (\boldsymbol{q} \cdot \boldsymbol{u}(\boldsymbol{R})) \rangle =$$

$$= \frac{1}{N} \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, s_1, s_2} \left\langle \left[\boldsymbol{q} \left(\boldsymbol{u}_{\boldsymbol{k}_1 s_1} + \boldsymbol{u}^\dagger_{\boldsymbol{k}_1 s_1} \right) \right] \left[\boldsymbol{q} \left(\boldsymbol{u}_{\boldsymbol{k}_2 s_2} e^{i\boldsymbol{k}_2 \boldsymbol{R} - i\omega_2 t} + \boldsymbol{u}^\dagger_{\boldsymbol{k}_2 s_2} e^{-i\boldsymbol{k}_2 \boldsymbol{R} + i\omega_2 t} \right) \right] \right\rangle$$

$$= \frac{1}{N} \sum_{\boldsymbol{k}, s} \left\langle \hat{a}^\dagger_{\boldsymbol{k}s} \hat{a}_{\boldsymbol{k}s} e^{-i\omega_{\boldsymbol{k}s} t} + \hat{a}_{\boldsymbol{k}s} \hat{a}^\dagger_{\boldsymbol{k}s} e^{i\omega_{\boldsymbol{k}s} t} \right\rangle e^{i\boldsymbol{k}\boldsymbol{R}}$$

$$= \frac{1}{N} \sum_{\boldsymbol{k}, s} \frac{(\boldsymbol{q}\boldsymbol{\epsilon}_s(\boldsymbol{k}))^2}{2M\omega_{\boldsymbol{k}s}} \left\langle (n_{\boldsymbol{k}s} + 1) e^{i\omega_{\boldsymbol{k}s} t} + n_{\boldsymbol{k}s} e^{-i\omega_{\boldsymbol{k}s} t} \right\rangle e^{i\boldsymbol{k}\boldsymbol{R}}.$$

From this we find the structure factor

$$S^{(1)} = e^{-2W} \frac{(\boldsymbol{q}\boldsymbol{\epsilon}_s(\boldsymbol{q}))^2}{2M\omega_{\boldsymbol{q}s}} \left[(n_{\boldsymbol{k}s}+1)\delta(\omega+\omega_{\boldsymbol{q}s}) + n_{\boldsymbol{k}s}\delta(\omega-\omega_{\boldsymbol{q}s})\right].$$

The δ functions correspond to the conservation laws:

Generation (emission) of phonons $$\frac{k^2}{2m} = \frac{k'^2}{2m} + \omega_{\boldsymbol{q}s};$$

Absorption of phonons $$\frac{k^2}{2m} = \frac{k'^2}{2m} - \omega_{\boldsymbol{q}s}.$$

Conservation of momentum: ($\boldsymbol{K}$ is a reciprocal lattice vector)

$$\boldsymbol{k}' \pm \boldsymbol{q} = \boldsymbol{k} + \boldsymbol{K},$$

namely ($\omega_{\boldsymbol{q}} = \omega_{-\boldsymbol{q}}$)

$$\frac{k^2}{2m} = \frac{k'^2}{2m} \pm \omega_{\boldsymbol{k}-\boldsymbol{k}',s}.$$