Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 12
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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 $\boldsymbol{E} = \boldsymbol{E}_0 e^{i(\boldsymbol{q}\boldsymbol{r}-\omega t)} = -\nabla_{\vec{r}}\varphi(\vec{r}, t)$, 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 $\mathbf{q}$.

(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 $\mathbf{P} = \dfrac{\epsilon(\mathbf{q}, \omega) - 1}{4\pi}\mathbf{E}$. Then, identify the dielectric function $\epsilon(\mathbf{q}, \omega)$.

Category B

2. Debye-Waller factor $(5 + 5 + 5 + 10 = 25$ Points)

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

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

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

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

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

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

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.