Goethe-Universität Frankfurt
Fachbereich Physik

Lecturer: Prof. Dr. Roser Valentí, Room 1.130
Tutorial supervisor: Karim Zantout, Room 1.142

Frankfurt, 25.11.2019

Einführung in die Theoretische Festkörperphysik

Winter term 2019/2020

Exercise 6

(Due date: 02.12.2019)

Problem 1 (**Second order term in the Dulong-Petit law**) (3 points)

At high temperatures the specific heat of a 3D crystal consisting of one atom species can be described by the so-called Dulong-Petit law in first order of T^{-1}: $c_V^0 = 3nk_B$, where n is the density of the material and k_B is the Boltzmann constant. Considering terms in the second order of T^{-1} one obtains $c_V = c_V^0 \left(1 - \frac{A}{T^2}\right)$. Calculate A as a function of the phonon dispersion.

Problem 2 (**Estimation of the Debye temperature**) (3 points)

A neutron beam with wave length $\lambda_0 = 1$ Å along [001] direction hits a crystal with fcc crystal structure. The crystal has lattice parameters $a = 3.52$ Å and a single-atom basis. A part of the neutrons with wave length $\lambda_1 = 1.25$ Å is reflected in a direction that is tilted by 4° from the incoming direction.

a) Assume that only single neutrons take part in the scatterin process. Calculate their wave vector and energy.

b) Is a phonen created or absorbed during the scattering process?

c) Estimate the sound speed and the Debye temperature of the material from the energy and wave vector of the phonon.

Problem 3 (**Neutron Scattering and Phonons**) (4 points)

In this exercise, we will complete the derivation of the dynamical structure factor presented in the lecture notes equations (4.141) - (4.145). (*Hint:* This section of the notes has been updated to correct some minor typos.)

In the notes it is shown that the dynamical structure factor can be written $S(\vec{q},\omega) \approx S_{(0)}(\vec{q},\omega) + S_{(1)}(\vec{q},\omega)$, where:

(1)
$$S_{(0)}(\vec{q},\omega) = \frac{1}{N} e^{-2W} \int \frac{dt}{2\pi} e^{-i\omega t} \sum_{n,n'} e^{-i\vec{q}\cdot(\vec{R}_{n0} - \vec{R}_{n'0})}$$

(2)
$$S_1(\vec{q},\omega) = \frac{1}{N} e^{-2W} \int \frac{dt}{2\pi} e^{-i\omega t} \sum_{n,n'} e^{-i\vec{q}\cdot(\vec{R}_{n0} - \vec{R}_{n'0})} \langle (\vec{q}\cdot\vec{u}_n(0))(\vec{q}\cdot\vec{u}_{n'}(t))\rangle$$

a) Show that $S_{(0)}(\vec{q},\omega)$ can be written:

(3)
$$S_{(0)}(\vec{q},\omega) = e^{-2W} \delta(\omega) N \sum_{\vec{G}} \delta_{\vec{q},\vec{G}}$$

b) Writing the atomic displacements in terms of phonon creation an annihilation operators:

$$\vec{u}_n = \sum_{\vec{k},j} \sqrt{\frac{\hbar}{2MN\omega_j(\vec{k})}} \left(a_{\vec{k},j} + a^\dagger_{-\vec{k},j}\right) \vec{e}_j(\vec{k})\; e^{i\vec{k}\cdot\vec{R}_{n0}} \tag{4}$$

show that $S_{(1)}(\vec{q},\omega)$ can be written:

$$S_1(\vec{q},\omega) = \frac{\hbar e^{-2W}}{2M} \sum_{\vec{k},j} \delta_{\vec{q}-\vec{k},\vec{G}} \frac{(\vec{q}\cdot\vec{e}_j(\vec{k}))^2}{\omega_j(\vec{k})} \Big\{(1+\langle a^\dagger_{\vec{k},j} a_{\vec{k},j}\rangle)\delta(\omega-\omega_j(\vec{k})) + \langle a^\dagger_{-\vec{k},j} a_{-\vec{k},j}\rangle\delta(\omega+\omega_j(\vec{k}))\Big\} \tag{5}$$

You may use the properties: $\omega_j(\vec{k}) = \omega_j(-\vec{k})$ and $\vec{e}_j(\vec{k}) = \vec{e}_j(-\vec{k})$.