

## PROBLEM SHEET 4

### Introduction to Condensed Matter Theory

*(To be submitted on Wednesday, 10.06.2015)*

1. **Ehrenfest Theorem:** The Ehrenfest theorem states that the expectation values of quantum mechanical operator under certain circumstances obey the classical laws of motion. We have also derived the dispersion relation in the previous exercises. Here, we will examine when and why such assumption is justified.

(a) For this, take any operator  $\hat{O}$ . Remember that the time evolution in the heisenberg picture is:

$$\frac{d\hat{O}}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{O}] + \frac{\partial \hat{O}}{\partial t} \quad (1)$$

What can you say about the time evolution of the expectation value  $d\langle \hat{O} \rangle / dt$ ? [1]

(b) Let us now examine for the sake of simplicity a Hamiltonian of the form  $\hat{H} = \hat{p}^2 / 2m + V(\hat{x})$ . Write the differential equation for the time evolution of the expectation values of position and momentum operator, and from it derive the equation of motion [3]

$$m \frac{d^2}{dt^2} \langle \hat{x} \rangle = \langle F(\hat{x}) \rangle \quad (2)$$

[ Remember that force is defined as the negative gradient of the potential.]

(c) As you can see, this is almost like the expression of the expectation values of the classical equation of motion. To see the exact agreement, develop the expectation value of the force using the expectation value of the position operator and find out for which system the following applies: [2]

$$\langle F(\hat{x}) \rangle = F(\langle \hat{x} \rangle) \quad (3)$$

2. **Density of states and the Debye model** (a) Consider a square lattice of atoms that have mass  $m$  separated by a distance  $a$  from each other. The effective potential for displacements of nearest neighbours is described by the spring constant  $K$ . Write the Hamiltonian and show that for periodic boundary conditions, the following dispersion relation is valid:

$$\omega(k) = 2\sqrt{\frac{K}{m}} \left[ \sin^2\left(\frac{k_1 a}{2}\right) + \sin^2\left(\frac{k_2 a}{2}\right) \right]^{\frac{1}{2}} \quad (4)$$

For  $k \rightarrow 0$  does the phonons spread isotropically or anisotropically? [4]

(b) The density of states  $n(\omega)$  describes the number of possible phononic states in the frequency range  $[\omega, \omega + d\omega]$  per unit cell. Give the expression for the density of states for a general  $d$ -dimensional crystal and explain it. [2]

(c) Use your knowledge of the previous subtasks to show that the density of states of the phonons in the two-dimensional lattice can be written as  $n(\omega) = \frac{1}{a^2} \sqrt{\frac{m}{k}} \bar{n}(\bar{\omega})$  with  $\bar{\omega} = \frac{1}{2} \sqrt{\frac{m}{K}} \omega$  where  $\bar{n}(\bar{\omega})$  and  $\bar{\omega}$  are dimensionless and  $\bar{n}(\bar{\omega})$  is given by [2]

$$\bar{n}(\bar{\omega}) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \delta(\bar{\omega} - \sqrt{\sin^2(\frac{k_1}{2}) + \sin^2(\frac{k_2}{2})}) \quad (5)$$

(d) In the expression for the density of states in a general d dimensional crystal, how is this  $n(\omega)$  generally normalized? [1]

(e) The internal energy of the system U is calculated as

$$U(T) = U(T=0) + N \int_0^{\infty} d\omega n(\omega) \hbar\omega \frac{1}{e^{\beta\hbar\omega} - 1} \quad (6)$$

where  $\beta = 1/k_B T$  (with the Boltzmann constant  $k_B$  and the temperature T). The second term in the integral describes the probability of occupation of a state with frequency  $\omega$  at temperature T.

In the Debye approximation it is assumed that at low temperatures, the linear dispersion relation for the entire Brillouin zone applies. Why is this assumption justified (atleast) for the calculation of internal energy? Write the expression for the corresponding density of states  $n_D(\omega)$ . [2]

(f) As a further approximation, we do not consider a longer Brillouin zone but a circle of radius  $k_D$ . The so-called Debye frequency  $\omega_D$  is defined as a cut-off frequency, so the Debye density of states has the same norm as the original density of states:

$$\int_0^{\infty} n(\omega) d\omega = \int_0^{\omega_D} n_D(\omega) d\omega \quad (7)$$

Calculate  $\omega_D$ . [1]

(g) Show with the help of the previous task that the internal energy can be written as

$$U(T) = U(0) + 4Nk_B \frac{T^3}{T_D^2} \int_0^{T_D/T} \frac{x^2}{e^x - 1} dx \quad (8)$$

where the Debye temperature is defined as  $\hbar\omega_D = k_B T_D$  and  $x = \hbar\omega\beta$ . [2]