
Exercise 10 for Theoretical Solid State Physics in Summer 2023

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Submission: 21.06.2023, 12:00 in the P.O. Box Popkov on D.10 (by e-mail)

Discussion: 21.06.2023, 14:15

1. One dimensional lattice with a two-atomic basis (10 points)

Consider a one-dimensional Bravais lattice with two ions per unit cell, with equilibrium positions na and $na + d$. We take the two ions to be identical, but take $d \leq \frac{a}{2}$. For simplicity we assume that only nearest neighbours interact. As a consequence the force between neighbouring ions depends on whether the distance is d or $a - d$. The harmonic potential energy can be written in the form

$$U = \frac{K}{2} \sum_n (u_1(na) - u_2(na))^2 + \frac{G}{2} \sum_n (u_2(na) - u_1(na + a))^2,$$

where $u_1(na)$ ($u_2(na)$) is the displacement of the ion which oscillates about the site na ($na + d$). Due to $d \leq \frac{a}{2}$ we have the relation $K \geq G$. Calculate the equations of motion and the dispersion relation assuming periodic boundary conditions. Analyse this relation!

2. Debye interpolation (10 points)

The partition function for the harmonic crystal is given by

$$Z = \text{tr} e^{-\beta \mathbf{H}} = \prod_{\vec{q} \in \text{BZ}} \prod_{s=1}^{3r} \text{tr} e^{-\beta \omega_s(\vec{q}) (\mathbf{b}_{\vec{q}s}^\dagger \mathbf{b}_{\vec{q}s} + \frac{1}{2})}.$$

(a) Calculate the free energy and show that it can be written as

$$F = E_0 + VT \int_0^\infty d\omega D(\omega) \ln(1 - e^{-\beta\omega}).$$

What is the internal energy?

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- (b) In the lecture you have seen that the specific heat c_V shows universal behavior for low and high temperatures T . We now look for a simple model for interpolating between low and high T . We assume a functional form of the density of states extrapolated from low energies and introduce a cut-off frequency ω_D in such a way that the condition

$$\int_0^{\infty} d\omega D(\omega) = \frac{3N_{\text{at}}}{V}, \quad (1)$$

is satisfied (why?). This leads to

$$D(\omega) = \frac{3\omega^2}{2\pi^2\bar{v}^3} \Theta(\omega_D - \omega) \quad (2)$$

where ω_D is fixed by condition (1). Use the function

$$A(x) = \frac{3}{x^3} \int_0^x dt \frac{t^3}{e^t - 1}$$

and calculate the internal energy and the specific heat. What does this mean physically? Draw c_V .