Exercise 10 for Theoretical Solid State Physics in Summer 2021

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Discussion: 28.06.2021, 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

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

   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

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

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

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

   What is the internal energy?

(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

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

is satisfied (why?). This leads to

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

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

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

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