Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 3**

Hand in: Mon 05.11.2018 *(questions marked as ∗ are optional)*
Discussion date: Fri 09.11.2018

4. Density of states of the mono-atomic chain

Consider a chain of atoms with mass m and nearest neighbour coupling κ and lattice periodicity (at rest) a. The dispersion relation for the chain is given by

$$\omega(q) = \omega_0 |\sin(\frac{qa}{2})|, \tag{1}$$

where $\omega_0 = 2\sqrt{\kappa/m}$.

(a) ∗ Derive and sketch the dispersion relation using the result from Problem 2, Sheet 2.

Hint: Pay attention that in moving from lattice periodicity $2a$ to a, the first Brillouin's zone doubles; do take care of this expansion (which we ignored in the lecture).

(b) (10pts) Show that the density of states per unit cell of the band is given by

$$g(\omega) = \frac{2}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}}. \tag{2}$$

Sketch the g as a function of ω.

(c) (10pts) Compute the density of states of the phonon band in Debye's approximation. Compare the obtained result with that of (b) to see when the approximation is good.

(d) (10pts) How does the specific heat at (very) low temperature behave with respect to temperature? Do verify the approximations you made.

Hint: At very low temperature, which part of the band gives most important contribution to the specific heat?

5. Low temperature specific heat in d-dimension

Consider a crystal in d-dimension of n atoms per unit cell.

(a) (5pts) How many acoustic bands and how many optical bands are there?

(b) (10pts) How does the specific heat at (very) low temperature behave with respect to temperature?

(c) ∗ What is the specific heat at (very) high temperature according to the Dulong–Petit law?