

## Tutorial 7, Statistical Mechanics: Concepts and applications 2016/17 ICFP Master (first year)

Maurizio Fagotti, Olga Petrova, Werner Krauth  
*Tutorial exercises*

### I. WORKSHEET: HARMONIC SOLID

Source: B. Jancovici, *Phys. Rev. Lett.* **19**, 20 (1967)

#### 1. The harmonic solid model

**Reminder:** The equipartition theorem states that the average energy for a simple harmonic oscillator is given by

$$\langle E \rangle = \langle E_{\text{kinetic}} \rangle + \langle U_{\text{potential}} \rangle = D \left( \frac{k_B T}{2} + \frac{k_B T}{2} \right) = D k_B T, \quad (1)$$

where  $D$  is the dimensionality of the problem.

**The model:** Consider a crystal in which the atoms are arranged in an ordered way: at  $T = 0$ , they are all located at their respective lattice sites  $\vec{R}_j$ . For the time being, let us assume the lattice to be a one-dimensional chain with periodic boundary conditions, so that  $R_j = ja$ , where  $a$  is the lattice constant that we take to be 1, and  $R_{j+N} = R_j$ . At  $T > 0$ , the atoms positions deviate from the associated lattice sites by some displacement  $x_j$ :

$$r_j = R_j + x_j. \quad (2)$$

The atoms have some sort of potential energy  $U$ , that we can expand in a Taylor series around the atoms' equilibrium positions  $R_j$ . The lowest order non-trivial contribution is going to be quadratic, resulting in the so-called harmonic approximation in which the systems energy is given by

$$E = \frac{m}{2} \sum_j \dot{x}_j^2 + \frac{K}{2} \sum_j (x_j - x_{j+1})^2. \quad (3)$$

- (a) Perform the Fourier transform of the position variables to find the normal modes of the system. Apply the FT to the potential energy and show how it enables us to factorize the problem.
- (b) Compute the quadratic displacement of a given atom  $\langle x_n^2 \rangle$ , then the quadratic displacement between different atoms  $\langle (x_n - x_m)^2 \rangle$ . What is the physical meaning of the results?

**Hint:** In the thermodynamic limit  $N \rightarrow \infty$ , replace the sum  $(1/N) \sum_{0 \leq k \leq \pi}$  with an integral  $\int_0^\pi \frac{dk}{2\pi}$ .

- (c) Consider the  $2D$  case, where the calculations are carried out in much the same way. Again, use the FT of  $\vec{x}_j$  to find the normal modes and factorize the potential energy term.
- (d) Find the quadratic displacement of a given atom in a given direction  $\langle (\hat{r} \cdot \vec{x}_n)^2 \rangle$ . What is the difference between  $D = 2$  and  $D > 2$  cases?
- (e) Calculate the quadratic displacement between different atoms in a given direction  $\langle (\hat{r} \cdot (\vec{x}_n - \vec{x}_m))^2 \rangle$ . Is there long range positional order in  $D = 2$ ?  $D > 2$ ?

(f) Consider the the following expectation value

$$\langle (\vec{r}(\vec{R} + \vec{a}_j) - \vec{r}(\vec{R})) \cdot (\vec{r}(\vec{R}' + \vec{a}_j) - \vec{r}(\vec{R}')) \rangle \quad (4)$$

where  $\vec{a}_j$  is one of the primitive vectors that generate the Bravais lattice. This is a measure of the spatial correlation of the “local orientation” of the system. If this correlation vanishes in the limit of large distance, it means that thermal fluctuations had spoiled the long-range propagation of the local crystalline orientation.