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Simulation numérique en physique statistique
TD n° 4

The structure factor

Références

[1] Principles of condensed matter physics, P. M. Chaikin and T. C. Lubensky, Cambridge Univ. Press

1 Generalities on the structure factor

The structure factor is an essential quantity which describes the spacial correlations between particles in condensed matter systems [1]. Let us consider N particles within a box of volume V. We introduce the density function

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i),$$

where $\mathbf{r}_i$ is the position of particle i. The structure factor is defined as

$$S(\mathbf{k}) = \frac{1}{N}\langle \rho(\mathbf{k})\rho(-\mathbf{k})\rangle,$$

where $\rho(\mathbf{k})$ is the Fourier transform of the density and $\langle .. \rangle$ indicates an ensemble average.

▷ **1-1** Write an explicit form of the structure factor in terms of $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.

▷ **1-2** Under what conditions $S(\mathbf{k}) \to 1$ when $\mathbf{k} \to \infty$?

▷ **1-3** Derive the relation between $S(\mathbf{k})$ and the pair distribution function $g(\mathbf{r})$.

▷ **1-4** One considers a simulation box of size L with periodic boundary conditions. What is the minimal wave-vectors accessible in the simulation ? What are the consequences ?

▷ **1-5** One considers now a subvolume D smaller than L, and one is interested in the fluctuations in particle number within this volume, more precisely in $(\langle N^2\rangle - \langle N\rangle^2)/\langle N\rangle$. Relate this quantity to the function $h(\mathbf{r}) = g(\mathbf{r}) - 1$ for an infinite system ($L \to \infty$) and then for a finite system of size L. Discuss the finite size corrections for this quantity.

2 Thermal fluctuations of a 1D chain

▷ **2-1** Let us consider a perfect 1D regular lattice of N particles separated by a distance d at zero temperature. Calculate $\rho(\mathbf{k})$ and deduce from this the structure factor of the chain.

▷ **2-2** Discuss the shape of the structure factor in the thermodynamic limit when $N \to \infty$.

▷ **2-3** Now we raise the temperature of the chain. Justify that the 1D cristal can not stay perfect but that defects will appear due to thermal fluctuations of the particles within the chain. It is convenient to describe the positions of the particles of this now imperfect lattice by $\mathbf{r}_i = id + \mathbf{u}_i$, where $\mathbf{u}_i$ is the displacement of each particle with respect to its position in the perfect lattice. Write the expression of the structure factor for such a lattice at fine temperature assuming that particles interact with their neighbors through an harmonic potential.

3 Structure factor near a critical point

▷ **3-1** We now go back to the general situation in 3D, but we consider the behavior of the structure factor near a critical point. Justify that for this case, the pair correlation function $g(r)$ for 2 points separated by a distance r scales as $r^{-(1+\eta)}$ for r sufficiently small. Deduce from this, the behavior of $S(\mathbf{k})$ at large $\mathbf{k}$.