ICFP M2 - Statistical physics 1 – TD n° 7
Crystalline order in low dimensions

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The goal of this tutorial is to illustrate the importance of thermal fluctuations in low dimensional systems. Indeed, as we will see, thermal fluctuations in dimension $d = 1$ and $d = 2$ are much stronger than in three dimensions. This fact that thermal fluctuations destroy long-range order in (short range) interacting systems was first realized by R. Peierls. Here, we will show that, in agreement with Peierl's argument, there can not exist any long range crystalline order in one and two dimensions. This tutorial was inspired by the lectures given by J. Dalibard at Collège de France [1].

1 Peierl's argument in dimension $d = 1$

We consider an infinite one-dimensional chain of atoms, whose positions are denoted by x_i (where i is the label of the atom). They are ordered such that $\ldots < x_{j-1} < x_j < x_{j+1} < \cdots$. We assume that the interactions are between nearest neighbors only (interactions are usually short-ranged in solids) and described by a potential $U(x)$ such that the total energy of interactions reads

$$V_{\rm int} = \sum_{i\in\mathbb{Z}} U(x_{j+1} - x_j) \; . \tag{1}$$

We suppose that $U(x)$ has a single minimum at $x = a$ such that at $T = 0$ the atoms form a perfect one-dimensional lattice with lattice spacing a. The goal is now to understand the effects of finite temperature $T > 0$.

1.1 Heuristics

Before doing a complete exact computation, we first build a simple heuristic argument. Suppose that x_0 is fixed, and we define δ_j as the displacement of the j-th atom from its $T = 0$ equilibrium position, i.e.

$$x_j = x_{j-1} + a + \delta_j \; . \tag{2}$$

We assume that the δ_j's are small and independent from each other.

1. Obtain the estimate

$$\langle \delta_j^2 \rangle \sim \frac{k_B\, T}{\kappa} \; , \text{with } \kappa = U''(a) \; , \tag{3}$$

   where here (and in the following), $\langle \cdots \rangle$ denotes an average over thermal fluctuations.

2. We define Δ_j as

$$x_j = x_0 + j\, a + \Delta_j \; . \tag{4}$$

   Show that $\Delta_j^2 \sim (k_B\, T/\kappa)\, j$.

3. Deduce from the previous question that the crystalline order is lost for $j \geq \kappa a^2/(k_B T)$.

1.2 The classical harmonic chain

We now assume that $|x_{j+1} - x_j - a| \ll a$ and we denote by u_j the displacement of the j-th atom from its $T = 0$ equilibrium position $X_j = ja$, i.e.

$$x_j = u_j + X_j \ . \tag{5}$$

We restrict ourselves to small deviations around the $T = 0$ equilibrium configuration and write the total energy of the system (kinetic + interactions) of N atoms as

$$E_{1d} = \sum_{j=1}^{N} \left[\frac{1}{2} m \dot{u}_j^2 + \frac{\kappa}{2} (u_{j+1} - u_j)^2 \right] \ , \tag{6}$$

where m is the mass of the atoms and κ is defined in (3). It is useful to consider a system with a finite number N of atoms with periodic boundary conditions, i.e. $u_{N+1} \equiv u_1$. For simplicity we consider N even and decompose u_j in Fourier modes $\hat{u}_q$ as

$$u_j = \frac{1}{\sqrt{N}} \sum_q e^{iqX_j} \hat{u}_q \tag{7}$$

where the sum over q runs over $q = -\frac{\pi}{a}, \cdots, -\frac{2\pi}{Na}, 0, +\frac{2\pi}{Na}, \cdots, \frac{\pi}{a}$ (this is where we used that N is even).

1. Show that the total energy E_{1d} in (6) reads, in terms of $\hat{u}_q$

$$E_{1d} = \sum_q \left[\frac{1}{2} m \, \dot{\hat{u}}_q \, \dot{\hat{u}}_{-q} + \frac{1}{2} m \, \omega_q^2 \hat{u}_q \hat{u}_{-q} \right] \ , \ \text{ with } \ \omega_q = 2 \frac{\kappa}{m} |\sin \frac{q\,a}{2}| \ . \tag{8}$$

2. At equilibrium, show that the correlations between the Fourier modes is given by

$$\langle \hat{u}_q \, \hat{u}_{q'} \rangle = \frac{k_B T}{m \omega_q^2} \delta_{q',-q} \ . \tag{9}$$

3. Compute the 2-point correlations of the displacements $\langle (u_j - u_0)^2 \rangle$ and show that

$$\langle (u_j - u_0)^2 \rangle = \frac{k_B \, T}{m} \frac{4}{N} \sum_{\mathbf{q}} \frac{\sin^2(qX_j/2)}{\omega_q^2} \tag{10}$$

which, in the limit $N \to \infty$ can be written as

$$\langle (u_j - u_0)^2 \rangle \sim C_{1d}(j) \ , \ C_{1d}(j) = 4 \frac{k_B T a}{m} \int_{-\pi/a}^{\pi/a} \frac{\sin^2(qX_j/2)}{\omega_q^2} \, \frac{dq}{2\pi} \ . \tag{11}$$

The segment $[-\pi/a, +\pi/a]$ corresponds to what is usually called the first Brillouin zone.

4. Obtain finally that for $j \gg 1$

$$C_{1d}(j) \sim \frac{k_B T}{\kappa} \, j \ , \tag{12}$$

in agreement with the above heuristic argument.

2 Two-dimensional crystals

We now discuss the case of two-dimensional crystals and consider a two-dimensional version of the model in (6). In this case, at $T = 0$, the atoms stay at the sites of a $2d$ square lattice of lattice spacing a, indexed by $\boldsymbol{j} = (j_x, j_y)$ where $j_x = 0, 1, \cdots, N$ and $j_y = 0, 1, \cdots N$ (with N even, for simplicity). The equilibrium position of the atoms is labeled by $\mathbf{R}_{\boldsymbol{j}} = a(j_x \hat{\mathbf{x}}_x + j_y \hat{\mathbf{y}})$ where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors in the x and y directions respectively. As done before in the $1d$ case, we consider periodic boundary conditions both in the x and y directions (the system is thus defined on a torus). At $T > 0$, the position of the atoms is labelled by $\mathbf{r}_{\boldsymbol{j}}$ which is conveniently parameterized by the displacement $\mathbf{u}_j$ with respect to the equilibrium positions, i.e.

$$\mathbf{r}_{\boldsymbol{j}} = \mathbf{R}_{\boldsymbol{j}} + \mathbf{u}_{\boldsymbol{j}} \ . \tag{13}$$

As in the $1d$ model (1), we consider nearest neighbor interactions (between two neighboring sites $\boldsymbol{j}$ and $\boldsymbol{j}'$). In the limit where $|\mathbf{u}_{\boldsymbol{j}} - \mathbf{u}_{\boldsymbol{j}'}| \ll a$, we can restrict ourselves to the following harmonic model

$$E_{2d} = \sum_{\boldsymbol{j}} \frac{1}{2} m \dot{\mathbf{u}}_{\boldsymbol{j}}^2 + \sum_{\langle \boldsymbol{j}, \boldsymbol{j}' \rangle} \frac{\kappa}{2} (\mathbf{u}_{\boldsymbol{j}} - \mathbf{u}_{\boldsymbol{j}'})^2 \ , \tag{14}$$

where $\sum_{\langle \boldsymbol{j}, \boldsymbol{j}' \rangle}$ stands for a sum over all pairs of sites, indexed by the vectors $(\boldsymbol{j}, \boldsymbol{j}')$, which are nearest neighbors.

2.1 Correlation functions

1. Following the rationale developed for $d = 1$, show that, at equilibrium, the 2-point correlation is given by

$$\langle (\mathbf{u}_{\boldsymbol{j}} - \mathbf{u}_{\mathbf{0}})^2 \rangle = \frac{8 k_B T}{m N^2} \sum_{\mathbf{q} = (q_x, q_y)} \frac{\sin^2(\mathbf{q} \cdot \mathbf{R}_{\boldsymbol{j}}/2)}{\omega_{\mathbf{q}}^2} \ , \text{ with } \ \omega_{\mathbf{q}}^2 = \frac{\kappa}{m} (4 - 2\cos(q_x\, a) - 2\cos(q_y\, a)) \ , \tag{15}$$

   where the sum over $\mathbf{q}$ runs over $q_x = -\frac{\pi}{a}, \cdots, -\frac{2\pi}{Na}, 0, +\frac{2\pi}{Na}, \cdots, \frac{\pi}{a}$ and similarly for q_y.

2. In the large N limit obtain that

$$\langle (\mathbf{u}_{\boldsymbol{j}} - \mathbf{u}_{\mathbf{0}})^2 \sim C_{2d}(\boldsymbol{j}) \ , \tag{16}$$

   with

$$C_{2d}(\boldsymbol{j}) = \frac{8 k_B T a^2}{m} \int_{ZB} \frac{\sin^2(\mathbf{q} \cdot \mathbf{R}_{\boldsymbol{j}}/2)}{\omega_{\mathbf{q}}^2} \frac{d^2 q}{(2\pi)^2} \tag{17}$$

   where $\int_{ZB}$ denotes the integral over the first $2d$ Brillouin zone, i.e. $(q_x, q_y) \in [-\pi/a, +\pi/a] \times [-\pi/a, +\pi/a]$

3. Show that for $|\boldsymbol{j}| \gg 1$, the $2d$ correlation function behaves as

$$C_{2d}(\boldsymbol{j}) \sim \frac{2}{\pi} \frac{k_B T}{\kappa} \ln \left(\frac{|\mathbf{R}_{\boldsymbol{j}}|}{a} \right) \ , \tag{18}$$

   and compare with the $1d$ result for C_{1d} in Eq. (12).

4. What would be the corresponding result in dimension $d = 3$? Comments.

2.2 Bragg peaks and quasi-order

To test experimentally the presence of crystalline order, a standard approach is to measure the diffraction of a wave (photon, phonon, electrons, neutrons, etc) with an incidental wave vector $\mathbf{k}_i$. For a perfect crystal spanned by the two vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, one expects to observe so called "Bragg peaks" in the directions $\mathbf{k} = \mathbf{k}_i + \mathbf{Q}$ where $\mathbf{Q} \cdot \hat{\mathbf{x}} \equiv 0 \bmod 2\pi$ as well as $\mathbf{Q} \cdot \hat{\mathbf{y}} \equiv 0 \bmod 2\pi$ (in other words, $\mathbf{Q}$ belongs to the reciprocal lattice). We want to investigate what is the fate of these Bragg peaks in presence of thermal fluctuations.

The starting point of our analysis is the expression of the diffracted intensity along the $\mathbf{k}$-direction which is given by

$$I(\mathbf{k}) = \left\langle \Big| \sum_{\boldsymbol{j}} e^{i\mathbf{k}\cdot(\mathbf{R}_{\boldsymbol{j}}+\mathbf{u}_{\boldsymbol{j}})} \Big|^2 \right\rangle , \tag{19}$$

where the sum over $\boldsymbol{j}$ runs over all the sites of the $2d$ lattice. From now on, we work with the infinite system, corresponding to the limit $N \to \infty$ of the system with periodic boundary conditions studied above.

1. Using the fact that the fluctuations of the positions $\mathbf{u}_{\boldsymbol{j}}$ are Gaussian, show that

$$I(\mathbf{k}) = N \sum_{\boldsymbol{j}\in\mathbb{Z}^2} e^{i\mathbf{k}\cdot\mathbf{R}_{\boldsymbol{j}}} \exp\left(-\frac{k^2}{4} \langle (\mathbf{u}_{\boldsymbol{j}} - \mathbf{u}_{\mathbf{0}})^2 \rangle \right) . \tag{20}$$

2. At $T = 0$ show that $I(\mathbf{k})$ is a sum of Dirac-delta peaks, the so called "Bragg-peaks" (for simplicity suppose that the incidental wave-vector $\mathbf{k}_i$ is orthogonal to the plane).

3. Using Poisson summation formula, show that

$$I(\mathbf{k}) = N \sum_{\mathbf{Q}} \int d^2\mathbf{r}\, e^{i(\mathbf{k}-\mathbf{Q})\cdot\mathbf{r}} \exp\left(-\frac{k^2}{4} \langle (\mathbf{u}_{\boldsymbol{r}} - \mathbf{u}_{\mathbf{0}})^2 \rangle \right) , \tag{21}$$

   where the sum over $\mathbf{Q}$ runs over the vectors belonging to the reciprocal lattice. We recall that for a function f such that $|f|^2$ is integrable over $\mathbb{R}$, the Poisson summation formula states that

$$\sum_{n\in\mathbb{Z}} f(n) = \sum_{k\in\mathbb{Z}} \hat{f}(k) , \quad \text{where } \hat{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-2i\pi kx}\, dx . \tag{22}$$

4. Let $\mathbf{Q}^*$ be a specific vector belonging to the reciprocal lattice. Using the result in (18), together with (21), show that for $|\mathbf{k} - \mathbf{Q}^*| \ll a^{-1}$

$$I(\mathbf{k}) \sim \frac{1}{|\mathbf{k} - \mathbf{Q}^*|^{2-\eta_{\mathbf{Q}^*}}} , \quad \text{with} \quad \eta_{\mathbf{Q}^*} = \frac{(\mathbf{Q}^*)^2 k_B T}{2\pi\kappa} . \tag{23}$$

   Such algebraic singularities (at variance with delta peaks) are associated to the notion of "quasi-order".

References

[1] J. Dalibard, *Peierls et l'ordre cristallin en basse dimension*, `http://www.phys.ens.fr/~dalibard/CdF/2017/notes_cours_1.pdf`