Crystal Symmetry and Time Scales

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Abstract

The relation between the notion of crystalline symmetry and characteristic time intervals when this symmetry could be observed is analyzed. Several time scales are shown to exist for a system of interacting particles. It is only when the observation time is much larger than the mesoscopic fluctuation time, the notion of crystalline symmetry becomes physically meaningful. The ideas are concretized by a two-phase lattice model.

1 Characteristic Time Scales

Crystalline symmetry is a well-defined geometric notion. But a crystal as such is a physical object consisting of many moving particles. In what sense these particles form a crystalline lattice with a given symmetry? An intuitive answer to this question would be that it is the average positions of particles which form a crystalline lattice, with the averaging performed over sufficiently large time. But, to be mathematically correct, it is necessary to concretize what does mean "sufficiently large" with respect to the observation time. The aim of this report is to demonstrate that the minimal time scale providing the lower threshold for the observation time is the mesoscopic fluctuation time.

There are several characteristic time scales for a system of interacting particles [1]. The smallest typical time is the interaction time

\[ \tau_{\text{int}} \sim \frac{a_s}{v}, \]  

(1)

in which \( a_s \) is an effective interaction radius, or effective particle size, or scattering length, and \( v \) is a characteristic particle velocity, say, sound velocity. When observing
a system of particles during an observation time $\tau_{obs}$ that is smaller than $\tau_{int}$, the motion of these particles looks absolutely random, with no preferable positions in space.

Another important scale is the local-equilibrium time

$$\tau_{loc} \sim \frac{\lambda}{v},$$

where $\lambda$ is a mean free path. The latter is connected with the scattering length $a_s$ and the average density of particles, $\rho$, as $\lambda \sim (\rho a_s^2)^{-1}$. The average density $\rho \sim a_0^{-3}$, with $a_0$ being a mean interparticle distance. Hence, $\lambda \sim a_0^3/a_s^2$, from where

$$\tau_{loc} \sim \left( \frac{a_0}{a_s} \right)^3 \tau_{int}. $$

During the local-equilibrium time, particles interact with each other, so that the state of local equilibrium is being evolved.

At a very short time $t$, one has the dynamic stage, when

$$0 < t < \tau_{int},$$

and particles move randomly. No spatial symmetry in the positions of particles can be noticed for the observation time in the diapason (4). The second time interval corresponds to the kinetic stage, when

$$\tau_{int} < t < \tau_{loc}. $$

At this stage, interparticle correlations begin arising due to interactions, but the overall motion looks yet rather disorganized, resembling the Brownian motion. In solids, $a_0$ is just slightly larger than $a_s$, so that the local-equilibrium time (3) is only a little longer than the interaction time, $\tau_{loc} \sim \tau_{int}$. The kinetic stage (5) is practically absent in solids. One has the hydrodynamic stage, when

$$\tau_{loc} < t < \infty. $$

It is at this stage when the averaged motion of particles is commonly assumed to define a crystalline lattice symmetry, under the appropriate external conditions.

However, in general, it is not the local-equilibrium time (3) that gives the lower threshold for the observation time, in order that the lattice symmetry be well defined. The actual lower threshold is much larger than $\tau_{loc}$. There exists one more time scale that can be called the mesoscopic fluctuation time

$$\tau_f \sim \frac{l_f}{a_0} \tau_{loc},$$

2
in which \( l_f \) is a linear size of a quasiequilibrium fluctuation [1]. The fluctuation is termed mesoscopic because of its intermediate size, being in the interval \( a_0 \ll l_f \ll L \), where \( L \) is a characteristic length of the system. Since \( l_f \gg a_0 \), one has \( \tau_f \gg \tau_{loc} \).

In this way, the hydrodynamic stage (6) consists of two qualitatively different parts. One is the *mesoscopic stage*, when

\[
\tau_{loc} < t < \tau_f .
\]  

(8)

Here, crystalline symmetry cannot yet be rigorously defined for the whole system, although the main part of the latter may already be approximately described by a kind of symmetry. At the *macroscopic stage*, when

\[
\tau_f < t < \infty ,
\]

(9)

the averaged motion of particles can be correctly characterized by assigning a concrete spatial symmetry. It is the mesoscopic fluctuation time (7) that defines the lower threshold for the observation time which is necessary for making the notion of symmetry physically meaningful. In this regard, sufficiently large observation time implies

\[
\tau_{obs} \gg \tau_f .
\]

(10)

Only averaging over the observation time satisfying the inequality (10) provides a mathematically correct definition of the related lattice symmetry.

## 2 Two-Phase Lattice Model

In order to exemplify the existence of mesoscopic fluctuations, let us consider a lattice model for which such fluctuations not only do exist but their presence makes the system more stable. Lattice models describe the physics of solids where an essential concentration of vacancies can arise. These vacancy defects appear in crystals with high anharmonicity. Among such objects, we could mention quantum crystals [2–6], crystallized plasma [7], crystallized white dwarfs [8], crystals near liquid-solid transition [1,9,10] and crystals close to vitrification [1,11]. Mesoscopic fluctuations of heterophase nature are common for liquid crystals [12].

It is worth noting that mesoscopic heterophase fluctuations exist not only in crystals but also in other materials. Thus, they are clearly observed by neutron scattering experiments in many magnetic alloys [13,14]. Even in such classical ferromagnets as Fe and Ni, there appears local magnetic order in their paramagnetic phase, which is also a sort of mesoscopic fluctuations [15,16]. Similar phenomena occurs in high-temperature superconductors where it is often termed phase separation [17–22]. More examples can be found in Ref. [1].

Now, let us turn to the lattice model to be analyzed in what follows. Consider a system of \( N \) particles in volume \( V \). Each particle can occupy one and only one
lattice site of a given crystalline lattice. Not all lattice sites are occupied, but some of them are vacant. The distribution of vacancies through the volume is not uniform. Some parts of the system contain more vacancies than other, which results in essentially different density of particles in the corresponding regions. The location and shapes of these parts with different density are not fixed, but fluctuate in space and time, forming a system with mesoscopic density fluctuations [23]. Thus, we have a heterophase system with coexisting dense and dilute phases. Such a system can serve as a cartoon of a crystal with regions of disorder [24].

Let us label the quantities related to the dense phase with the index 1 and those corresponding to the dilute phase, by the index 2. For instance, the average number of particles pertaining to the dense phase is \(N_1\), occupying the volume \(V_1\), while the average number of particles in the dilute phase is \(N_2\), inside the volume \(V_2\). The total number of particles and the system volume are conserved:

\[
N = N_1 + N_2, \quad V = V_1 + V_2.
\]  

(11)

Because of the presence of vacancies, the number of lattice sites, \(N_0\), is larger than the total number of particles \(N\). Hence, the density of sites is larger than that of particles:

\[
\rho_0 > \rho, \quad \rho_0 \equiv \frac{N_0}{V}, \quad \rho \equiv \frac{N}{V}.
\]  

(12)

By definition, the dense phase has a larger density of particles than the dilute phase:

\[
\rho_1 > \rho_2, \quad \rho_\nu \equiv \frac{N_\nu}{V_\nu} \quad (\nu = 1, 2).
\]  

(13)

Introducing the geometric probabilities of the corresponding phases,

\[
w_\nu \equiv \frac{V_\nu}{V}, \quad w_1 + w_2 = 1,
\]  

(14)

the mean density of particles can be written as

\[
\rho = w_1 \rho_1 + w_2 \rho_2.
\]  

(15)

For what follows, it is convenient to define the dimensionless densities

\[
n_\nu \equiv \frac{\rho_\nu}{\rho_0}, \quad n \equiv \frac{\rho}{\rho_0} = \frac{N}{N_0},
\]  

(16)

for which Eq. (15) reduces to

\[
n = w_1 n_1 + w_2 n_2.
\]  

(17)

A system with mesoscopic heterophase fluctuations is quasiequilibrium and has to be described by a quasiequilibrium Gibbs ensemble [1], with a statistical operator
\[ \rho(\xi) \sim e^{-Q(\xi)}, \] where \( Q(\xi) \) is a quasihamiltonian and the set \( \xi = \{\xi_{i}(r)\} \) of manifold indicators characterizes a distribution of phases in space. This phase distribution is frozen at the mesoscopic stage (8), when no lattice symmetry can be defined. Going to the macroscopic stage (9) implies averaging over all phase configurations. This averaging can be defined [1] as functional integration over the set \( \xi = \{\xi_{\nu}(r)\} \) of the manifold indicator functions. In the process of that integration, the notion of the heterophase Hamiltonian \( \overline{H} \) arises, defined by the relation

\[ \int e^{-Q(\xi)} \mathcal{D}\xi \equiv e^{-\beta \overline{H}}, \] \hspace{1cm} (18)

in which \( \beta \equiv T^{-1} \) is inverse temperature, \( k_B \equiv 1 \). From Eq. (18), one has

\[ \overline{H} = -T \ln \int e^{-Q(\xi)} \mathcal{D}\xi. \] \hspace{1cm} (19)

The \( i \)-site of the lattice, pertaining to the part filled by the \( \nu \)-phase, is characterized by the variable \( e_{i\nu} \), taking the value \( e_{i\nu} = 1 \) if the site is occupied by a particle and the value \( e_{i\nu} = 0 \) when the site is empty. For the heterophase Hamiltonian (19), we obtain

\[ \overline{H} = H_{1} \oplus H_{2}, \] \hspace{1cm} (20)

which is a sum of the phase-replica Hamiltonians

\[ H_{\nu} = w_{\nu} \sum_{i=1}^{N_{0}} (K_{i} - \mu) e_{i\nu} + \frac{1}{2} w_{\nu}^{2} \sum_{i \neq j}^{N_{0}} \Phi_{ij} e_{i\nu} e_{j\nu}, \] \hspace{1cm} (21)

where \( K_{i} \) is kinetic energy; \( \mu \), chemical potential; and \( \Phi_{ij} \) is interaction potential. The phase probabilities \( w_{\nu} \) are defined from the minimization of the thermodynamic potential

\[ y = -\frac{1}{N} \ln \operatorname{Tr} e^{-\beta \overline{H}}, \] \hspace{1cm} (22)

in which, for taking account of the normalization \( w_{1} + w_{2} = 1 \), it is convenient to introduce

\[ w \equiv w_{1} \quad w_{2} \equiv 1 - w. \] \hspace{1cm} (23)

Then \( w \) is given by the equations

\[ \frac{\partial y}{\partial w} = 0, \quad \frac{\partial^{2} y}{\partial w^{2}} > 0. \] \hspace{1cm} (24)

In terms of the occupation operators \( e_{i\nu} \), the densities (13) are

\[ \rho_{\nu} = \frac{1}{V} \sum_{i=1}^{N_{0}} < e_{i\nu} >, \] \hspace{1cm} (25)
where $< \ldots >$ implies the statistical averaging, and the densities (16) become

$$n_\nu = \frac{1}{N_0} \sum_{i=1}^{N_0} < e_{i\nu} > .$$

(26)

Recall that, by definition, $\nu = 1$ corresponds to the dense phase while $\nu = 2$, to the dilute phase, so that $\rho_1 > \rho_2$ and $n_1 > n_2$.

It is possible to pass to quasispin representation by introducing the variable $\sigma_{i\nu} = \pm 1$, defined by the relations

$$\sigma_{i\nu} \equiv 2e_{i\nu} - 1, \quad e_{i\nu} = \frac{1}{2}(1 + \sigma_{i\nu}) .$$

(27)

Then the Hamiltonian (21) takes the form

$$H_\nu = U_\nu + \frac{1}{8} w_\nu^2 \sum_{i \neq j}^{N_0} \Phi_{ij} \sigma_{i\nu} \sigma_{j\nu} - \frac{1}{2} w_\nu \sum_{i=1}^{N_0} h_{i\nu} \sigma_{i\nu} ,$$

(28)

where

$$U_\nu \equiv \frac{1}{2} w_\nu \sum_{i=1}^{N_0} (K_i - \mu) + \frac{1}{8} w_\nu^2 \sum_{i \neq j}^{N_0} \Phi_{ij} ,$$

$$h_{i\nu} \equiv \mu - K_i = \frac{1}{2} w_\nu \frac{1}{N_0} \sum_{i \neq j}^{N_0} \Phi_{ij} .$$

The form (28) corresponds to the Ising model in an external field.

To accomplish concrete calculations, let us consider the Kac-type interaction potential $\Phi_{ij} = \Phi_{ij}(N_0)$, for which

$$\lim_{N_0 \to \infty} \Phi_{ij}(N_0) = 0 , \quad \lim_{N_0 \to \infty} \left| \frac{1}{N_0} \sum_{i \neq j}^{N_0} \Phi_{ij}(N_0) \right| < \infty .$$

(29)

For this kind of potentials, the problem as is known [25], can be solved asymptotically exactly in the thermodynamic limit, when $N_0 \to \infty$, $V \to \infty$, so that $N_0/V \to const$. In the case of such long-range potentials, the mean-field decoupling

$$< \sigma_{i\nu} \sigma_{j\nu} > = \delta_{ij} + (1 - \delta_{ij}) < \sigma_{i\nu} > < \sigma_{j\nu} >$$

(30)

becomes asymptotically exact.

### 3 Numerical Results and Conclusions

With the decoupling (30), we can calculate all thermodynamic characteristics of the model. In terms of the occupation operators $e_{i\nu}$, this decoupling is equivalent to the equality

$$< e_{i\nu} e_{j\nu} > = \frac{1}{2} \delta_{ij}( < e_{i\nu} > + < e_{j\nu} > ) + (1 - \delta_{ij}) < e_{i\nu} > < e_{j\nu} > .$$
Calculations result in a system of transcendental equations which we have analyzed numerically. Dimensionless densities $n_1 \equiv a$, $n_2 \equiv b$, $(a > b)$, as functions of temperature $T$, in units of $\Phi \equiv \frac{1}{N_0} \sum_{i \neq j}^{N_0} \Phi_{ij}$, are presented in Fig. 1, for different mean densities. Note that from the condition of heterophase stability, that is the second of Eqs. (24), it follows that $\Phi > 0$. Fig. 2 shows the probability of the dense phase vs. temperature. The shifted chemical potential $\mu_*$, defined by the equations $\mu_* \equiv \frac{\mu - K}{\Phi}$, $K \equiv \frac{1}{N_0} \sum_{i=1}^{N_0} K_i$, is given in Fig. 3. The pressure, $P$, specific heat, $C_V$, and isothermal compressibility, $\kappa_T$, are shown in Figs. 4 to 6, respectively. All curves in Figs. 1 to 6 end at the points where the probability of the dense phase becomes zero, after which the heterophase system looses its stability, since the phase probabilities, by definition, must be always positive. Finally, in Fig. 7, the thermodynamic potential $\omega_w \equiv \frac{yT}{\Phi}$ is drawn for the case of the heterophase system and also this potential, $\omega_1$, for the pure dense system when $w = 1$. As is seen, one always has $\omega_w < \omega_1$, which means that the heterophase system is thermodynamically more stable than the pure system.

In this way, a heterophase system, exhibiting mesoscopic fluctuations, is thermodynamically more stable than a pure system without these fluctuations. At the same time, the existence of mesoscopic fluctuations implies the occurrence of local instability [1]. In the present case, such instabilities are related to the fluctuational grouping of vacancies in some parts of the system, which forms fluctuating disordered regions locally destroying crystalline symmetry. It is only for large observation times, satisfying the inequality (10), when the system displays, on average, a perfect symmetry of the lattice, while for times shorter than the lifetimes of mesoscopic fluctuations, an ideal lattice symmetry cannot be observed. However, such a temporal breaking of symmetry makes the system more stable in the long run.

The results exemplified here by a lattice model can be generalized to other physical systems. To our mind, the same conclusions concern not only simple physical systems but, even to a greater extent, all complex systems, such as societies. Thus, a society allowing the occurrence of mesoscopic fluctuations can be called democratic, while that one prohibiting any deviation from the prescribed symmetry is dictatorial. In the long run, democracy is more stable than dictatorship.
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Figure Captions

**Fig. 1.** The density of the dense phase (solid curve) and of the dilute phase (dashed curve) as functions of temperature.

**Fig. 2.** The probability of the dense phase vs. temperature.

**Fig. 3.** The shifted chemical potential vs. temperature.

**Fig. 4.** The dimensionless pressure vs. temperature.

**Fig. 5.** Specific heat vs. temperature.

**Fig. 6.** Isothermal compressibility vs. temperature.

**Fig. 7.** Dimensionless thermodynamic potentials for the heterophase system (two lower curves) and for the pure dense system (two upper curves).