ON THE IMPOSSIBILITY OF CRYSTALLINE ORDERING

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Abstract

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E. M. SOROKINA

ON THE IMPOSSIBILITY OF CRYSTALLINE ORDERING

IN ONE- AND TWO-DIMENSIONAL CLASSICAL SYSTEMS

(Presented by Academician N. N. Bogolyubov, 21 V 1969)

The concept of the separation of a state of statistical equilibrium, introduced by N. N. Bogolyubov ([1]) in the statistical mechanics of quantum systems, is evidently also applicable in classical statistical mechanics. In this case the quasi-averages of the corresponding dynamical quantities $A(p, q)$, understood as

$$\lim_{\nu\to 0} \int A(p,q) \exp\left[-\frac{\mathcal{H}_\nu(p,q)}{\theta}\right] dp\, dq \Big/ \int \exp\left[-\frac{\mathcal{H}_\nu(p,q)}{\theta}\right] dp\, dq = \langle A\rangle, \quad (1)$$

where $\mathcal{H}_\nu(p, q) = \mathcal{H} + \nu\mathcal{H}'$ is the Hamiltonian of the system with an included external field that removes the degeneracy; $p = \{p_1, \dots, p_N\}$; $q = \{q_1, \dots, q_N\}$ are canonically conjugate variables, and the limiting transition $\nu \to 0$ is performed after the limiting statistical transition $N \to \infty$, $V \to \infty$, $N/V \to n = \text{const}$.

We shall consider the problem of the existence of crystalline ordering in one- and two-dimensional classical systems described by the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{\substack{i,j=1\\ i\neq j}}^{N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|), \quad (2)$$

where $p_i, \mathbf{r}_i$ are the momentum and coordinate of the i-th particle, and $\Phi(|\mathbf{r}_i - \mathbf{r}_j|)$ is the pair-interaction potential.

An analogous problem for a one-dimensional quantum system was considered by us in ([2]).

In the proof given below we shall rely on an inequality that is a classical analogue of the N. N. Bogolyubov inequality ([1]), obtained in ([3]) with the aid of the classical Green functions introduced in ([4]). Another derivation of the classical inequality is given in ([5]), where it is illustrated by the example of a classical Heisenberg ferromagnet.

Introduce the local density of the number of particles

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

and its Fourier transform ρ_q by the relation

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_q \rho_q \exp(-i\mathbf{q} \cdot \mathbf{r}); \qquad \rho_q = \int \rho(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r})\, d\mathbf{r} = \sum_{i=1}^{N} \exp(i\mathbf{q} \cdot \mathbf{r}_i). \tag{3}$$

In the presence of a separated state of statistical equilibrium—crystalline ordering—the quasi-average $\langle \rho(\mathbf{r}) \rangle$ is a quantity periodic with the lattice period, i.e., there exists a vector $\mathbf{G} \neq 0$ from the set of reciprocal-lattice vectors for which the quasi-average is nonzero—

$\langle \rho_G / V \rangle$. The indicated degeneracy, as is well known, is connected with the law of conservation of momentum, or, equivalently, with the translational invariance of the Hamiltonian (2).

We next introduce the local momentum-density quantity $\mathbf{j}(\mathbf{r})$ and its Fourier transform $\mathbf{j}_q$:

$$\mathbf{j}(\mathbf{r}) = \sum_{i=1}^{N} \mathbf{p}_i \delta(\mathbf{r} - \mathbf{r}_i) = \frac{1}{V} \sum_q \mathbf{j}_q \exp(-i\mathbf{q} \cdot \mathbf{r}),$$

$$\mathbf{j}_q = \int \mathbf{j}(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r})\, d\mathbf{r} = \sum_{i=1}^{N} \mathbf{p}_i \exp(i\mathbf{q} \cdot \mathbf{r}_i).$$

The classical analogue of Bogoliubov' s inequality has the form (3):

$$\langle B^* B \rangle \geq \theta\, |\langle \{Q, B\} \rangle|^2 / |\langle \{Q, \{Q^*, \mathcal{H}\}\} \rangle|, \tag{4}$$

where $B(p, q)$, $Q(p, q)$ are certain dynamical quantities; $\{...\}$ denotes the Poisson brackets:

$$\{A, B\} = \sum_{i=1}^{N} \left[\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right],$$

θ is the temperature in energy units.

We shall consider this inequality for the dynamical quantity B

$$B = \rho_{k+\mathbf{G}} = \sum_{i=1}^{N} \exp[i(\mathbf{k}+\mathbf{G},\mathbf{r}_i)], \qquad B^* = \sum_{i=1}^{N} \exp[-i(\mathbf{k}+\mathbf{G},\mathbf{r}_i)] = \rho_{-\mathbf{k}-\mathbf{G}}, \tag{5}$$

choosing as Q the quantity

$$Q = \left(\frac{\mathbf{k}}{k}\cdot\mathbf{j}_{-\mathbf{k}}\right) = \sum_{i=1}^{N}\left(\frac{\mathbf{k}}{k}\cdot\mathbf{p}_i\right)\exp(-i\mathbf{k}\cdot\mathbf{r}_i), \tag{6}$$

$$Q^* = \left(\frac{\mathbf{k}}{k}\cdot\mathbf{j}_{k}\right) = \sum_{i=1}^{N}\left(\frac{\mathbf{k}}{k}\cdot\mathbf{p}_i\right)\exp(i\mathbf{k}\cdot\mathbf{r}_i),$$

which is an "almost integral of motion" in the sense of (2). With respect to the vector $\mathbf{G}$ we assume, in accordance with what was said above, that $\langle\rho_G/V\rangle \neq 0$.

Calculating the Poisson brackets for the corresponding dynamical quantities, substituting them into (4), and dividing by N, so that all terms of the inequality are of zeroth order in N, we obtain:

$$\left\langle \frac{1}{N}\sum_{\substack{i,j\\ i\neq j}} \exp[i(\mathbf{k}+\mathbf{G},\mathbf{r}_i-\mathbf{r}_j)]\right\rangle + 1 \geq \left\{\theta\left(\frac{\mathbf{k}}{k},\mathbf{k}+\mathbf{G}\right)^2 \left|\int_{(v)}\langle\rho(\mathbf{r})\rangle e^{-i\mathbf{G}\mathbf{r}}\,d\mathbf{r}\right|^2\right\}\times$$

$$\times\left\{\left[\left\langle\frac{1}{N}\sum_{i=1}^{N}\frac{3(\mathbf{p}_i\cdot\mathbf{k})^2}{m}\right\rangle + \left\langle\frac{1}{N}\sum_{\substack{i,j\\ i\neq j}}(1-\cos(\mathbf{k},\mathbf{r}_i-\mathbf{r}_j))\right.\right.\right.$$

$$\left.\left.\left.\times\left(\frac{\mathbf{k}}{k}\cdot\frac{\partial}{\partial(\mathbf{r}_i-\mathbf{r}_j)}\right)^2\Phi(|\mathbf{r}_i-\mathbf{r}_j|)\right\rangle\right]\right\}^{-1} =$$

$$= \frac{\theta\left(\frac{\mathbf{k}}{k},\mathbf{k}+\mathbf{G}\right)^2 v^2\left|\langle\frac{\rho_G}{V}\rangle\right|^2}{3k^2\theta + \int_{(v)} d\mathbf{R}\int_{(V)} d\mathbf{r}\,\widetilde{D}_2(\mathbf{R},\mathbf{r})\,(1-\cos(\mathbf{k}\cdot\mathbf{r}))\left(\frac{\mathbf{k}}{k}\cdot\nabla\right)^2\Phi(\mathbf{r})}. \tag{7}$$

where

$$\widetilde{D}_2((\mathbf{r}_1+\mathbf{r}_2)/2, \mathbf{r}_1-\mathbf{r}_2) =$$

$$= D_2(\mathbf{r}_1, \mathbf{r}_2) = \left\{ N(N-1) \int \exp[-H(p,q)/\theta]\, dp\, \frac{dq}{d\mathbf{r}_1 d\mathbf{r}_2} \right\} \times$$

$$\times \left\{ \iint \exp\left[-\frac{H(p,q)}{\theta}\right] dp\, dq \right\}^{-1}$$

is the pair correlation function, periodic in the first argument with the lattice period; $v = V/N$ is the volume of the elementary cell of a simple lattice.

The inequality written above is analogous to that obtained in work ([2]) for a quantum system. Multiplying it by a positive function $h(\mathbf{k}) = h(k)$:

$$h(k) = \frac{1}{(2\pi)^d} \int \mathcal{H}(r) \exp(-i\mathbf{k}\cdot\mathbf{r})\, d\mathbf{r}; \qquad \mathcal{H}(r) = \int h(k) \exp(-i\mathbf{k}\cdot\mathbf{r})\, d\mathbf{r}$$

($d = 1, 2, 3$ is the dimensionality of the system), localized in the neighborhood of $\mathbf{k} = 0$, so that $\mathcal{H}(r)$ is a monotonically decreasing function of r, we integrate the resulting inequality over all $\mathbf{k}$:

$$\int dk\, h(k) \left\langle \frac{1}{N} \sum_{i \neq j} \exp[i(\mathbf{k}+\mathbf{G}, \mathbf{r}_i + \mathbf{r}_j)] \right\rangle + \mathcal{H}(0) \geq$$

$$\geq \theta v^2 \left| \left\langle \frac{\rho_G}{V} \right\rangle \right|^2 \int \frac{dk\, h(k)(\mathbf{k}/k, \mathbf{k}+\mathbf{G})^2}{3k^2\theta + \int_{(v)} d\mathbf{R} \int_{(V)} d\mathbf{r}\, \widetilde{D}_2(\mathbf{R}, \mathbf{r})(1-\cos(\mathbf{k}\cdot\mathbf{r})) \left(\frac{\mathbf{k}}{k}\cdot\nabla\right)^2 \Phi(r)}. \tag{8}$$

The integral over $\mathbf{k}$ on the right-hand side diverges in the one- and two-dimensional cases. The left-hand side has the form

$$\left\langle \frac{1}{N} \sum_{\substack{i,j \\ i \neq j}} \exp[i(\mathbf{G}, \mathbf{r}_i - \mathbf{r}_j)] \mathcal{H}(|\mathbf{r}_i - \mathbf{r}_j|) \right\rangle + \mathcal{H}(0). \tag{9}$$

Repeating verbatim the reasoning of ([2]), we see that in the one-dimensional case it is bounded by the quantity $2\pi h(0)/2a + \mathcal{H}(0)$, where a is some constant such that $\alpha/a = 1/\varkappa \ll 1$; a is the lattice spacing.

Let us now show how the left-hand side of (8) can be estimated in the two-dimensional case. (Without loss of generality we shall assume that the two-dimensional lattice is square, with spacing a.) As is known, consideration of a crystal lattice by an approach based on perturbation theory (the harmonic approximation) assumes the deviations of atoms from their equilibrium positions to be small. We use a weaker assumption: assuming, as in the one-dimensional case, that neighboring atoms cannot approach to a distance smaller than some fixed $\alpha = a/\varkappa$, where $\varkappa$ may be large: $|\mathbf{r}_i - \mathbf{r}_{i+1}| \geq \alpha$, we shall suppose that arbitrary atoms i, j cannot approach each other by more than the equilibrium distance between them divided by $\varkappa = a/\alpha$. Numbering the atoms of the square lattice by indices $i = (i_1, i_2)$, $j = (j_1, j_2)$, we write this condition in the form

$$|\mathbf{r}_i - \mathbf{r}_j| \equiv |\mathbf{r}_{(i_1,i_2)} - \mathbf{r}_{(j_1,j_2)}| \geq$$

$$\geq \frac{1}{\varkappa}\sqrt{a^2(i_1-j_1)^2 + a^2(i_2-j_2)^2} = \alpha\sqrt{(i_1-j_1)^2 + (i_2-j_2)^2}, \qquad (10)$$

With the aid of (10) we estimate (9):

$$\left\langle \frac{1}{N}\sum_{\substack{i,j\\ i\neq j}} \exp[-i(\mathbf{G}, \mathbf{r}_i - \mathbf{r}_j)]\mathcal{H}(|\mathbf{r}_i - \mathbf{r}_j|) \right\rangle + \mathcal{H}(0) \leq$$

$$\leq \frac{1}{N}\sum_{(i_1,i_2)\neq(j_1,j_2)} \mathcal{H}\left(\alpha\sqrt{(i_1-j_1)^2 + (i_2-j_2)^2}\right) + \mathcal{H}(0) \leq$$

$$\leq \int_0^\infty\int_0^\infty \mathcal{H}\left(\alpha\sqrt{x^2+y^2}\right)\,dx\,dy + \mathcal{H}(0) = \frac{(2\pi)^2}{4\alpha^2}\,h(0) + \mathcal{H}(0).$$

Thus, the left-hand side of (8) is bounded above by the quantity $\frac{(2\pi)^2}{(2a)^2}\,h(0) + \mathcal{H}(0)$, whence, analogously to how this was done in (2) for the one-dimensional case, we conclude that the quasi-average $\langle \rho_{\mathbf{G}}/V\rangle$ is equal to zero at a temperature θ different from zero, i.e., that crystalline ordering is impossible in a two-dimensional system. The arguments presented apply fully also to the two-dimensional quantum case, since they rely only on the form of inequality (7), analogous to that obtained in (2).

Let us note that the integral over $\mathbf{k}$ on the right-hand side of (8) in a two-dimensional system diverges logarithmically and is of order $\ln N$ with respect to N as $N \to \infty$, which indicates the possibility of the existence of submacroscopic crystalline flakes, the number N in which may be very large.

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Mathematical Institute named after V. A. Steklov
Academy of Sciences of the USSR
Moscow

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Note: Figure translations are in progress. See original paper for figures.