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B. I. SADOVNIKOV, E. M. SOROKINA

ON THE IMPOSSIBILITY OF CRYSTALLINE ORDERING IN ONE-DIMENSIONAL QUANTUM SYSTEMS

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N. N. Bogolyubov' s theorem on a singularity of the type $1/k^2$ (1) is one of the effective methods for studying systems with broken symmetry (2). Recently, in a number of works, N. N. Bogolyubov' s inequality has been applied to prove the impossibility of phase transitions in certain one- and two-dimensional systems (3,4). In the present paper we consider a proof of the impossibility of crystalline ordering in one-dimensional quantum systems, based on N. N. Bogolyubov' s inequality.

Consider a dynamical system of N identical Bose or Fermi particles contained in a volume V, whose Hamiltonian has the form:

$$H = -\frac{1}{2m}\int_{(V)} \psi^+(\mathbf{r})\Delta\psi(\mathbf{r})\,d\mathbf{r} - \lambda\int_{(V)} \psi^+(\mathbf{r})\psi(\mathbf{r})\,d\mathbf{r} +$$

$$+\frac{1}{2}\int_V \psi^+(\mathbf{r}_1)\psi^+(\mathbf{r}_2)\Phi(|\mathbf{r}_1-\mathbf{r}_2|)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)\,d\mathbf{r}_1\,d\mathbf{r}_2, \qquad (1)$$

where λ is the chemical potential; $\Phi(|\mathbf{r}_1-\mathbf{r}_2|)$ is the interaction potential of a pair of particles; $V = L^d$ is the volume of the system; $d = 1, 2, 3$ is its dimensionality. The field operators $\psi(\mathbf{r})$, $\psi^+(\mathbf{r})$ are represented by quasi-discrete sums:

$$\psi(\mathbf{r}) = \frac{1}{V^{1/2}}\sum_{(\mathbf{k})} a_k e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad \psi^+(\mathbf{r}) = \frac{1}{V^{1/2}}\sum_{(\mathbf{k})} a_k^+ e^{-i\mathbf{k}\cdot\mathbf{r}} \qquad (2)$$

in which the operators a_k, a_k^+ satisfy the usual Bose or Fermi permutation relations, $\mathbf{k} = \frac{2\pi}{L}\{n_x, n_y, n_z\}$; n_x, n_y, n_z are integers.

We shall assume that at temperatures below some critical temperature the system under consideration is in a state of crystalline ordering. This state has lower symmetry than the Hamiltonian (1) with respect to the translation group and therefore is degenerate. As is known, this degeneracy is removed by introducing into the Hamiltonian (1) some infinitely small additional term, which we shall not write down, bearing in mind, however, in what follows the corresponding averages in the sense of "quasi-averages" (^{1}).

As shown in (^{1}), for retarded and advanced temperature Green' s functions (see, for example, (^{5})) in the energy representation, at $E = 0$, the following inequality holds:

$$|\langle\langle A; B\rangle\rangle_{E=0}| \leq |\langle\langle A; A^+\rangle\rangle_{F=0}|\, |\langle\langle B^+; B\rangle\rangle_{E=0}|\,, \tag{3}$$

Putting here $A(t) = i\,\partial Q(t)/\partial t$ and using the spectral representations for the Green' s functions and correlation functions (see (^{5})),

one can give inequality (3) the form

$$\langle BB^+ + B^+B\rangle \geqslant 2\theta\, \frac{|\langle [Q, B]_-\rangle|^2}{\langle [[Q, [Q^+, H]_-]_-\rangle}, \tag{4}$$

where θ is the temperature in energy units.

Let us return to the consideration of the crystalline state. The particle-number density is defined as the average of the operator $\rho(\mathbf{r}) = \psi^+(\mathbf{r})\psi(\mathbf{r})$,

$$\int_{(V)} \rho(\mathbf{r})\, d\mathbf{r} = N;$$

introducing the operator of the Fourier component of the particle-number density ρ_q by the relation

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{(\mathbf{q})} \rho_q e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{5}$$

we obtain (in the momentum representation)

$$\rho_q = \sum_{(\mathbf{k})} a_k^+ a_{k+\mathbf{q}}. \tag{6}$$

The operator of the total momentum of the system is

$$P = \int \mathbf{j}(\mathbf{r})\, d\mathbf{r},$$

where, as is known,

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i}\, [\psi^+(\mathbf{r})\nabla\psi(\mathbf{r}) - (\nabla\psi^+(\mathbf{r}))\psi(\mathbf{r})]; \tag{7}$$

introducing the Fourier component $\mathbf{j}_q$ by the relation

$$\mathbf{j}(\mathbf{r}) = \frac{1}{V} \sum_{(\mathbf{q})} \mathbf{j}_q e^{i\mathbf{q}\cdot\mathbf{r}},$$

we obtain for $\mathbf{j}_q$

$$\mathbf{j}_q = \sum_{(\mathbf{k})} \frac{2\mathbf{k} + \mathbf{q}}{2} a_k^+ a_{k+\mathbf{q}}. \tag{8}$$

Let us note that the particle-number density $\langle \rho(\mathbf{r}) \rangle$ in a crystal is a function periodic with the lattice spacing. Therefore there exists a vector $\mathbf{G}_i \neq 0$ from the set of reciprocal-lattice vectors for which the quasi-average $\langle \rho_G / V \rangle$ is nonzero.

It is of interest to consider inequality (13) for the correlation function $\langle \rho_{G+\mathbf{k}} \rho_{-\mathbf{G}-\mathbf{k}} \rangle$, i.e., to set

$$B = \rho_{G+\mathbf{k}}^+ = \rho_{-\mathbf{G}-\mathbf{k}}. \tag{9}$$

For the greatest effectiveness of inequality (4), one should strive to make the denominator on the right-hand side as small as possible with respect to $\mathbf{k}$. Therefore, as the operator Q, one should choose an operator Q_k which, for $\mathbf{k} = 0$, turns into an integral of motion (commutes with the Hamiltonian). Such an "almost integral of motion" in our problem is the operator $\mathbf{j}_k$ (see (8)), which for $\mathbf{k} = 0$ becomes $\mathbf{j}_0 = P$, the total-momentum operator, commuting with the Hamiltonian (1). As the operator Q_k we choose the "projection" of this operator onto the direction $\mathbf{k}$:

$$Q_k = \left(\frac{\mathbf{k}}{k} \cdot \mathbf{j}_k \right). \tag{10}$$

Let us introduce into consideration the "pair correlation function" $F_2(\mathbf{r}_1, \mathbf{r}_2) = \langle \psi^+(\mathbf{r}_1) \psi^+(\mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \rangle$. Being written in the variables $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, it is, obviously, periodic in the argument $\mathbf{R}$:

$$F_2(\mathbf{r}_1 + \mathbf{a}, \mathbf{r}_2 + \mathbf{a}) = F_2(\mathbf{r}_1, \mathbf{r}_2) = F_2(\mathbf{R}, \mathbf{r}) = F_2(\mathbf{R} + \mathbf{a}, \mathbf{r}).$$

The function

$$\frac{1}{N(N-1)} F_2(\mathbf{r}_1, \mathbf{r}_2)$$

is the diagonal element of the statistical operator of a complex of two particles in the $\mathbf{r}$-representation. With the aid of this operator, as is known (^{6}), one can calculate quantum-statistical averages of quantities of binary type. It is not difficult

note that $\langle \rho_{G+k}\rho_{-G-k}\rangle$ is

$$\begin{aligned}\langle \rho_{G+k}\rho_{-G-k}\rangle &= \int_{(V)}\int_{(V)} d\mathbf{r}_1 d\mathbf{r}_2\, F_2(\mathbf{r}_1,\mathbf{r}_2)e^{-i(G+k,\mathbf{r}_1-\mathbf{r}_2)} + N \\ &= N\left(\int_{(V)} d\mathbf{r}\int_{(v)} d\mathbf{R}\,\widetilde{F}_2(\mathbf{R},\mathbf{r})\, e^{-i(G+k,\mathbf{r})}+1\right) = \left\langle \sum_{i,j;\,i\neq j} e^{-i(G+k,\mathbf{r}_i-\mathbf{r}_j)}\right\rangle + N.\end{aligned} \tag{11}$$

Computing the corresponding commutators on the right-hand side of inequality (4), where the operators B and Q are defined by formulas (9) and (10), we obtain an inequality for $\langle \rho_{G+k}\rho_{-G-k}\rangle$, which, after division by N, and bearing in mind the performance of the limiting statistical transition $N\to\infty$, $V\to\infty$, $N/V = n = 1/v = \text{const}$, gives

$$\begin{aligned}\frac{1}{N}\langle \rho_{G+k}\rho_{-G-k}\rangle &= \left\langle \frac{1}{N}\sum_{i,j;\,i\neq j} e^{-i(G+k)(\mathbf{r}_i-\mathbf{r}_j)}\right\rangle + 1 \\ &\geq \left[\theta\left|\int_{(v)}\langle\rho(\mathbf{r})\rangle e^{-iG\cdot\mathbf{r}}\,d\mathbf{r}\right|^2\left(\frac{\mathbf{k}}{k},\,\mathbf{k}+\mathbf{G}\right)^2\right]\Bigg/\left[\frac{k^4}{4m}+\frac{1}{N}\sum_{(\mathbf{p})}\frac{3(\mathbf{p}\cdot\mathbf{k})^2}{m}\langle a_p^+a_p\rangle\right. \\ &\qquad\left.+\int_{(V)} d\mathbf{r}\int_{(v)} d\mathbf{R}\,\widetilde{F}_2(\mathbf{R},\mathbf{r})(1-\cos(\mathbf{k}\cdot\mathbf{r}))\left(\frac{\mathbf{k}}{k}\cdot\nabla\right)^2\Phi(\mathbf{r})\right].\end{aligned} \tag{12}$$

Let us multiply this inequality by a positive, sufficiently regular function $h(\mathbf{k})$ (without loss of generality $h(\mathbf{k}) = h(|\mathbf{k}|)$), localized in a neighborhood of $\mathbf{k} = 0$. Its Fourier transform $\mathcal{H}(|\mathbf{r}|)$, defined by the relation

$$\mathcal{H}(\mathbf{r}) = \int h(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{k}, \qquad h(\mathbf{k}) = \frac{1}{(2\pi)^d}\int \mathcal{H}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\,d\mathbf{r}, \qquad d = 1,2,3, \tag{13}$$

is, obviously, a positive monotonically decreasing function of $|\mathbf{r}|$. We integrate the resulting inequality over all $\mathbf{k}$. The integrand on the right-hand side as $k\to 0$ is of order $1/k^2$; therefore the integral over $\mathbf{k}$ on the right-hand side of the inequality diverges in the one- and two-dimensional cases.

Let us turn to the left-hand side of the inequality. Clearly, we can speak of crystalline ordering in the system when the deviations of the atoms from the equilibrium (most probable) position are such that the distance between neighboring atoms does not become smaller than some arbitrarily small but fixed distance a, which we can choose to be several times smaller than the lattice spacing.

In the one-dimensional case, naturally numbering the atoms in accordance with their arrangement along the straight line, we write this condition in the form

$$|\mathbf{r}_i - \mathbf{r}_{i+1}| \geq a, \tag{14}$$

whence it follows that

$$|\mathbf{r}_i - \mathbf{r}_j| \geq a|i-j|. \tag{15}$$

Let us estimate in the one-dimensional case, with the aid of this relation, the left-hand side of the inequality obtained ($N \to \infty$), taking into account that $\mathcal{H}(r)$ is a positive monotonically decreasing function:

$$\begin{aligned}\int dk\, h(k) \left\{ \left\langle \frac{1}{N} \sum_{i,j;\, i\neq j} e^{-i(G+k)(r_i - r_j)} \right\rangle + 1 \right\} &= \frac{1}{N} \sum_{i,j;\, i\neq j} e^{-iG(r_i-r_j)} \mathcal{H}(|r_i - r_j|) + \mathcal{H}(0) \\ &\leq \frac{1}{N} \sum_{i,j;\, i\neq j} \mathcal{H}(a|i-j|) + \mathcal{H}(0) \\ &\leq \int_0^\infty \mathcal{H}(ay)\, dy + \mathcal{H}(0) = \frac{2\pi h(0)}{2a} + \mathcal{H}(0).\end{aligned}$$

Thus, in the one-dimensional case the left-hand side is bounded above by the constant quantity $2\pi h(0)/2a + \mathcal{H}(0)$ and exceeds the right-hand side, which, as we have shown, diverges in the one-dimensional case. Consequently, the exact inequality (12), obtained on the basis of spectral representations for the correlation functions and Green' s functions, is satisfied in one-dimensional systems at temperatures $\theta \neq 0$ only in the case when the quasimean

$$\langle \rho_G / V \rangle \cdot v = \int_{(v)} \langle \rho(r) \rangle e^{-iGr}\, dr, \qquad v = L/N,$$

which enters the right-hand side, is identically equal to zero. This means that the quasimean $\langle \rho(r) \rangle = N/L = \text{const}$, and crystalline ordering in one-dimensional systems at $\theta \neq 0$ is impossible.

Let us emphasize here that our result has been obtained without using the harmonic approximation and rests only on the obvious assumption (14), corresponding to the absence of "points of condensation" in the crystal.

We note that inequality (3) is valid for the Green' s functions introduced in work (7) for the statistical mechanics of classical systems, and obtaining an analogous result for a classical crystalline system presents no difficulty.

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Moscow State University
named after M. V. Lomonosov

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

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