Symmetry properties of the ground state of the system of interacting spinless bosons

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We perform the symmetry analysis of the properties of the ground state of a finite system of interacting spinless bosons for the three most symmetric boundary conditions (BCs): zero BCs with spherical and circular symmetries, as well as periodic BCs. The symmetry of the system can lead to interesting properties. For instance, the density of a periodic Bose system is an exact constant: \( \rho(r) = \text{const.} \). Moreover, in the case of perfect spherical symmetry of BCs, the crystalline state cannot produce the Bragg peaks. The main result of the article is that symmetry properties and general quantum-mechanical theorems admit equally both crystalline and liquid ground state for a Bose system of any density.

Keywords: Bose system; ground state; symmetry.

1 Introduction

As is known, it is impossible analytically and very difficult numerically to find directly and reliably the solution for the ground state (GS) of a dense Bose system. The only exception is a one-dimensional (1D) system of spinless point bosons: the analytical structure of the ground-state wave function (WF) of such a system is known \([1, 2, 3]\). For all possible values of the system parameters, the ground state of this system corresponds to a liquid (gas) \([1, 4]\). For such a system, gaseous and liquid states are indistinguishable, see \([1]\) for details.

In what follows, we will consider symmetry properties of GS of a system of interacting spinless bosons for several ideal boundary conditions (BCs): zero BCs with rotational symmetry and periodic BCs (such idealized BCs enables one to use corresponding mathematical theorems). In these cases, the properties of the system are rather bizarre and not visual. We will also try to clarify whether the symmetry analysis allows us to find out the nature of the ground state of a Bose system of a given density: is it a liquid or a crystal?

The outline of the article is as follows. The general analysis of the symmetry properties of one-dimensional, two-dimensional (2D), and three-dimensional (3D) systems of identical
particles is made in Sect. 2. Further, we investigate the symmetry properties of the GS of a system of spinless bosons for the following cases: a periodic 3D system (Sect. 3), a ball-shaped 3D system (Sect. 4), and a perfectly circular 2D system (Sect. 5). In particular, in Sect. 5, we find the structure of the wave functions of a 2D system of spinless bosons with zero BCs on a circle. Some conclusions comprise Sect. 6. In Appendix, we adduce the proof of the nondegeneracy of the GS of a 1D system of two spinless bosons and point out conditions of validity of this proof.

2 Symmetry analysis: general remarks

Symmetry analysis enable us to draw some exact conclusions about properties of the system. Below, we will investigate the symmetry properties of the ground state of a system of interacting spinless bosons under ideal BCs: periodic ones and zero BCs with rotational symmetry. Such an analysis will allow us to comprehend the properties of GS of real systems, for which BCs have lower symmetry. We consider only spinless bosons since certain mathematical theorems work just for such particles. Our analysis is valid for such inert elements as $^4$He, Ne, Ar, Kr, and Xe. For neon, argon, krypton, and xenon, we have in mind isotopes corresponding to zero atomic spin (consequently, zero nuclear spin, for atoms in the ground state) and an infinite (or very long) lifetime: these are $^{20}$Ne, $^{22}$Ne, $^{36}$Ar, $^{38}$Ar, $^{40}$Ar, $^{78}$Kr, $^{80}$Kr, $^{82}$Kr, $^{84}$Kr, $^{86}$Kr, $^{124}$Xe, $^{126}$Xe, $^{128}$Xe, $^{130}$Xe, $^{132}$Xe, $^{134}$Xe, and $^{136}$Xe [6, 7].

It is noted in the book by J. Elliott and P. Dawber that GS of a system should be invariant under all transformations of each of the symmetry groups of the given system [8] (in this case, the system means the boundary-value problem: the Hamiltonian plus BCs). In other words, GS should be the most symmetric state of the system or enter the set of the most symmetric states. Here it is implicitly assumed that there is no spontaneous symmetry breaking.

Two theorems are valid for a system of interacting particles, which is described by the Schrödinger equation with zero BCs: (1) The node theorem by R. Courant: if the eigenstates $\Psi_j$ are numbered ($j = 1, 2, \ldots, \infty$) in the order of increasing energies $E_j$, then the function $\Psi_j$ has no more than $j - 1$ nodes [5, 9]. (2) The theorem by R. Courant and D. Hilbert: the ground state is non-degenerate [5]. These theorems hold under the following conditions: all $\Psi_j$ are one-component and real; the system is finite; the particles do not have a spin or an intrinsic multipole moment; and the requirement for the total interatomic potential: $- \infty < \int dr_1 \cdots dr_N U(r_1, \ldots, r_N) |\Psi_0(r_1, \ldots, r_N)|^2 < \infty$ (see Appendix below). For a majority of real-life systems, at least one of these conditions is violated. However, all conditions hold for the atoms of inert elements $^4$He, Ne, Ar, Kr, and Xe (for the interatomic potentials of inert elements see [10, 11, 12, 13]; we do not consider hydrogen, because $^2$H molecules possess intrinsic quadrupole moment, which violates the conditions of the theorems).

We note that these two theorems work for complex WFs as well. In the sense that as the stationary Schrödinger equation does not contain complex numbers, the complete set of WFs
can be constructed so that all these WFs are real. The theorems have been proved for a system of particles that possesses no definite (Bose or Fermi) symmetry with respect to permutations: i.e. the complete set of WFs contains the Bose symmetric, Fermi symmetric, and all other WFs. However, the boundary-value problem is invariant under the permutation group $S_N$. Therefore, the complete collection of WFs can be set such that all WFs transform according to irreducible representations of the group $S_N$ [8, 14]. The degeneracy multiplicity of the given state is equal to the dimension of the irreducible representation the state transforms by [8, 14]. Therefore, a non-degenerate state corresponds to a one-dimensional representation. As GS is non-degenerate, the wave function of GS must transform according to a one-dimensional representation. The group $S_N$ has exactly two such representations: one corresponds to Bose symmetry, the other to Fermi symmetry [8, 14]. GS must have the highest symmetry, so the ground-state WF must transform according to the identity representation of the group $S_N$. Such a representation corresponds to Bose symmetry. Therefore, those conclusions of the theorems by Courant and Hilbert that concern the GS properties are conclusions about the GS properties of a Bose system.

Note also that 1D and 2D systems of $N$ identical particles can have special properties. In works [15, 16], it was made an analysis of the “reduced” configuration space $M_N = (R^N - \Delta)/S_N$ obtained from the ordinary configuration space $R^N$ of $N$ particles by identifying those points from $R^N$, that differ only by permutation of coordinates $r_1, \ldots, r_N$, and subtracting the set $\Delta$ (this is a subspace of the space $R^N$, consisting of the points for which the coordinates of two atoms coincide: $r_j = r_p$ for any $j \neq p$). Let the space $R$ have dimensionality $d$. From the standpoint of the properties of the space $M_N$, the type of particle statistics is defined by one-dimensional irreducible representations of the first homotopy group $\pi_1(M_N)$ [15, 17]. For $d \geq 3$ we have $\pi_1(M_N) = S_N$, so for a 3D system ($d = 3$) only Fermi and Bose statistics are possible. However, for a 2D system ($d = 2$), the group $\pi_1(M_N)$ is isomorphic to the infinite non-abelian braid group $B_N$ [17, 18]. One-dimensional irreducible representations of the group $B_N$ have the form $\chi_\theta = e^{-i\theta}$, where $\theta$ takes an infinite number of values in the interval $[0, 2\pi[$. The values $\theta = 0$ and $\theta = \pi$ correspond to Bose and Fermi statistics, respectively. The remaining values of $\theta$ correspond to fractional (anomalous) statistics. In this case, fractional statistics reveals itself both in the symmetry of WF (e.g., $\Psi(r_1, r_2) = e^{i\theta}\Psi(r_2, r_1)$ for $N = 2$ [so called $\theta$ symmetry]; more precisely, the phase $\theta$ arises when two particles are moved resulting in the exchange [17]) and in the energy distribution of states and thermodynamics [17]. We remark that anomalous statistics was also introduced without using the symmetry properties of WFs [19, 20, 21].

WFs obeying fractional statistics are multivalued. These WFs usually differ from each other by a constant factor that takes several different values in the phase space. Such WFs describe several different states of the same energy. It corresponds to a degenerate state of the system.
Such anomalous WFs must be eigenfunctions for a given boundary-value problem. Since the Hamiltonian of a 2D system of identical particles is invariant under the group $S_N$ (rather than the more extensive group $B_N$), only Bose and Fermi statistics are realized as a rule. However, WFs with the $\theta$ symmetry do not correspond to the $S_N$ symmetry of the Hamiltonian. Therefore, WFs satisfying fractional statistics are possible only in the case of spontaneous symmetry change. We suppose that spontaneous symmetry change (or breakdown) occurs solely if at least one of the conditions of Courant-Hilbert’s theorem is violated. Indeed, since the anomalous states are degenerate, they cannot correspond to the genuine GS of the system (according to Courant-Hilbert’s theorem). Consequently, if the GS is degenerate, then the conditions of the theorem are violated. For characteristic problems leading to WFs with the $\theta$ symmetry, the conditions of Courant-Hilbert’s theorem are actually violated (see Appendix below). Note that solutions corresponding to anomalous statistics have been obtained theoretically and justified experimentally (see monograph [17] and reviews [22, 23]).

For 1D systems, a connection with anomalous statistics has also been found. In particular, the energy distribution of states for a system of spinless point bosons (potential $U(x_j - x_l) = 2c\delta(x_j - x_l)$) coincides with the distribution for an ideal gas with generalized fractional statistics [24, 25], at any temperature $T$. For such a system, WFs have Bose symmetry, and the unconventional statistics manifests itself in the energy distribution of states and, consequently, in thermodynamic formulae. However, the thermodynamic formulae for such a system depend on the way of introducing quasiparticles [26]. One can specify free quasiparticles in such a way they to obey pure Bose statistics (for $N = \infty$, $T \rightarrow 0$) [27]. Now let us imagine that we consider two arbitrary quasiparticles, with momenta $k_1$ and $k_2$ say, as one quasiparticle with momentum $k_3 = k_1 + k_2$. Accordingly, we consider two quasiparticles with momentum $k_1$ and two quasiparticles with momentum $k_2$ as two quasiparticles, each having momentum $k_3 = k_1 + k_2$. And so on. We will obtain another ensemble of quasiparticles, with a slightly different distribution of quasiparticles on energies and with other occupation numbers. Therefore, Bose statistics will be violated. Evidently, in this way, one can obtain an infinite number of quasiparticle ensembles with different statistics. In most cases, such an ensemble will not obey Bose, Fermi, or fractional statistics. Thus, the results in [24, 25, 27] show that for $T \rightarrow 0$ there are ways of introducing quasiparticles in which we arrive at Bose statistics or fractional statistics. And just as importantly, the two approaches must be equivalent: experiments give only a single dependence of heat capacity on $T$, which must be derived theoretically in both approaches. Indeed, the approach with fractional statistics [24, 25] is built on Yang-Yang’s approach [28] and thence is equivalent to the latter. The Bose approach [27] also is equivalent to Yang-Yang’s approach, as shown in [29]. Consequently, the approaches [24, 25] and [27] have indeed to be equivalent. For non-small $T$, Bose quasiparticles are well-defined [30] but strongly interact with each other, which greatly complicates the thermodynamic description. In this case, “quasiparticles” in the approach
with fractional statistics do not interact with each other even at large $T$, which is a surprising and nontrivial property. It is natural to call quasiparticles, corresponding to the most simple description of the system, elementary excitations \[20\]. Therefore, elementary excitations of the 1D system of spinless point bosons are Bose quasiparticles at $T \to 0$ and quasiparticles, satisfying generalized fractional statistics, at non-small $T$. These properties are interesting. We also remark that the 1D Calogero–Sutherland system of the particles interacting with a $(x_j - x_l)^{-2}$ potential can be thermodynamically described, at any temperature, as an ideal gas of (quasi) particles with fractional statistics \[24, 25, 31, 32\].

Thus, 1D and 2D systems of identical particles can have nontrivial statistical properties. However, below we consider only 2D and 3D systems of identical particles for which the conditions of Courant-Hilbert’s theorem hold. For such systems, there is no spontaneous symmetry change, wave functions correspond to irreducible representations of the group $S_N$, and GS is described by a nodeless single-valued WF. In that case, anomalous statistics may in principle be obtained for an “equivalent” system, which can be matched to the given system similarly to the analysis in \[24, 25, 31, 32\]. Below we are interested in the properties of an initial real-life system. As is seen from the aforesaid, the symmetry of the ground-state WFs of such a system must correspond to Bose statistics.

So, GS of a system of spinless bosons must be described by a nodeless non-degenerate WF belonging to the set of functions that are invariant under all transformations of symmetry groups of the boundary-value problem. Let us consider the properties of wave functions for several boundary-value problems and check whether crystalline and liquid GS meet these requirements.

Since the symmetry of the boundary-value problem means the symmetry of both the Hamiltonian and the boundary conditions, we will consider idealized BCs corresponding to symmetries of the Hamiltonian: (i) periodic BCs and (ii) zero ones with rotational symmetry (3D ball and 2D disk).

We will consider only finite systems (since for an infinite system Courant-Hilbert’s theorem does not work, generally speaking, and spontaneous symmetry breaking is possible).

### 3 Periodic 3D system of spinless bosons

The Hamiltonian

\[
\hat{H} = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \Delta r_j + \frac{1}{2} \sum_{j \neq l} U(|r_i - r_j|)
\]

(1)

is invariant under the continuous group of translations $T(3)$, the continuous group of rotations $SO(3)$, the group of permutations $S_N$, and the group of inversions $C_i$ (the latter contains two elements: inversion $I$ and $I^2 = 1$; here and below, we consider that any symmetry transformation applies to all coordinates $r_1, \ldots, r_N$). Since the space is isotropic and uniform,
the invariance of $\hat{H}$ under the groups $SO(3)$ and $T(3)$ would survive if $\hat{H}$ also includes three-particle interaction \cite{33, 34, 35, 36} and possible many-particle ones. Periodic BCs are invariant under the groups $T(3)$, $S_{N}$, and $C_{i}$, but are not under the group $SO(3)$. The ground-state WF reads

$$
\Psi_{0} = e^{S_{0}}, \quad \Psi_{0}(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}) = \sum_{j_{1}j_{2}} S_{2}(\mathbf{r}_{j_{1}} - \mathbf{r}_{j_{2}}) + \sum_{j_{1}j_{2}j_{3}} S_{3}(\mathbf{r}_{j_{1}} - \mathbf{r}_{j_{2}}, \mathbf{r}_{j_{2}} - \mathbf{r}_{j_{3}}) + \ldots
$$

$$
+ \sum_{j_{1}j_{2}\ldots j_{N}} S_{N}(\mathbf{r}_{j_{1}} - \mathbf{r}_{j_{2}}, \mathbf{r}_{j_{2}} - \mathbf{r}_{j_{3}}, \ldots, \mathbf{r}_{j_{N-1}} - \mathbf{r}_{j_{N}}).
$$

Such a WF can describe both a liquid \cite{26, 37, 38, 39, 40} and a crystal \cite{41, 42, 43, 44}. This WF is invariant under the groups $T(3)$, $S_{N}$, and $C_{i}$. The transition from the liquid GS to the crystalline one leads to the appearance of long-range crystalline order in the two-particle and higher correlation functions. Thus, the properties of the crystalline and liquid GS are in agreement with the theorems by Courant and Hilbert and with Elliott-Dawber’s statement.

We note that any state of the system with the total momentum $\mathbf{P} \neq 0$ must be degenerate because $[\hat{H}, \hat{\mathbf{P}}] = 0, [\hat{H}, \hat{\mathbf{I}}_{r}] = 0$, but $[\hat{\mathbf{P}}, \hat{\mathbf{I}}_{r}] = -2\hat{\mathbf{I}}_{r}\hat{\mathbf{P}} \neq 0$ (here, $\hat{\mathbf{I}}_{r}$ denotes the coordinate inversion operator: $\hat{\mathbf{I}}_{r}\hat{\Psi}(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}) = \hat{\Psi}(-\mathbf{r}_{1}, \ldots, -\mathbf{r}_{N})$). On states with zero $\mathbf{P}$ the operators $\hat{\mathbf{P}}$ and $\hat{\mathbf{I}}_{r}$ commute with each other. Only such states can be non-degenerate. The condition $\mathbf{P} = 0$ is satisfied for the ground state \cite{2, 3} and an infinite number of excited states. All such states are invariant under the groups $T(3)$, $S_{N}$, and $C_{i}$. These are the most symmetric states of the system.

The ground state of a Bose crystal is most often described by the localized ansatz \cite{45, 46}

$$
\Psi_{0}^{c} \approx e^{S_{0}} \sum_{P_{c}} \prod_{j=1}^{N} \varphi(\mathbf{r}_{j} - \mathbf{R}_{j}),
$$

where $\mathbf{r}_{j}$ and $\mathbf{R}_{j}$ are the coordinates of atoms and lattice sites, respectively, $N$ is the number of atoms in the system, $\varphi(\mathbf{r}) = e^{-\alpha r^{2}/\bar{d}^{2}}$ ($\bar{d}$ stands for the average interatomic distance), $P_{c}$ denotes all possible permutations of coordinates $\mathbf{r}_{j}$, and $e^{S_{0}}$ corresponds to the isotropic liquid solution with $S_{0}$ \cite{3}. Such ansatz can be considered as an approximate solution under zero BCs. It gives satisfactory agreement with experiments \cite{45, 47}.

Interestingly, for any pure state (including GS) of a periodic Bose system, the concentration is an exact constant: $n(\mathbf{r}) = \text{const}$ \cite{48, 49, 50, 51}. This property is related to translation invariance and can be proved easily \cite{50, 51}. For a system with $T > 0$, this can be proved analogously to the analysis in \cite{50}, using the formula $n(\mathbf{r}) = \text{const} \cdot \int d\mathbf{r}_{2} \ldots d\mathbf{r}_{N} \sum_{j} e^{-E_{j}/k_{B}T} |\Psi_{j}(\mathbf{r}, \mathbf{r}_{2}, \ldots, \mathbf{r}_{N})|^{2}$ and property $\Psi(\mathbf{r} + \delta\mathbf{r}, \ldots, \mathbf{r}_{N} + \delta\mathbf{r}) = (1 + i\mathbf{p}\delta\mathbf{r})\Psi(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}) = e^{i\mathbf{p}\delta\mathbf{r}}\Psi(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N})$. In this case, the crystalline ordering is hidden: it manifests itself in long-range oscillations (with periods of a crystal) of the two-particle and higher distribution functions, not in the density.
As an example, consider \( N \) free spinless bosons in the state \(|\Psi_c\rangle = |N_{k_x}, N_{-k_x}, N_{k_y}, N_{-k_y}, N_{k_z}, N_{-k_z}, N_{k=0}\rangle\), where \( N_k \) is the number of Bose particles with momentum \( \hbar k \). Let us set \( N_{k_x} = N_{-k_x} = N_{k_y} = N_{-k_y} = N_{k_z} = N_{-k_z} = J \) and \( N_{k=0} = N - 6J \). Such a state is described by the second quantized operator

\[
\hat{\psi}(r, t) = V^{-1/2} \left( \hat{a}_{k_x} e^{i k_x x} + \hat{a}_{-k_x} e^{-i k_x x} + \hat{a}_{k_y} e^{i k_y y} \right.
\]

\[
\left. + \hat{a}_{-k_y} e^{-i k_y y} + \hat{a}_{k_z} e^{i k_z z} + \hat{a}_{-k_z} e^{-i k_z z} + \hat{0} \right).
\]

After some evaluation, we find the two-particle distribution function:

\[
g_2(r_1, r_2) \equiv C_g \langle \Psi_0^6 | \hat{\psi}^+(r_1, t) \hat{\psi}^+(r_2, t) \hat{\psi}(r_1, t) \hat{\psi}(r_2, t) | \Psi_0^6 \rangle
\]

\[
= C_g V^{-2} \left[ N^2 - N - 6J^2 + 4J F_3 \cdot (JF_3 + N - 6J) \right],
\]

where

\[
F_3 = \cos[k_x(x_1 - x_2)] + \cos[k_y(y_1 - y_2)] + \cos[k_z(z_1 - z_2)],
\]

\( C_g = V^2/(N^2 - N) \). Here, the normalization is \( \int d\mathbf{r}_1 d\mathbf{r}_2 g_2(\mathbf{r}_1, \mathbf{r}_2) = V^2 \). It is a translationally invariant crystal-like solution with a rectangular 3D lattice. The amplitude of oscillations of the function \( g_2(\mathbf{r}_1, \mathbf{r}_2) \) is greatest at \( J = N/6 \), i.e. when \( N_{k=0} = 0 \). Such a state corresponds to WF with many nodes. In this case, GS corresponds obviously to the state \(|\Psi_0\rangle = |N_{k=0}\rangle\) with \( N_{k=0} = N \). We may expect that, at nonzero interatomic interaction, the state \(|\Psi^c\rangle = |N_{k_x}, N_{-k_x}, N_{k_y}, N_{-k_y}, N_{k_z}, N_{-k_z}, N_{k=0}\rangle\) (where \( N_k \) is the number of phonons with momentum \( \hbar k \)) also corresponds to a crystal with a nodal WF. The exact crystalline solution \([4]\) for a 1D system of point bosons indicates it (this solution has the same structure). Such a crystal can be regarded as a liquid with a condensate of phonons (this interpretation is correct at least for the 1D system of point bosons). In this case, the condensate of phonons creates a lattice. On the other hand, the lattice forms by a network of nodes of WF. D. Kirzhnits and Yu. Nepomnyashchii have called such a solution by “coherent crystal” \([56, 57]\). The energy of a state with a multi-node WF considerably exceeds the GS energy of the system. It is yet unclear, whether such coherent crystal can be stable and exist in Nature.

### 4 Ball-shaped 3D system of spinless bosons

Consider a 3D system of spinless bosons placed in a sphere with zero BCs (\( \Psi = 0 \) on the boundary). Such a system has the form of an ideal ball. The Hamiltonian \( \hat{H} \) \([2]\) is invariant
leads to the formula $\hat{L}$ we do not distinguish between the numbers $r$ and $l$. The representations with integer and half-integer $j$ are, respectively, one- and two-valued \[8, 14, 63, 64\]. The scalar WFs can transform only by irreducible representations of the rotation group $SO(3)$ \[8, 14\] (this is true for unitary representations; as the group $SO(3)$ is compact, its representations are equivalent to unitary ones \[14, 63\]). This group is characterized by the complete collection of irreducible representations $g \to \hat{T}_l(g)$ with $l = 0, 1/2, 1, 3/2, 2, \ldots, \infty$ and the dimension $2l + 1$ (here, $g$ is an element of the group). The representations with integer and half-integer $l$ are, respectively, one- and two-valued \[8, 14, 63, 64\]. The scalar WFs can transform only by the representations with integer $l$. In this case, $\hat{L}^2 \Psi^{(l)} = \hbar^2 l(l + 1) \Psi^{(l)} \[8, 14\]$ (in this article, we do not distinguish between the numbers $L$ and $l$). The rotation operator is defined by the formula \[61, 62\]

$$\hat{R}\Psi(r_1, \ldots, r_N) = \Psi(\hat{r}_1, \ldots, \hat{r}_N),$$

(8)

where $r_j$ and $\hat{r}_j = Ar_j$ are the coordinates of a vector before and after a rotation. Eq. (8) leads to the formula $\hat{R} = e^{i\varphi \hat{L}/\hbar} \[61, 62\]$. The wave functions, invariable under any rotation $\hat{R} \Psi \equiv e^{i\varphi \hat{L}/\hbar} \Psi = \Psi$, i.e., $\hat{L} \Psi = 0$, transform according to the identity representation $g \to \hat{T}_0(g)$: $\hat{T}_0(g) \Psi = \Psi$ for any element $g$ of the group $SO(3)$. The irreducible representation $g \to \hat{T}_1(g)$ is characterized by the orthonormal basis $\Psi^{(l)}_1, \Psi^{(l)}_2, \ldots, \Psi^{(l)}_{2l+1}$. In this case, $\hat{T}_l(g) \Psi^{(l)}_j = \sum_{p=1}^{2l+1} T^{(l)}_{pj}(g) \Psi^{(l)}_p$ for any element $g$ of the group $SO(3)$, where $T^{(l)}(g)$ are the matrices of constants and realize the representation $g \to \hat{T}_l(g) \[8, 14\]$. For each representation $g \to \hat{T}_l(g)$, all functions $\Psi^{(l)}_p$ correspond to the same energy. Indeed, let $\Psi^{(l)}_j$ be an eigenfunction of the Schrödinger equation with energy $E$:

$$\hat{H} \Psi^{(l)}_j = E \Psi^{(l)}_j.$$  

(9)

Let us act by the operator $\hat{T}(g) = \hat{R}^{-1}(g) = \hat{R}(g^{-1}) \[8, 63\]$ on this equation. Since $\hat{R}(g) \hat{H} - \hat{H} \hat{R}(g) = 0$ for any rotation $g$, the last equality holds also for the rotation $g^{-1}$. From whence, we get $\hat{T}(g) \hat{H} - \hat{H} \hat{T}(g) = 0$. Therefore,

$$E \hat{T}(g) \Psi^{(l)}_j = \hat{T}(g) E \Psi^{(l)}_j = \hat{T}(g) \hat{H} \Psi^{(l)}_j = \hat{H} \hat{T}(g) \Psi^{(l)}_j.$$  

(10)
That is, the function $\hat{T}(g)\Psi_j^{(l)}$ is also an eigenfunction of the Schrödinger equation with energy $E$. We now substitute the expansion $\hat{T}(g)\Psi_j^{(l)} \equiv [\hat{T}_0(g) \oplus \hat{T}_1(g) \oplus \ldots \oplus \hat{T}_\infty(g)]\Psi_j^{(l)} = \hat{T}_1(g)\Psi_j^{(l)} = \sum_{p=1}^{2l+1} \tau_p^{(l)}(g)\Psi_p^{(l)}$ in formula (10). Since the basis functions $\Psi_p^{(l)}$ are independent of one another, we get that all functions $\Psi_p^{(l)}$ are eigenfunctions of the Schrödinger equation with energy $E$. Therefore, such a state is $(2l+1)$-fold degenerate. We note that an accidental degeneracy $E_0 = E_{j\neq 0}$ is impossible because, in this case, all states of the system would be degenerate, which contradicts the theorem on the nondegeneracy of GS. Thus, only the state with $L = 0$ is non-degenerate. This state transits into itself at any rotation and transforms according to the identity representation of the group $SO(3)$.

We remark that the first way of the proof follows, in fact, from the second (group) way since the operators $\hat{L}_\xi$ ($\xi = x, y, z$) are connected with the generators $\hat{I}_\xi$ of the group $SO(3)$ by the relation $\hat{L}_\xi = i\hbar \hat{I}_\xi$ [8, 14]. The group analysis is the most general and establishes the connection between the symmetry of a boundary-value problem and the properties of wave functions.

Since GS of the system of spinless bosons is non-degenerate [5] (see also Appendix below), it must correspond to a state with $L = 0$. This state is isotropic in the sense that WF does not change under any rotation of all $r_j$ around the center of the system. In this case, the atomic arrangement relative to each other may be anisotropic and correspond to a crystal, for instance. Such an anisotropy manifests itself in the two-particle distribution function and higher ones. That is, a state with $L = 0$ may correspond both to a liquid and a crystal (in Section 5, this question is considered for a 2D system in greater detail). At first, the author of the present article was unconscious that the condition $L = 0$ is compatible with a crystalline solution and arrived at the wrong conclusion [65] that the symmetry analysis forbids the crystalline GS with a nodeless WF.

All distribution functions $g_j(r_1, \ldots, r_j)$ of a ball-shaped system are invariant under rotations for any pure state of the system. Consider, for example, the two-particle distribution function for a $j$-th state:

$$g_2(r_1, r_2) = V^2 \int_G d\mathbf{r}_3 \ldots d\mathbf{r}_N |\Psi_j(r_1, \ldots, r_N)|^2,$$

(11)

where $G = V^{N-2}$ is the domain of the variables $r_3, \ldots, r_N$. Now express all $r_j$ in the form $r_j = A^{-1} \mathbf{r}_j$, where $A$ denotes the matrix of rotation around the coordinate origin (center of the ball). In this case, the Jacobian is $J = det(A^{-1}) = 1$, and the boundary surface passes into itself (hence, $V = \hat{V}$ and $G = \hat{G}$). At any rotation, the state of such a system passes into an equivalent one. Therefore, the relation $e^{i\beta} \Psi_j(r_1, \ldots, r_N) = \Psi_j(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ must hold (here, $\beta$ is a constant, depending on rotation angles; $\beta = 0$ for states with $L = 0$). In the issue we obtain

$$g_2(r_1, r_2) = V^2 \int_G d\mathbf{r}_3 \ldots d\mathbf{r}_N |\Psi_j(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \equiv g_2(\mathbf{r}_1, \mathbf{r}_2),$$

(12)
that is, \( g_2(\mathbf{r}_1, \mathbf{r}_2) \) is isotropic. One can show similarly that the particle number density \( n(\mathbf{r}) \) and all higher distribution functions are also isotropic under rotations around the center of the ball.

A crystal is commonly defined as a system that (i) gives the Bragg peaks when scattering X-rays (the main criterion), (ii) permits the existence of transverse phonons, and (iii) does not flow (except for the supersolid state). The Bragg peaks are sharp peaks of the structure factor \( S(\mathbf{k}) \) which is connected with \( g_2(\mathbf{r}_1, \mathbf{r}_2) \) by the equation

\[
S(\mathbf{k}) = \langle \rho_\mathbf{k} \rho_{-\mathbf{k}} \rangle = 1 + \frac{1}{N} \sum_{j,l=1,...,N} \frac{1}{V^2} \int d\mathbf{r}_l d\mathbf{r}_j g_2(\mathbf{r}_l, \mathbf{r}_j) e^{-i\mathbf{k}(\mathbf{r}_l - \mathbf{r}_j)}. \tag{13}
\]

Here, the integration over coordinates \( \mathbf{r}_l, \mathbf{r}_j \) is to be performed over the volume \( V \) of the system. Since the particles are indistinguishable, we obtain

\[
S(\mathbf{k}) = 1 + \frac{N - 1}{V^2} \int d\mathbf{r}_1 d\mathbf{r}_2 g_2(\mathbf{r}_1, \mathbf{r}_2) e^{-i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)}. \tag{14}
\]

For uniform systems, \( g_2(\mathbf{r}_1, \mathbf{r}_2) = g_2(\mathbf{r}_1 - \mathbf{r}_2) \). Then (14) leads to the well-known formula

\[
S(\mathbf{k})|_{\mathbf{k} \neq 0} = 1 + n \int d\mathbf{r}(g_2(\mathbf{r}) - 1)e^{-i\mathbf{k}\mathbf{r}}, \tag{15}
\]

where \( g_2(\mathbf{r}) - 1 \) is the two-particle correlation function. Our system is finite and generally nonuniform. Therefore, we will base ourselves on the general formula (14), which is valid for a finite system of any form. Let us rotate in Eq. (14) the coordinates \( \mathbf{r}_l, \mathbf{r}_j \) similarly to the above analysis for \( g_2(\mathbf{r}_1, \mathbf{r}_2) \) and use the property \( A^{-1} = A^T \) [68]. Then we find \( \mathbf{k}\mathbf{r} = \mathbf{k}(A^{-1}\hat{\mathbf{r}}) = \mathbf{k}(A^T \hat{\mathbf{r}}) = (A\mathbf{k})\hat{\mathbf{r}} = \hat{\mathbf{k}}\mathbf{r} \) and \( S(\mathbf{k}) = S(\hat{\mathbf{k}}) \). That is, the structure factor is isotropic and depends only on \( |\mathbf{k}| \). Consequently, a state with \( L = 0 \) does not give the Bragg peaks. In this case, the functions \( g_{j \geq 2}(\mathbf{r}_1, \ldots, \mathbf{r}_j) \) may exhibit a crystal structure with long-range order in the mutual arrangement of atoms. Under rotation of all coordinates, such a structure rotates as a whole. As a result, the functions \( g_{j \geq 2}(\mathbf{r}_1, \ldots, \mathbf{r}_j) \) do not alter.

## 5 Perfectly circular 2D system of spinless bosons

Let the system be inside a circle of radius \( R \) with zero BCs. The Hamiltonian

\[
\hat{H} = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \left[ \frac{1}{\rho_j} \frac{\partial}{\partial \rho_j} \left( \rho_j \frac{\partial}{\partial \rho_j} \right) + \frac{1}{\rho_j^2} \frac{\partial^2}{\partial \varphi_j^2} \right] + \frac{1}{2} \sum_{j,l=1 \atop j \neq l}^{N} U(|\mathbf{r}_l - \mathbf{r}_j|) \tag{16}
\]

is invariant under the rotation group \( SO(2) \) and the groups \( T(2), S_N, C_i \). The group \( SO(2) \) is compact and abelian, so all its irreducible representations are one-dimensional [8, 14]. In this case, the dimensions of irreducible representations do not help to ascertain which states are non-degenerate. One can establish it otherwise. Since \([\hat{H}, \hat{L}_z] = 0 \) (where \( \hat{L}_z = -i\hbar \sum_{j=1}^{N} \frac{\partial}{\partial \varphi_j} \) is the operator of the total angular momentum of the system), the complete set of wave
functions can be constructed so they to be the eigenfunctions of the operators $\hat{H}$ and $\hat{L}_z$. Introduce the phase inversion operator $\hat{I}_\varphi$: $\varphi_j \to -\varphi_j$ for all $j = 1, \ldots, N$. The states $\Psi(\varphi_1, \ldots, \varphi_N)$ and $\hat{I}_\varphi \Psi(\varphi_1, \ldots, \varphi_N) = \Psi(-\varphi_1, \ldots, -\varphi_N)$ correspond to the same energy $E$ (because $[\hat{H}, \hat{I}_\varphi] = 0$), but different eigenvalues of the operator $\hat{L}_z$: $L_z = \hbar m_L$ and $L_z = -\hbar m_L$, respectively. Therefore, all states with $m_L \neq 0$ are doubly degenerate. Only states with $m_L = 0$ are non-degenerate. The degeneracy is related here to the fact that $[\hat{H}, \hat{L}_z] = 0$, but $[\hat{L}_z, \hat{I}_\varphi] = -2\hat{I}_\varphi \hat{L}_z \neq 0$. Below we find a general form of the wave functions of such a system and argue that the structure of WFs with $m_L = 0$ tolerates both crystalline and liquid solution.

5.1 Wave functions for a perfectly circular 2D system of spinless bosons

For periodic BCs, the wave functions of weakly excited states of the Bose system and equations for them are obtained in [26, 40, 69]. For another BCs, wave functions of a Bose system and equations for these WFs presumably have not been obtained (except in the case of a 1D system of point bosons [2, 3, 70, 71]). Let us find the general structure (without equations) of the WFs of a 2D Bose system under zero BCs on a circle.

Consider a 2D system of interacting spinless bosons, which is described by the Hamiltonian (16) and lies in the circle of radius $R$. Let BCs be zero ones: $\Psi(r_1, \ldots, r_N) = 0$ provided $\rho_j \equiv |r_j| = R$ for any $j$. Each eigenfunction of this boundary-value problem can be expanded in the wave functions of free bosons (found for the same boundary-value problem) since they form a complete set of Bose symmetric functions. At a switched-off interaction, the Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \sum_{j=1}^N \left[ \frac{1}{\rho_j} \frac{\partial}{\partial \rho_j} \left( \rho_j \frac{\partial}{\partial \rho_j} \right) + \frac{1}{\rho_j^2} \frac{\partial^2}{\partial \varphi_j^2} \right] \psi = E \psi. \quad (17)$$

For free particles $E \geq 0$, so we put $E = \frac{k^2 \hbar^2}{2m}$ with $k > 0$. Then Eq. (17) takes the form

$$\sum_{j=1}^N \left[ \frac{1}{\rho_j} \frac{\partial}{\partial \rho_j} \left( \rho_j \frac{\partial}{\partial \rho_j} \right) + \frac{1}{\rho_j^2} \frac{\partial^2}{\partial \varphi_j^2} \right] \psi + k^2 \psi = 0. \quad (18)$$

When $N = 1$ we set $k \rho = z$ and $\psi(z, \varphi) = e^{il\varphi} f(z)$. The condition $\psi(z, \varphi = 0) = \psi(z, \varphi = 2\pi)$ gives $l = 0; \pm 1; \pm 2; \ldots; \pm \infty$. In the issue at $N = 1$, Eq. (18) leads to the Bessel equation

$$z^2 \frac{d^2 f}{dz^2} + \frac{df}{dz} + (z^2 - l^2) f = 0. \quad (19)$$

Its general solution is $f(z) = c_j J_l(z) + c_y Y_l(z)$, where $J_l(z)$ and $Y_l(z)$ are the Bessel function and the Weber function, respectively [72, 73, 74]. In view of the relations $J_{-l}(z) = (-1)^l J_l(z)$ and $Y_{-l}(z) = (-1)^l Y_l(z)$ [74] one can write $f(z) = c_j J_{|l|}(z) + c_y Y_{|l|}(z)$. Since $Y_{|l|}(z \to 0) \to \infty$, we reject the Weber function. Thus, Eq. (18) with $N = 1$ has the solutions $\psi_{l,k}(z) = e^{il\varphi} J_l(k \rho)$ $(l = 0; \pm 1; \ldots; \pm \infty)$ with the boundary condition $\psi_{l,k}(\rho = R) = 0$. Similarly, separating
variables, we find the solutions of Eq. (18) for $N > 1$ particles:

$$\psi_{\{l_j\}, \{k_j\}}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = c_{\{l_j\}, \{k_j\}} \sum_P e^{il_1\varphi_1 + \ldots + il_N\varphi_N} \prod_{j=1}^N J_{l_j}(k_j \rho_j),$$  \hspace{1cm} (20)

where $\sum_{j=1}^N k_j^2 = k^2$, $\sum_{j=1}^N l_j = l_z$, $c_{\{l_j\}, \{k_j\}}$ is a normalization constant, $\sum_P$ denotes the sum over all possible permutations of coordinates $(\varphi_1, \rho_1), \ldots, (\varphi_N, \rho_N)$. Here $l_z = L_z/h$ is fixed; it is the quantum number of the total angular momentum of the system. The sets $\{k_j\} = (k_1, \ldots, k_N)$ for each set $\{l_j\}$ must be found from the BC $J_{|l_1|}(k_1 R) = \ldots = J_{|l_N|}(k_N R) = 0$ (there is no need to take the equation $\sum_{j=1}^N k_j^2 = k^2$ into account, since $k^2$ is arbitrary). Each set $\{l_j\}$ must correspond to an infinite number of sets $\{k_j\}$ (because $J_l(z)|_{z \geq r_1, |l|} \approx \sqrt{\frac{2}{\pi z}} \cos \left(z - \frac{\ell \pi}{2} - \frac{\pi}{4}\right)$ \cite{72, 73, 74} and $z = k_j \rho \leq k_j R$ takes values on the segment $[0, \infty]$ since $k_j \in [0, \infty]$). The functions (20) form a complete set of orthonormal functions. The general solution corresponding to a given $l_z$ is a superposition of solutions (20) with all possible $\{l_j\} = (l_1, \ldots, l_N)$, satisfying the condition $\sum_{j=1}^N l_j = l_z$, and all $\{k_j\}$ for each set $\{l_j\}$:

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{\{l_j\}} \sum_{\{k_j\}} b(l_1, \ldots, l_N; k_1, \ldots, k_N) \psi_{\{l_j\}, \{k_j\}}(\mathbf{r}_1, \ldots, \mathbf{r}_N),$$  \hspace{1cm} (21)

where $l_j = 0; \pm 1; \ldots; \pm \infty$, $j = 1, \ldots, N$, and $b(l_1, \ldots, l_N; k_1, \ldots, k_N)$ are constants. The boundary condition $J_{|l_1|}(k_1 R) = \ldots = J_{|l_N|}(k_N R) = 0$ must be satisfied for each function (20).

As the two-particle distribution function is isotropic, for each state it must have the form $g_2(\mathbf{r}_1, \mathbf{r}_2) = f_1(\rho_1, \rho_2) + \Phi(\varphi_1 - \varphi_2)f_2(\rho_1, \rho_2)$, where $f_1$, $f_2$, and $\Phi$ are some functions. It is essential that $\Phi(\varphi_1 - \varphi_2) \neq \text{const}$, otherwise the dependence on angles would drop out, which is unphysical: such dependence is always present in real-life systems because the correlations between two atoms cannot depend only on $\rho_1$ and $\rho_2$. As is seen from the properties of the function $e^{il\varphi}$ and the Bessel functions, if in the total WF (21) the main weight falls on terms with $|l_1|, \ldots, |l_N| \sim 1$ then the solution should describe a liquid. A crystalline solution with any $l_z$ (including $l_z = 0$) may correspond to WF (21) with the main contribution from harmonics corresponding to $k_j \simeq 2\pi/a$ and $|l_j|$ of various magnitude from $\sim 1$ to $\sim \sqrt{N}$ (here, $a$ denotes the crystal lattice spacing).

States with $l_z \neq 0$ are degenerate and therefore must be excited states of the system. For such states, the total WF (21) can be written in the form $\psi = \psi_q \psi_0$, where $\psi_q$ is a nodeless WF of the ground state of the system and $\psi_q$ describes a single quasiparticle or a set of interacting quasiparticles. In this case, GS is that of states with $l_z = 0$, which has the lowest energy. We may expect from physical considerations that, at weak coupling, the function $\psi_q$ for a single quasiparticle is approximately reduced to the solution for a free particle: $\psi_q = \psi_{l_z k_q} \approx \frac{\epsilon_{l_z k_q}}{\sqrt{N}} \sum_j e^{i\varphi j} J_{|l_z|}(k_q \rho_j)$ \cite{75}. 

6 Conclusions

We have found that the perfect symmetry of a boundary-value problem can lead to unconventional properties of the system. In particular, the density $\rho(r) = mn(r)$ of a periodic system turns out to be a constant, and the two-particle distribution function of a system with rotational symmetry is always isotropic (therefore, a scattering will not produce the Bragg peaks). That is, perfect symmetry hides those inner properties of the system, which “break” this symmetry. In the examples above, these are nonuniformity and anisotropy. In real-life 1D and 2D systems, external fields necessarily violate the translation invariance of the Hamiltonian. While a real 3D system can be periodic only if it is the entire Universe. Therefore in realizable systems, $\rho(r)$ should not be a constant. Similarly with rotational symmetry: for real systems, the ideal rotational symmetry of BCs is at least slightly broken. In this case, a rotation does not transfer the system into an equivalent state, and the task becomes similar to that with strongly broken rotational symmetry. As a consequence, for the crystalline state, the two-particle distribution function should be anisotropic, and the Bragg peaks must be observed.

Another result is that symmetry together with Courant-Hilbert’s theorem narrows the possible properties of the ground state vastly but does not enable a choice to be made between crystalline and liquid ground state: both are equally permissible. We remark that the symmetry analysis cannot be used for real-life BCs, not having ideal symmetry. Because the symmetry analysis requires that both the Hamiltonian and the boundary conditions have the same symmetry.

The symmetry analysis allows one to ascertain an interesting property: the liquid to crystal transition does not imply spontaneous symmetry breaking (SSB). Indeed, the term “spontaneous symmetry breaking” is applied when the system transits from the state possessing the symmetry of the Hamiltonian to a state with lower symmetry. However, for the above-considered systems, the crystalline and liquid states are invariant under all symmetry transformations of the Hamiltonian and BCs. In this case, the liquid to crystal transition implies a physical change in symmetry since such a transition leads to a change in the properties of distribution functions. In real systems, the symmetry of BCs is much lower than the symmetry of the Hamiltonian. Therefore, crystalline and liquid solutions at $T = 0$ also have lower symmetry, which corresponds to boundary conditions. In this case, we virtually cannot verify whether SSB occurs under the given phase transition. So it seems correct to associate the liquid-to-crystal transition with spontaneous symmetry reduction, distinguishing the latter from SSB. Reduction of symmetry at the liquid-to-crystal transition can be ascertained by those changes in the properties of thermodynamic quantities and the structure factor that are associated with changes in the behavior of the distribution functions $g_{j \geq 2}(r_1, \ldots, r_j)$. All these properties evidence that the crystal solution is invariant under some discrete rotation group being a subgroup of the continuous group $O(3) = SO(3) \times C_1$, but the liquid solution
is invariant under the group $O(3)$ itself.

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7 Appendix. Proof of the nondegeneracy of the ground state

Consider the theorem on the nondegeneracy of GS and constraints for this theorem. Although the theorem is well-known, its proof is less known, and the conditions for the applicability of this theorem were seemingly not discussed in the literature.

In the classical monograph by R. Courant and D. Hilbert [5], the node theorem has been proved for one spinless particle located in a finite two-dimensional volume with zero BCs. The proof can be easily generalized to the case of a large number of particles and any dimensionality of space. The proof in [5] admits the presence of a finite degeneracy ($E_j = E_{j-1}$; the degeneracy is finite if the volume of the system is finite; see [5], §2). If GS is doubly degenerate, then one of the states is described by a nodeless WF $\psi_1$ (according to the node theorem). WF $\psi_2$ of the second state can have a single node, according to the same theorem. On the other hand, $\psi_2$ should be orthogonal to $\psi_1$ and, therefore, must have at least one node. Thus, the node theorem [5] admits a degeneracy of the ground state.

The nondegeneracy of GS has been proved at the other place of book [5]. The proof is based on Jacobi’s method (see [5], §7). We will give it in a slightly more detailed form.

Consider the Schrödinger equation

$$-\Delta \psi + U(x, y)\psi - E\psi = 0 \tag{22}$$

for one particle located in a 2D region $G = (x, y)$ with zero BCs ($\psi(x, y) = 0$ on the boundary of the region $G$). Here, $U(x, y)$ is a potential, and we set $\hbar = 2m = 1$. If there exists a solution $\psi_1$ of Eq. (22) corresponding to the smallest eigenvalue $E_1$, then $\psi_1$ can be found by solving the following variation problem [5]: the inequality

$$D[\varphi] = \int_G dxdy(\varphi_x^2 + \varphi_y^2 + U\varphi^2) \geq E_1 \int_G dxdy\varphi^2 \tag{23}$$

must be satisfied for all functions $\varphi(x, y)$ that are equal to zero on the boundary of the region $G$ and have “good” properties ($\varphi$ is to be continuous, whereas $\varphi_x$ and $\varphi_y$ are to be piecewise continuous). Here, $\varphi_x \equiv \partial\varphi/\partial x$, $\varphi_y \equiv \partial\varphi/\partial y$. Inequality (23) becomes equality only for $\varphi(x, y) = c_1\psi_1(x, y)$, where $c_1 = \text{const}$. It follows from the node theorem that $\psi_1$ has no nodes [5].

Assume that GS is degenerate and corresponds to two functions: $\psi_1$ and $\psi_2$. In this case, $\psi_1$ has no nodes, and $\psi_2$ must have one node (as was noted above). In this case, from the
variation viewpoint, \( \psi_1 \) and \( \psi_2 \) satisfy condition (23) and the zero BCs, and \( \psi_2 \) additionally satisfies the condition of orthogonality of the functions \( \psi_1 \) and \( \psi_2 \). Since \( \psi_1 \) has a constant sign everywhere inside \( G \), we may set \( \psi_2(x, y) = \vartheta(x, y)\psi_1(x, y) \). Let us ascertain whether such a solution is possible. We set \( \varphi(x, y) = \eta(x, y)\psi_1(x, y) \) in \( D[\varphi] \) (23). Then

\[
D[\varphi] = \int_G dxdy[\psi_1^2(\eta_x^2 + \eta_y^2) + \eta_x^2(\psi_1^2 + \psi_{1y}^2) + 2\psi_1\psi_{1x}\eta_x + 2\psi_1\psi_{1y}\eta_y + U\eta^2\psi_1^2].
\] (24)

Let us use the relations \( 2\eta_x = (\eta_x^2)_x \), \( 2\eta_y = (\eta_y^2)_y \) and integrate the terms with \( \eta_x \) and \( \eta_y \) by parts. We obtain two integrals over the boundary, both are zero due to the zero BCs, and the remaining terms give

\[
D[\varphi] = \int_G dxdy[\psi_1^2(\eta_x^2 + \eta_y^2) - \eta^2\psi_1\Delta\psi_1 + U\eta^2\psi_1^2].
\] (25)

Since \( \psi_1 \) satisfies Eq. (22) with \( E = E_1 \), formula (25) is reduced to

\[
D[\varphi] = \int_G dxdy[\psi_1^2(\eta_x^2 + \eta_y^2)] + E_1\eta^2\psi_1^2 \geq E_1 \int_G dxdy \varphi^2.
\] (26)

The equality is obtained only for \( \eta(x, y) = C = \text{const} \). Hence, the wave function corresponding to the energy \( E_1 \) can have only the form \( \text{const} \cdot \psi_1(x, y) \). Therefore, the solution \( \psi_2(x, y) = \vartheta(x, y)\psi_1(x, y) \) with \( \vartheta(x, y) \neq \text{const} \) is impossible. It proves that the lowest level is indispensably non-degenerate. In this case, any excited state \( \psi_{j>1}(x, y) \) can be degenerate (because \( \psi_{j>1}(x, y) \) has nodes and, therefore, the representation \( \varphi(x, y) = \eta(x, y)\psi_j(x, y) \) is inapplicable).

If we pass from \( x, y \) to \( r_1, \ldots, r_N \) in all formulae, the reasoning remains valid. Therefore, the conclusion about the nondegeneracy of GS is valid for systems with any \( N \) and for any dimensionality of space. The above analysis is carried out for a system under the zero BCs. We may expect that the main conclusion holds under any BCs.

An important point is the conditions under which this theorem works: (1) wave functions are real single-component; (2) the particle system is finite; (3) the particles do not have a spin, intrinsic dipole and higher multipole moment; (4) the total potential energy is finite: \( -\infty < \int dr_1 \cdots dr_N U(r_1, \ldots, r_N) |\Psi_0(r_1, \ldots, r_N)|^2 < \infty \). Conditions (1) and (2) are assumed in the proof. The violation of condition (4) makes impossible the transformation of inequality (23) into equality at finite \( E_1 \). Particles should be spinless because spin indirectly influences the structure of spatial WFs and energy levels of the system, which is not taken into account in the theorems by Courant and Hilbert. Particles cannot possess intrinsic multipole moment since the node theorem implies that the potential \( U \) depends solely on the spatial coordinates of the particles. More accurately: the theorem works if each particle has a moment whose magnitude and direction are fixed. However, in real systems of dimensionality \( \geq 2 \) the directions of the moments can change, which must lead to an additional strong degeneracy of states. If particles have the dipole or higher multipole moment, induced by interaction with
neighboring particles, the theorem remains valid (since such a moment is expressed in terms of the spatial coordinates of the particles \[76, 77, 78\]).

We note that Courant-Hilbert’s theorem on the nondegeneracy of GS has been proved only for the Schrödinger equation (22). This theorem also holds if the system is placed in an external field if it appears as a part of the potential \(U(x, y)\). But if the external fields lead to derivatives in the Schrödinger equation that are not reduced to \(const \cdot \Delta\), then the proof above does not work, and GS may be degenerate. In particular, the degeneracy of the lowest Landau level \[61, 62\] is related to the derivatives \(\partial/\partial x\) and \(\partial/\partial y\) (or \(\partial/\partial \varphi\)) in the Schrödinger equation. Therefore, this degeneracy does not contradict to Courant-Hilbert’s theorem. WFs with \(\theta\) symmetry also arise for the Schrödinger equation containing similar derivatives \[17\]. In both these cases, the external field is magnetic.

As another example, consider a ferromagnetic. Its GS corresponds to all codirectional atomic spins. In this case, spontaneous symmetry breaking occurs, and GS is infinitely degenerate under rotations, which contradicts Courant–Hilbert’s theorem. Low-lying levels of such a system are described by the exchange Hamiltonian \[79\]

\[
\hat{H} = -\frac{1}{2} \sum_{l \neq j} J(R_l - R_j) \hat{s}_l \hat{s}_j,
\]

(27)

where \(R_l\) denote the coordinates of lattice sites. In this instance, the violation of Courant–Hilbert’s theorem is related to the use of the spin operators \(\hat{s}_i\) (the potential \(U\) in (22) is an ordinary function). However, formally the Hamiltonian \[27\] follows from an ordinary Hamiltonian, which describes interacting nuclei and electrons, and contains no spin operators. Nevertheless, spin properties are present implicitly because the exchange interaction is a principal one only for atoms with the electronic shell of a certain structure. To comprehend this structure, one needs to take account of the Pauli principle and other properties of particles with a spin. In this instance, Courant–Hilbert’s theorem is violated because the particles have a spin. The theorem works exclusively for spinless particles.

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