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Multipole degrees of freedom in physics of high-spin quantum atomic gases

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We provide the general arguments that quantum atomic gases of interacting high-spin atoms represent a physical system in which the multipole (hidden) degrees of freedom may be manifested. Their manifestation occurs when the interatomic interaction is of non-local type. For a local interaction described by the *s*-wave scattering length, the multipole degrees of freedom do not reveal themselves. To illustrate our findings, we theoretically examine the phenomenon of Bose–Einstein condensation in an interacting gas of spin-1 atoms in an external magnetic field. This study is based on the SU(2) invariant Hamiltonian, which has a bilinear structure in the spin and quadrupole operators along with the scalar term. It is shown that depending on the conditions imposed on the interaction amplitudes (stability conditions), the ground state of the system may exhibit three different phases: quadrupolar, ferromagnetic, and paramagnetic. The basic thermodynamic characteristics affected by hidden degrees of freedom are found for all phases.

Keywords: high-spin atoms, quantum atomic gases, Bose–Einstein condensation.

1. Introduction

The spin degrees of freedom of the structural units of matter and their interaction significantly affect the collective properties of many-body systems giving rise to different magnetic states such as traditional ferromagnetic and antiferromagnetic [1, 2] phases in the simplest spin-1/2 systems, as well as nematic and other orderings [3–14] in high-spin systems. This fully applies ultracold atomic gases, especially since the connection between the spin and statistics is manifested exactly at low temperatures dividing the atoms into the bosons and fermions.

In particular, dilute Bose gases of alkali atoms undergo Bose–Einstein condensation (BEC) below some critical temperature. This unique phenomenon, consisting in accumulation of a macroscopic number of bosonic atoms in a single state, was experimentally proved [15–17] seventy years after its theoretical prediction [18]. Somewhat later, it was theoretically demonstrated that the spin degrees of freedom of atoms and their interaction lead to a number of features in the formation of BEC in ultracold spin-1 gases [19–22] including ferromagnetic and antiferromagnetic (polar) phases. The number of possible magnetically-ordered ground states increases as the atomic spin grows [23]. Spinor gases with BEC are unique in that they simultaneously manifest two different phenomena such as superfluidity and magnetism, both of which are associated with spontaneous symmetry breaking. Moreover, they can be used to observe a number of interesting phenomena. One can indicate, for example, the ability to control the speed of electromagnetic waves in ultracold gases with BEC applying an external magnetic field [24–26], including encryption and filtering of a useful electromagnetic signal [27]. The high-spin atomic Fermi gases ($S > 1/2$) also provide the possibility to study new spin-dependent phenomena. In particular, being loaded to an optical lattice, they represent the effective simulator of superfluid and magnetic phenomena, which are difficult to probe in real materials [28–30].

Usually, the interaction effects in ultracold quantum atomic gases with low-energy collisions of atoms are described by the *s*-wave scattering lengths. In this case, for spin-1 atoms, it is sufficient to consider two terms in the many-body interaction Hamiltonian with the corresponding coupling constants expressed through the scattering lengths [19, 21, 23]. The first one does not contain the spin operators at all, while the second term, bilinear in them, is of the Heisenberg form. At the same time, it is well known that in high-spin systems ($S \geqslant 1$), such as solid-state magnets, the spin-spin interaction has a more complicated character that

goes beyond the usual Heisenberg form [4]. In addition, their description requires to introducing the multipole degrees of freedom (quadrupole for $S = 1$, octupole for $S = 3/2$, and so on). To the best of our knowledge, although the multipole degrees of freedom were theoretically predicted for the solid-state magnets, there is still no strong experimental evidence of their manifestation despite attempts to detect them [31, 32].

Since the ultracold gases of high-spin atoms exhibit a very high control of the relevant physical parameters, a natural question arises as to under what conditions the multipole degrees of freedom are manifested in this kind of systems. This motivates us to examine a many-body Hamiltonian of pairwise interaction for spin-S atoms and apply it to study spin-1 BEC with quadrupole degrees of freedom in the framework of the Bogoliubov model for a weakly interacting Bose gas [33]. We show that the well-known scattering length approximation [34, 35] (local interaction) is insufficient to consider the interaction effects associated with quadrupole degrees of freedom. In order to study their manifestation, the interaction must be of the finite-range (non-local interaction) [36]. Even though the scattering-length approximation well describes the interaction effects in ultracold gases, it also has some disadvantages. In particular, it leads to divergences of the ground state energy or chemical potential computed within the Bogoliubov model for a weakly interacting Bose gas, so that some artificial renormalization procedure for the coupling constant is necessary to remove them [34, 35, 37]. For spinor condensates, the scattering length approximation does not reproduce the complete structure of the single-particle excitation spectra, making some of them independent of the interaction parameters [36]. The issue of non-local interaction has been recently discussed both for ultracold Bose [38, 39] and Fermi [40–42] gases.

2. Single-particle density matrix and multipole degrees of freedom

Let us consider the emergence of multipole description parameters by studying the single-particle density matrix of spin-S atoms,

$$f_{\alpha\beta}(\mathbf{p},\mathbf{p}') = \mathrm{Tr}\,\rho a^{\dagger}_{\mathbf{p}'\beta} a_{\mathbf{p}\alpha}. \tag{1}$$

Here $a^{\dagger}_{\mathbf{p}\alpha}$ and $a_{\mathbf{p}\alpha}$ are the creation and annihilation operators, where the momentum p and spin projection α specify the individual single-particle state. Depending on the statistics, these operators satisfy the bosonic commutation (in case of integer spin) or fermionic anticommutation (in case of half-integer spin) relations,

$$[a_{\mathbf{p}\alpha}, a^{\dagger}_{\mathbf{p}'\beta}]_B = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\alpha\beta}, \quad [a_{\mathbf{p}\alpha}, a_{\mathbf{p}'\alpha'}]_B = 0, \tag{2}$$

$$\{a_{\mathbf{p}\alpha}, a^{\dagger}_{\mathbf{p}'\beta}\}_F = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\alpha\beta}, \quad \{a_{\mathbf{p}\alpha}, a_{\mathbf{p}'\alpha'}\}_F = 0. \tag{3}$$

For non-equilibrium systems, the statistical operator $\rho = \rho(t)$ satisfies the Liouville equation,

$$i\hbar\frac{\partial\rho(t)}{\partial t} = [H, \rho(t)],$$

where H is the system Hamiltonian. If the system is in the equilibrium state, then ρ is replaced by the Gibbs statistical operator w defined by Eq. (11) (see below). Therefore, Eq. (1) provides a general definition of the single-particle density matrix, which is independent of statistics and is valid for both equilibrium and non-equilibrium systems.

The single-particle density matrix $f_{\alpha\beta}(\mathbf{p},\mathbf{p}')$ representing the square $n\times n$ matrix with $n = 2S+1$ can be decomposed over the complete set of n^2 independent $n\times n$ matrices. As such basis matrices, one can choose the identity matrix $I \equiv \delta_{\alpha\beta}$ and $n^2 - 1$ generators T^a of the SU(n) group. Therefore, we can write

$$f_{\alpha\beta}(\mathbf{p},\mathbf{p}') = f^0(\mathbf{p},\mathbf{p}')\delta_{\alpha\beta} + \sum_{a=1}^{(2S+1)^2-1} f^a(\mathbf{p},\mathbf{p}')T^a_{\alpha\beta}. \tag{4}$$

The generators T^a, being independent Hermitian ($T^a = T^{a\dagger}$) and traceless ($\mathrm{Tr}T^a \equiv T^a_{\alpha\alpha} = 0$; here and below, summation over repeated indices is assumed) matrices meet the following commutation relations (see, e.g., [1]):

$$[T^a, T^b] = if^{abc}T^c, \quad f^{abc} = -f^{bac} = f^{bca}, \tag{5}$$

where f^{abc} are the structure constants. Taking into account the following property of T^a:

$$T^a_{\alpha\beta}T^b_{\beta\alpha} = \frac{1}{2}\delta_{ab}, \quad a,b = 1,\ldots (2S+1)^2 - 1, \tag{6}$$

one finds the coefficients $f^0(\mathbf{p},\mathbf{p}')$ and $f^a(\mathbf{p},\mathbf{p}')$ in Eq. (4),

$$f^0(\mathbf{p},\mathbf{p}') = \frac{1}{2S+1}f_{\alpha\alpha}(\mathbf{p},\mathbf{p}'), \quad f^a(\mathbf{p},\mathbf{p}') = 2T^a_{\alpha\beta}f_{\beta\alpha}(\mathbf{p},\mathbf{p}').$$

Equation (1) allows to represent the scalar $f^0(\mathbf{p},\mathbf{p}')$ and vectorial $f^a(\mathbf{p},\mathbf{p}')$ parts of the single-particle density matrix in the form

$$f^0(\mathbf{p},\mathbf{p}') = \frac{1}{2S+1}\mathrm{Sp}\,\rho a^{\dagger}_{\mathbf{p}'\alpha}a_{\mathbf{p}\alpha},$$

$$f^a(\mathbf{p},\mathbf{p}') = 2\mathrm{Sp}\,\rho a^{\dagger}_{\mathbf{p}'\alpha}T^a_{\alpha\beta}a_{\mathbf{p}\beta}. \tag{7}$$

It is worth noting that the vectorial parameter $f^a(\mathbf{p},\mathbf{p}')$ of dimension $(2S+1)^2 - 1$ appear in a natural way, from purely mathematical considerations. This parameter is induced by the spin of the structural units of matter and it specifies the macroscopic state of a many-body system. For spatially homogeneous states, Eqs. (7) read

$$f^0(\mathbf{p},\mathbf{p}') = f^0(\mathbf{p})\delta_{\mathbf{p}\mathbf{p}'} = \frac{1}{2S+1}\mathrm{Sp}\,\rho a^{\dagger}_{\mathbf{p}\alpha}a_{\mathbf{p}\alpha}\delta_{\mathbf{p}\mathbf{p}'},$$

$$f^a(\mathbf{p},\mathbf{p}') = f^a(\mathbf{p})\delta_{\mathbf{p}\mathbf{p}'} = 2\mathrm{Sp}\,\rho a^{\dagger}_{\mathbf{p}\alpha}T^a_{\alpha\beta}a_{\mathbf{p}\beta}\delta_{\mathbf{p}\mathbf{p}'}. \tag{8}$$

Note that the quantity

$$\Sigma^a = 2\sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} T^a_{\alpha\beta} a_{\mathbf{p}\beta} \tag{9}$$

represents the generalization of the total spin operator

$$\mathbf{S} = \sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} \mathbf{S}_{\alpha\beta} a_{\mathbf{p}\beta}.$$

From the above point of view, the many-body system of spin-1/2 particles is very specific. Indeed, in this case, three Pauli matrices

$$\sigma^1 \equiv \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 \equiv \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma^3 \equiv \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{10}$$

can be chosen to be the generators of the SU(2) group, $T^a_{\alpha\beta} \equiv (1/2)\sigma^i_{\alpha\beta}$ $(a = i = 1, 2, 3)$. Therefore, according to Eq. (9), the system is completely described by a three component vector Σ^a related to the total spin by $\Sigma^a \equiv 2S^i$ $S^i_{\alpha\beta} = (1/2)\sigma^i_{\alpha\beta}$. The latter determines the physically observable magnetization vector. Note that no additional description parameters emerge in this case.

The situation becomes completely different for macroscopic systems of high-spin atoms ($S \geqslant 1$). In the simplest spin-1 case, according to Eq. (4), we should consider eight generators of the SU(3) group with the properties given by Eqs. (5), (6). These generators can be realized by a set of eight 3×3 Gell–Mann matrices $\lambda^a = 2T^a$ $(a = 1, \ldots, 8)$, which are Hermitian and traceless (see Eqs. (15) below). Now the macroscopic description parameter Σ^a of the system represents the eight-component vector. As we see below, its three components can be related with the total spin of the system or magnetization vector, while the remaining five components can be interpreted as the quadrupole operators associated with the quadrupole matrix.

It is evident that the number of operators associated with the internal symmetry increases as the spin of the structural units of matter grows. In particular, for spin-3/2 atoms (SU(4) group), we have $(2S+1)^2 - 1 = 15 = 3 + 5 + 7$ operators. Three of them should be associated with the spin components, other five and seven operators with quadrupole and octupole degrees of freedom, respectively.

Before studying the system with interatomic interaction, we consider an ideal gas of spin-1 atoms in equilibrium by performing calculation of the single-particle density matrix and by giving a physical interpretation of the Gell–Mann generators. The equilibrium state of a many-body system is completely described by the Gibbs statistical operator,

$$w = \exp\left[\Omega - \beta\left(H - \mu N\right)\right], \tag{11}$$

where H is the Hamiltonian of the system (it may include the interaction terms) and N is the particle number operator representing the additive integral of motion given by

$$N = \sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha}. \tag{12}$$

The grand thermodynamic potential Ω as a function of reciprocal temperature $\beta = 1/T$ and chemical potential μ is found from the normalization condition $\mathrm{Sp}\, w = 1$, which gives

$$\Omega = -\ln \mathrm{Sp} \exp\left[-\beta\left(H - \mu N\right)\right]. \tag{13}$$

The system is supposed to be at rest so that its translational and angular velocities are zero. Otherwise, two other integrals of motion such as the operators of total momentum and angular momentum should be introduced into the Gibbs exponent. Moreover, since the operators of the total momentum and angular momentum do not commute, the rotating system is inhomogeneous. Note that the statistical operator in the form of Eq. (11) describes only the normal equilibrium states. If the symmetry is spontaneously broken, then one should apply the Bogoliubov quasiaverage concept [44–48], which consists in adding infinitely small symmetry breaking terms in Eq. (11). In particular, for Bose condensed systems studied below, the method of quasiaverages and principle of spatial correlation weakening allow to justify the replacement of creation and annihilation operators by c-numbers.

Since the spin of an atom reveals in a magnetic field, let us find the single-particle density matrix for a homogeneous ideal gas in an external magnetic field **B** directed along z-axis, **B** = (0, 0, B). The Hamiltonian of such a system reads,

$$H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha} + g\mu_B B \sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} S^z_{\alpha\beta} a_{\mathbf{p}\beta}, \tag{14}$$

where $\varepsilon_{\mathbf{p}} = p^2/2m$ is the kinetic energy of an atom with mass m, g is the Landè hyperfine factor, $\mu_B = e\hbar/2m_e$ is the Bohr magneton (e is the elementary charge and m_e is the electron rest mass), and S^z is the z-component of the spin operator.

In the simplest case of spin-1/2 atoms, the equilibrium single-particle density matrix is determined by Eqs. (8), where ρ and T^a are replaced by the Gibbs statistical operator w and Pauli matrices $\sigma^i/2$, respectively. Then, the standard technique (see, e.g., [4]) for computing the corresponding quantities yields,

$$f^0(\mathbf{p}) = \frac{1}{2}\left[\frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu - \mu_B B] + 1} + \frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu + \mu_B B] + 1}\right],$$

$$f^i(\mathbf{p}) = \delta_{iz}\left[\frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu - \mu_B B] + 1} - \frac{1}{\exp[\varepsilon(p) - \mu + \mu_B B] + 1}\right].$$

Therefore, an external applied magnetic field induces magnetization $M^i = (g\mu_B/2)\sum_{\mathbf{p}} f^i(\mathbf{p})$ which turns to zero when $B = 0$.

Now we address the description of an ideal gas of spin-1 atoms in a magnetic field using the Hamiltonian determined by Eq. (14). In this case, the single-particle density matrix is decomposed over the complete set of 3×3 matrices. As such a basis, one can choose the identity matrix and eight linearly independent Gell–Mann matrices $\lambda^a = 2T^a \quad (a = 1, \ldots 8)$. The latter represent the generators of the SU(3) group and given by

$$\lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda^6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \qquad (15)$$

According to Eq. (8), the scalar and vectorial part of the single-particle density matrix become,

$$f^0(\mathbf{p}) = \frac{1}{3} \mathrm{Tr}\, w a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha}, \quad f^a(\mathbf{p}) = \mathrm{Tr}\, w a^\dagger_{\mathbf{p}\alpha} \lambda^a_{\alpha\beta} a_{\mathbf{p}\beta}. \qquad (16)$$

The spin-1 operators entering the Gibbs exponent through the Hamiltonian [see Eq. (14)] are expressed in terms of the Gell–Mann matrices as follows:

$$S^x = \frac{1}{\sqrt{2}}(\lambda^1 + \lambda^6) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$S^y = \frac{1}{\sqrt{2}}(\lambda^2 + \lambda^7) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

$$S^z = \frac{1}{2}(\lambda^3 + \sqrt{3}\lambda^8) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \qquad (17)$$

Again, applying the standard procedure to compute traces in Eq. (16), one obtains the following expression for the single-particle density matrix:

$$f_{\alpha\beta}(\mathbf{p}) = \frac{1}{3}\left[f_{-1}(\mathbf{p}) + f_0(\mathbf{p}) + f_1(\mathbf{p})\right]\delta_{\alpha\beta} + \\ + \frac{1}{2}\left[f_{-1}(\mathbf{p}) - f_0(\mathbf{p})\right]\lambda^3_{\alpha\beta} + \\ + \frac{1}{2\sqrt{3}}\left[f_{-1}(\mathbf{p}) + f_0(\mathbf{p}) - 2f_1(\mathbf{p})\right]\lambda^8_{\alpha\beta},$$

where

$$f_{-1}(\mathbf{p}) = \frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu - \mu_B B] - 1},$$

$$f_0(\mathbf{p}) = \frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu] - 1},$$

$$f_1(\mathbf{p}) = \frac{1}{\exp[\varepsilon(\mathbf{p}) - \mu + \mu_B B] - 1}.$$

Finally, taking into account Eqs. (17), we arrive at

$$f_{\alpha\beta}(\mathbf{p}) = \frac{1}{3}\left[f_{-1}(\mathbf{p}) + f_0(\mathbf{p}) + f_1(\mathbf{p})\right]\delta_{\alpha\beta} + \\ + \frac{1}{2}\left[f_{-1}(\mathbf{p}) - f_1(\mathbf{p})\right]S^z_{\alpha\beta} + \\ + \frac{1}{4}\left[f_{-1}(\mathbf{p}) - 2f_0(\mathbf{p}) + f_1(\mathbf{p})\right]\left[\lambda^3_{\alpha\beta} - \frac{1}{\sqrt{3}}\lambda^8_{\alpha\beta}\right]. \qquad (18)$$

The first two terms in Eq. (18) determine the atomic density and magnetization respectively, while the third term indicates the emergence of additional degrees of freedom induced in a many-body system by the spin of atoms. Therefore, a natural question arises as to what physical characteristics are sensitive to these additional parameters. It is clear that the single-particle density matrix itself cannot be measured experimentally. The only measurable physical quantity associated with internal degrees of freedom is the magnetization vector of the system. The latter is found to be

$$M^z = g\mu_B S^z_{\alpha\beta} \sum_{\mathbf{p}} f_{\beta\alpha}(\mathbf{p}) = g\mu_B \sum_{\mathbf{p}} (f_{-1}(\mathbf{p}) - f_1(\mathbf{p})).$$

However, this quantity is determined purely by the atomic spin and the mentioned additional parameters do not affect its structure. One can show that they also do not modify the heat capacity, pressure, and other characteristics of an ideal gas. Therefore, in order to predict the physical characteristics that might reveal additional degrees of freedom it is necessary, first of all, to take into account properly the interatomic interaction that involves these degrees of freedom.

Before starting to solve the declared problem, let us find out, at least in spin-1 case, the physical interpretation of all operators λ^a required to describe a many-body system. To this end, we take the realization of spin-1 operators in the vector (Cartesian) basis $|x\rangle, |y\rangle, |z\rangle$,

$$\langle i \,|\, k \rangle = \delta_{ik}, \quad S^i \,|\, k \rangle = i\varepsilon_{ikl} \,|\, l \rangle, \qquad (19)$$

so that S^i meet the commutation relations for spin operators $[S^i, S^k] = i\varepsilon_{ikl} S^l$ and $S^2 = S(S+1)I$. Then, Eq. (19) gives

$$\langle k \,|\, S^i \,|\, l \rangle \equiv (S^i)_{kl} = -i\varepsilon_{ikl},$$

wherefrom

$$S^x=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},\quad S^y=\begin{pmatrix}0&0&i\\0&0&0\\-i&0&0\end{pmatrix},\quad S^z=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix}. \tag{20}$$

Performing the comparison of Eqs. (20) with Eqs. (15) we have $S^x\equiv\lambda^7$, $S^y\equiv-\lambda^5$, and $S^z\equiv\lambda^2$. The other five Gell–Mann operators are found to be

$$\lambda^1=-\{S^x,S^y\},\quad \lambda^3=(S^y)^2-(S^x)^2,\quad \lambda^4=-\{S^x,S^z\},$$

$$\lambda^6=-\{S^y,S^z\},\quad \lambda^8=\sqrt{3}(S^z)^2-\frac{2}{\sqrt{3}}I, \tag{21}$$

where $\{a,b\}=ab+ba$ and I is the unit 3×3 matrix. As the next step, consider the traceless quadrupole matrix, $\mathcal{Q}^{ik}\equiv S^iS^k+S^kS^i-(4/3)\delta_{ik}$ (see, e.g., [40]). In this way, one can easily seen that it is completely specified by the above five Gell–Mann operators,

$$\mathcal{Q}^{ik}=\begin{pmatrix}-\lambda^3-\lambda^8/\sqrt{3}&-\lambda^1&-\lambda^4\\-\lambda^1&\lambda^3-\lambda^8/\sqrt{3}&-\lambda^6\\-\lambda^4&-\lambda^6&2\lambda^8/\sqrt{3}\end{pmatrix}. \tag{22}$$

For this reason, operators given by Eq. (21) are interpreted as quadrupole operators. These five quantities can be organized to form a five-component vector

$$q^b=(-\lambda^1,-\lambda^3,-\lambda^4,-\lambda^6,\lambda^8).$$

Hence, in case of spin-1 system, there are eight many-body operators associated with internal symmetry [compare to Eq. (9)],

$$\Lambda^a=\sum_{\mathbf{p}}a^\dagger_{\mathbf{p}\alpha}\lambda^a_{\alpha\beta}a_{\mathbf{p}\beta},\quad a=1,\ldots 8. \tag{23}$$

They can be split into the total spin operator of the system,

$$S^i=\sum_{\mathbf{p}}a^\dagger_{\mathbf{p}\alpha}S^i_{\alpha\beta}a_{\mathbf{p}\beta},\quad S^i=(S^x=\lambda^7,S^y=-\lambda^5,S^z=\lambda^2), \tag{24}$$

and quadrupole operator,

$$Q^b=\sum_{\mathbf{p}}a^\dagger_{\mathbf{p}\alpha}q^b_{\alpha\beta}a_{\mathbf{p}\beta},\quad q^b=(-\lambda^1,-\lambda^3,-\lambda^4,-\lambda^6,\lambda^8). \tag{25}$$

Note that the multipole (quadrupole) operators are uniquely determined by the spin operator of the quantum system.

3. Many-body Hamiltonian of pairwise interaction

SU(2) invariant Hamiltonian. To understand the structure of a many-body Hamiltonian of pairwise interaction, which would include both spin and quadrupole operators, consider a collision of two identical atoms with spin $S=1$. In general case, when colliding, two bosonic atoms can couple to form the states with total spin $\mathcal{S}=0,1,2$. Let $g_{\mathcal{S}}$ be the coupling constants corresponding to three-channel scattering. Following [28], we write the interaction Hamiltonian in the form $V=g_0P_0+g_1P_1+g_2P_2$, where $P_{\mathcal{S}}$ is the projection operator onto a two-body state with the total spin angular momentum $\mathcal{S}$, which has the following properties: $P_{\mathcal{S}}P_{\mathcal{S}'}=\delta_{\mathcal{S}\mathcal{S}'}$ and $P_{\mathcal{S}}^2=1$. The projection operators are found from the following system of coupled equations:

$$\mathbf{S}_1\cdot\mathbf{S}_2=-2P_0-P_1+P_2,\quad (\mathbf{S}_1\cdot\mathbf{S}_2)^2=P_2+P_1+4P_0,$$

$$P_0+P_1+P_2=1. \tag{26}$$

The first two equations follow from the relation: $\mathbf{S}_1\cdot\mathbf{S}_2=\sum_{\mathcal{S}=0}^{2}\lambda_{\mathcal{S}}P_{\mathcal{S}}$, where $\lambda_{\mathcal{S}}=\frac{1}{2}\big[\mathcal{S}(\mathcal{S}+1)-2S(S+1)\big]$, while the third equation represents the completeness condition for the projection operator. The solution of Eqs. (26) is found to be

$$P_0=\frac{1}{3}\Big[(\mathbf{S}_1\cdot\mathbf{S}_2)^2-1\Big],\quad P_1=1-\frac{1}{2}\Big[(\mathbf{S}_1\cdot\mathbf{S}_2)+(\mathbf{S}_1\cdot\mathbf{S}_2)^2\Big],$$

$$P_2=\frac{1}{3}+\frac{1}{2}(\mathbf{S}_1\cdot\mathbf{S}_2)+\frac{1}{6}(\mathbf{S}_1\cdot\mathbf{S}_2)^2.$$

Therefore, the interaction Hamiltonian under consideration becomes [46],

$$V=c_0+c_1(\mathbf{S}_1\cdot\mathbf{S}_2)+c_2(\mathbf{S}_1\cdot\mathbf{S}_2)^2, \tag{27}$$

with

$$c_0=g_1+\frac{1}{3}(g_2-g_0),\quad c_1=\frac{1}{2}(g_2-g_1),$$

$$c_2=\frac{1}{3}\left(g_0-\frac{3g_1}{2}+\frac{g_2}{2}\right). \tag{28}$$

As we see, for three-channel scattering characterized by the total spin $\mathcal{S}=0,1,2$, the interaction Hamiltonian is specified by both bilinear and biquadratic terms in the spin operators.

If the interaction between the atoms is of local character and parameterized by the *s*-wave scattering length $a_{\mathcal{S}}$ so that $g_{\mathcal{S}}=4\pi\hbar^2a_{\mathcal{S}}/m$, then the scattering with $\mathcal{S}=1$ is forbidden, since in *s*-state of relative motion the unit angular momentum is ruled out because the wave function must be symmetric under exchange ot two atoms. In this case $P_1=0$ and the biquadratic term in spin operators becomes $(\mathbf{S}_1\cdot\mathbf{S}_2)^2=2-(\mathbf{S}_1\cdot\mathbf{S}_2)$ so that the interaction Hamiltonian reduces to the form [21], $V=\tilde{c}_0+\tilde{c}_2(\mathbf{S}_1\cdot\mathbf{S}_2)$, where $\tilde{c}_0=1/3(g_0+2g_2)$ and $\tilde{c}_2=1/3(g_2-g_0)$. Therefore, for local interaction parameterized by *s*-wave scattering length, the Hamiltonian is of the Heisenberg type: it contains the spin-independent term and the term, which is bilinear in the spin operators. This is in contrast to Eq. (27), which does not employ the scattering-length approximation.

Now we formulate a many-body Hamiltonian of pairwise interaction constructed from both spin and quadrupole operators and show that its structure is consistent with Eq. (27). Taking into account Eqs. (24) and (25) and employing the general rules for constructing two-body operators in the second quantization method we represent the interaction Hamiltonian in the following general form, which does not imply parameterization by the scattering length:

$$V = V_U + V_J + V_K, \tag{29}$$

with

$$V_U = \frac{1}{2\mathcal{V}} \sum_{\mathbf{p}_1,\cdots\mathbf{p}_4} U(\mathbf{p}_1 - \mathbf{p}_3) a^\dagger_{\mathbf{p}_1\alpha} a^\dagger_{\mathbf{p}_2\beta} a_{\mathbf{p}_3\alpha} a_{\mathbf{p}_4\beta} \delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4}, \tag{30}$$

$$V_J = \frac{1}{2\mathcal{V}} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} J(\mathbf{p}_1 - \mathbf{p}_3) a^\dagger_{\mathbf{p}_1\alpha} a^\dagger_{\mathbf{p}_2\beta} S^i_{\alpha\gamma} S^i_{\beta\delta} a_{\mathbf{p}_3\gamma} a_{\mathbf{p}_4\delta} \delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4}, \tag{31}$$

$$V_K = \frac{1}{2\mathcal{V}} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} K(\mathbf{p}_1 - \mathbf{p}_3) a^\dagger_{\mathbf{p}_1\alpha} a^\dagger_{\mathbf{p}_2\beta} q^b_{\alpha\gamma} q^b_{\beta\delta} a_{\mathbf{p}_3\gamma} a_{\mathbf{p}_4\delta} \delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4}, \tag{32}$$

where $U(\mathbf{p})$, $J(\mathbf{p})$, and $K(\mathbf{p})$ are the Fourier transforms of the corresponding interaction energies and $\mathcal{V}$ is the volume of the system. The Hamiltonian given by Eqs. (29)–(32) is SU(2) invariant, since $[V, S^i] = 0$, where S^i is the total spin operator determined by Eq. (24). Next, employing the formulae below that relate the Gell–Mann matrices to squares and mixed products of the spin components:

$$(S^x)^2 = \frac{1}{2}\left(-\lambda^3 - \frac{1}{\sqrt{3}}\lambda^8 + \frac{4}{3}\right),$$

$$(S^y)^2 = \frac{1}{2}\left(\lambda^3 - \frac{1}{\sqrt{3}}\lambda^8 + \frac{4}{3}\right), \quad (S^z)^2 = \frac{1}{3}\left(\sqrt{3}\lambda^8 + 2\right)$$

and

$$S^xS^y = -\frac{1}{2}\left(\lambda^1 - i\lambda^2\right), \quad S^yS^x = -\frac{1}{2}\left(\lambda^1 + i\lambda^2\right),$$

$$S^xS^z = -\frac{1}{2}\left(\lambda^4 - i\lambda^5\right), \quad S^zS^x = -\frac{1}{2}\left(\lambda^4 + i\lambda^5\right),$$

$$S^yS^z = -\frac{1}{2}\left(\lambda^6 - i\lambda^7\right), \quad S^zS^y = -\frac{1}{2}\left(\lambda^6 + i\lambda^7\right),$$

we arrive at following quantity entering the interaction Hamiltonian [see Eq. (32)]:

$$\frac{1}{2} q^b_{\alpha\gamma} q^b_{\beta\delta} = S^i_{\alpha\sigma} S^i_{\beta\rho} S^k_{\sigma\gamma} S^k_{\rho\delta} + \frac{1}{2} S^i_{\alpha\gamma} S^i_{\beta\delta} - \frac{4}{3}\delta_{\alpha\gamma}\delta_{\beta\delta}.$$

Therefore, a comparison of Eq. (27) to Eqs. (29)–(32) allows us to conclude that the involvement of the quadrupole degrees of freedom specified by the generators of the SU(3) group is equivalent to emergence of the biquadratic terms in the interaction Hamiltonian.

SU(3) invariant Hamiltonian. Since for ultracold gases the interaction parameters can be adjusted using the Feshbach resonance [49, 50], one can achieve the equality, $J(\mathbf{p}) = K(\mathbf{p})$, so that the interaction Hamiltonian takes the form,

$$V_{SU(3)} = \frac{1}{2\mathcal{V}} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} U(\mathbf{p}_1 - \mathbf{p}_3) a^\dagger_{\mathbf{p}_1\alpha} a^\dagger_{\mathbf{p}_2\beta} a_{\mathbf{p}_3\alpha} a_{\mathbf{p}_4\beta} \delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4} +$$

$$+ \frac{1}{2\mathcal{V}} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} J(\mathbf{p}_1 - \mathbf{p}_3) a^\dagger_{\mathbf{p}_1\alpha} a^\dagger_{\mathbf{p}_2\beta} \lambda^a_{\alpha\gamma} \lambda^a_{\beta\delta} a_{\mathbf{p}_3\gamma} a_{\mathbf{p}_4\delta} \delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4}. \tag{33}$$

This Hamiltonian is SU(3) invariant since $[V_{SU(3)}, \Lambda^a] = 0$, where Λ^a is determined by Eq. (23) [this becomes obvious if we use Eqs. (2) and (5)].

The structure of a more general SU(n) invariant Hamiltonian can also be understand in the framework of the phenomenological quasiparticle approach in which the energy of the system is considered to be a functional of the single-particle density matrix, like in the normal Fermi-liquid theory [51, 52]. In the case of low density systems, we can take the energy functional quadratic in the single-particle density matrix,

$$E(f) = E_0(f) + E_{\text{int}}(f), \tag{34}$$

with

$$E_0(f) = \sum_{\mathbf{p}_1,\mathbf{p}_2} \varepsilon_{\alpha_1\alpha_2}(\mathbf{p}_1,\mathbf{p}_2) f_{\alpha_2\alpha_1}(\mathbf{p}_2,\mathbf{p}_1),$$

$$E_{\text{int}}(f) = \frac{1}{2} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} f_{\alpha_1\alpha_2}(\mathbf{p}_1,\mathbf{p}_2) \times$$

$$\times F_{\alpha_2\alpha_1;\alpha_4\alpha_3}(\mathbf{p}_2,\mathbf{p}_1;\mathbf{p}_4,\mathbf{p}_3) f_{\alpha_3\alpha_4}(\mathbf{p}_3,\mathbf{p}_4), \tag{35}$$

where $\varepsilon_{\alpha_1\alpha_2}(\mathbf{p}_1,\mathbf{p}_2)$ is the quasiparticle energy representing the first variational derivative of the energy functional $E(f)$. Since the interaction amplitude $F_{\alpha_2\alpha_1;\alpha_4\alpha_3}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_4,\mathbf{p}_3)$ represents the second variational derivative of the energy functional with respect to $f_{\alpha_1\alpha_2}(\mathbf{p}_1,\mathbf{p}_2)$, it has the following property:

$$F_{\alpha_2\alpha_1;\alpha_4\alpha_3}(\mathbf{p}_2,\mathbf{p}_1;\mathbf{p}_4,\mathbf{p}_3) = F_{\alpha_4\alpha_3;\alpha_2\alpha_1}(\mathbf{p}_4,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_1). \tag{36}$$

If to require the SU(n) symmetry of the interaction term in the energy functional, then one can write

$$F_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3) = F^{(1)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)\delta_{\alpha_1\alpha_2}\delta_{\alpha_4\alpha_3} +$$

$$+ F^{(2)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3) T^{(a)}_{\alpha_1\alpha_2} T^{(a)}_{\alpha_4\alpha_3}, \tag{37}$$

where the amplitudes $F^{(1)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)$ and $F^{(2)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)$, according to Eq. (36), satisfy the following symmetry conditions:

$$F^{(1)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=F^{(1)}(\mathbf{p}_4,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_2),$$

$$F^{(2)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=F^{(2)}(\mathbf{p}_4,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_2) \qquad (38)$$

and can be expressed in terms of the interaction amplitude $F_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)$ as follows [see Eq. (6)]:

$$F^{(1)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=\frac{1}{(2S+1)^2}F_{\alpha\alpha;\beta\beta}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3),$$

$$F^{(2)}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=$$

$$=\frac{1}{S(S+1)}T^a_{\alpha_3\alpha_4}T^a_{\alpha_2\alpha_1}F_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3). \qquad (39)$$

On the other hand, the general quantum-mechanical Hamiltonian describing the pair interaction of quasiparticles has the form [48]:

$$V_\Phi=\frac{1}{4\mathcal{V}}\sum_{\mathbf{p}_1\cdots\mathbf{p}_4}a^\dagger_{\mathbf{p}_1\alpha_1}a^\dagger_{\mathbf{p}_2\alpha_2}\times$$

$$\times\,\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)a_{\mathbf{p}_3\alpha_3}a_{\mathbf{p}_4\alpha_4}. \qquad (40)$$

For definiteness, we consider quasiparticles to be bosons. Therefore, the interaction amplitude should have the following symmetry properties:

$$\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)=\Phi_{\alpha_2\alpha_1;\alpha_3\alpha_4}(\mathbf{p}_2,\mathbf{p}_1;\mathbf{p}_3,\mathbf{p}_4)=$$

$$=\Phi_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3). \qquad (41)$$

The similar properties can also be written for fermions,

$$\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)=\Phi_{\alpha_3\alpha_4;\alpha_2\alpha_1}(\mathbf{p}_2,\mathbf{p}_1;\mathbf{p}_4,\mathbf{p}_3),$$

$$\Phi_{\alpha_2\alpha_1;\alpha_3\alpha_4}(\mathbf{p}_2,\mathbf{p}_1;\mathbf{p}_3,\mathbf{p}_4)=\Phi_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=$$

$$=-\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4).$$

Therefore, the choice of bosonic quasiparticles does not limit the generality of the further consideration.

As the next step, we require the equality between the interaction part of the energy functional given by Eq. (35) and the expectation value of the introduced quasiparticle Hamiltonian V_Φ:

$$E_{\text{int}}(f)=\text{Tr}\,\rho_0(f)V_\Phi, \qquad (42)$$

where $\rho_0(f)$ is the statistical operator of an ideal nonequilibrium gas of quasiparticles [48],

$$\rho_0(f)=\exp\left[\Omega-\sum_{\mathbf{p},\mathbf{p}'}a^\dagger_{\mathbf{p}\alpha}A_{\mathbf{p}\alpha\mathbf{p}'\beta}a_{\mathbf{p}'\beta}\right].$$

Here the quantities Ω and $A_{\mathbf{p}\alpha\mathbf{p}'\beta}$, being the functionals of the single-particle density matrix, are determined by the following relations, respectively, $\text{Sp}\,\rho_0(f)=1$ and $f_{\alpha\beta}(\mathbf{p},\mathbf{p}')=\text{Sp}\,\rho_0(f)a^\dagger_{\mathbf{p}'\beta}a_{\mathbf{p}\alpha}$. The von Neumann entropy $S=\text{Sp}\,\rho_0(f)\ln\rho_0(f)$ is in agreement with its combinatorial expression, $S=-\text{Tr}[f\ln f-(1+f)\ln(1+f)]$, where trace is taken over the single-particle states specified by the momentum and spin projection. The statistical operator $\rho_0(f)$ satisfies the principle of spatial correlation weakening and the Bloch–De Dominicis (or Wick's) theorem is applied for it [45]. It was employed to derive the kinetic equations and collision integrals for weakly interacting quantum gases [48, 53, 54] and was generalized to examine the superfluid states for both Fermi [55] and Bose systems [56]. Therefore, application of the Bloch–De Dominicis theorem to Eq. (42) gives the following relation between the interaction amplitudes :

$$\frac{1}{\mathcal{V}}\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_4,\mathbf{p}_3)=\frac{1}{2}\Big[F_{\alpha_1\alpha_3;\alpha_2\alpha_4}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)+F_{\alpha_2\alpha_3;\alpha_1\alpha_4}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)\Big]=$$

$$=\frac{1}{2}\Big[F^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)\delta_{\alpha_1\alpha_3}\delta_{\alpha_2\alpha_4}+F^{(1)}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)\delta_{\alpha_2\alpha_3}\delta_{\alpha_1\alpha_4}\Big]+$$

$$+\frac{1}{2}\Big[F^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)T^a_{\alpha_1\alpha_3}T^a_{\alpha_2\alpha_4}+F^{(2)}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)T^a_{\alpha_2\alpha_3}T^a_{\alpha_1\alpha_4}\Big]. \qquad (43)$$

where we have used Eqs. (41), (37). Therefore, the interaction Hamiltonian given by Eq. (40) can be written in the form,

$$V_\Phi=\frac{1}{4\mathcal{V}}\sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4}a^\dagger_{\mathbf{p}_1\alpha_1}a^\dagger_{\mathbf{p}_2\alpha_2}F^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)a_{\mathbf{p}_3\alpha_1}a_{\mathbf{p}_4\alpha_2}+\frac{1}{4\mathcal{V}}\sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4}a^\dagger_{\mathbf{p}_1\alpha_1}a^\dagger_{\mathbf{p}_2\alpha_2}F^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)T^a_{\alpha_1\alpha_3}T^a_{\alpha_2\alpha_4}a_{\mathbf{p}_3\alpha_3}a_{\mathbf{p}_4\alpha_4}. \qquad (44)$$

Now we require the interaction Hamiltonian (40) to be translationally invariant that is equivalent to its commutation with the total momentum of the system,

$$[V_\Phi,\,\mathbf{P}]=0,\quad \mathbf{P}=\sum_{\mathbf{p}}\mathbf{p}a^\dagger_{\mathbf{p}\alpha}a_{\mathbf{p}\alpha}.$$

The above condition can be satisfied by redefining the amplitude $\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)$ and, consequently, $F_{\alpha_2\alpha_3;\alpha_1\alpha_4}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)$ [see Eq. (43)] in the following manner:

$$\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4) =$$

$$= \tilde{\Phi}_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)\delta_{\mathbf{p}_1+\mathbf{p}_4;\mathbf{p}_2+\mathbf{p}_3},$$

$$F_{\alpha_2\alpha_3;\alpha_1\alpha_4}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4) =$$

$$= \tilde{F}_{\alpha_2\alpha_3;\alpha_1\alpha_4}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)\delta_{\mathbf{p}_1+\mathbf{p}_4;\mathbf{p}_2+\mathbf{p}_3},$$

where the Kronecker delta ensures the momentum conservation law. Therefore, Eq. (44) takes the form

$$V_\Phi = \frac{1}{4\mathcal{V}}\sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} a^\dagger_{\mathbf{p}_1\alpha_1}a^\dagger_{\mathbf{p}_2\alpha_2}\times$$

$$\times\tilde{F}^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)a_{\mathbf{p}_3\alpha_1}a_{\mathbf{p}_4\alpha_2}\delta_{\mathbf{p}_1+\mathbf{p}_4;\mathbf{p}_2+\mathbf{p}_3} +$$

$$+\frac{1}{4\mathcal{V}}\sum_{\mathbf{p}_1,\ldots,\mathbf{p}_4} a^\dagger_{\mathbf{p}_1\alpha_1}a^\dagger_{\mathbf{p}_2\alpha_2}\tilde{F}^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)\times$$

$$\times T^a_{\alpha_1\alpha_3}T^a_{\alpha_2\alpha_4}a_{\mathbf{p}_3\alpha_3}a_{\mathbf{p}_4\alpha_4}\delta_{\mathbf{p}_1+\mathbf{p}_4;\mathbf{p}_2+\mathbf{p}_3}, \qquad (45)$$

where the amplitudes $\tilde{F}^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)$ and $\tilde{F}^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)$ are also determined in accordance with Eqs. (39). It is worth noting that, according to Eq. (43), the interaction amplitude $\Phi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_3,\mathbf{p}_4)$ of the microscopic Hamiltonian are expressed in terms of the different components of the same amplitude $\tilde{F}_{\alpha_2\alpha_3;\alpha_1\alpha_4}(\mathbf{p}_2,\mathbf{p}_3;\mathbf{p}_1,\mathbf{p}_4)$ in the phenomenological expansion of energy in a series of the single-particle density matrix. This indicates one nature of the interaction forces $\tilde{F}^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)$ and $\tilde{F}^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4)$. In the case $S \geq 1$, the latter supplement and generalize the usual spin-spin interaction.

It should be noted that in spite of the fact that the Hamiltonian must be constructed of the operators of physical quantities, it is expressed in terms of abstract, perhaps, non-physical characteristics representing the generators T^a of the SU(n) group. However, their emergence is mathematically justified, since they (as well as identity operator) represent a complete set of matrices for the expansion of the single-particle density matrix and indicate the necessity to introduce additional description parameters along with the ordinary spin operator. As we have shown, for spin-1 system, all eight Gell–Mann generators of the SU(3) group have their physical meaning: three of them are the components of the spin operator and the remaining five operators specify the quadrupole degrees of freedom. For spin-S system, described by the SU(2S+1) group, there is no general recipe for extracting both spin operators and other multipole degrees of freedom from the generators T^a. Therefore, such a problem has to be solved for each specific spin-S system. However, we can always construct the spin-S matrices from the generators T^a and, thereby, to separate the bilinear spin-spin (exchange) interaction in the Hamiltonian.

Finally, the general pairwise interaction Hamiltonian in the form of Eq. (45) has a more general form than that given by Eq. (33). This is due to the fact that the Hamiltonian V_Φ describes the interaction between quasiparticles. However, it can be related to the traditional Hamiltonian of pairwise interaction by using the following relations between the interaction amplitudes:

$$\tilde{F}^{(1)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4) =$$

$$= \frac{1}{8}\left[U(\mathbf{p}_3-\mathbf{p}_1)+U(\mathbf{p}_3-\mathbf{p}_2)+U(\mathbf{p}_4-\mathbf{p}_1)+U(\mathbf{p}_4-\mathbf{p}_2)\right],$$

$$\tilde{F}^{(2)}(\mathbf{p}_1,\mathbf{p}_3;\mathbf{p}_2,\mathbf{p}_4) =$$

$$= \frac{1}{8}\left[J(\mathbf{p}_3-\mathbf{p}_1)+J(\mathbf{p}_3-\mathbf{p}_2)+J(\mathbf{p}_4-\mathbf{p}_1)+J(\mathbf{p}_4-\mathbf{p}_2)\right], \quad (46)$$

where $U(\mathbf{p})$ and $J(\mathbf{p})$ are the Fourier transforms of the corresponding functions $U(\mathbf{x}_1-\mathbf{x}_2)$ and $U(\mathbf{x}_1-\mathbf{x}_2)$ that specify the interaction of two particles at points $\mathbf{x}_1$ and $\mathbf{x}_2$. According to the above consideration, these functions can be related to phenomenological amplitudes describing the "density-density" interaction. Combining Eqs. (45) and (46) we arrive at the SU(n) symmetric interaction Hamiltonian having the structure of Eq. (33).

4. Manifestation of quadrupole degrees of freedom in magnetic phases of spin-1 condensate

In this section, we intend to demonstrate the manifestation of the "hidden" internal degrees of freedom on the physical characteristics of a specific many-body system with interatomic interaction. In particular, we study a non-ideal Bose gas of interacting spin-1 atoms on the basis of the obtained interaction Hamiltonian involving both spin and quadrupole operators and find the ground-state magnetic phases and excitations modified by quadrupole degrees of freedom. Therefore, the starting point is the following second-quantized Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + V, \quad \mathcal{H}_0 = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}\alpha}\left[(\varepsilon_{\mathbf{p}}-\mu)\delta_{\alpha\beta} - hS^z_{\alpha\beta}\right]a_{\mathbf{p}\beta},$$

$$S^z_{\alpha\beta} \equiv \lambda^2_{\alpha\beta}, \qquad (47)$$

where $h = g\mu_B B$ and the magnetic field B is chosen to be directed along z-axis, $\mathbf{B} = (0, 0, B)$. The interaction Hamiltonian $\mathcal{V}$ is given by Eqs. (29)–(32). Bose–Einstein condensation occurs when a macroscopic number N_0 of ultracold bosons accumulates in the lowest quantum state with zero momentum (N_0/N tends to non-zero value when both N and V go to infinity so that the density N/V is kept fixed). To describe such a phenomenon, we use the

Bogoliubov model [33] for a non-ideal Bose gas with condensate in which the creation and annihilation operators of atoms with zero momentum are considered to be *c*-numbers, $a_0^\dagger \to \sqrt{\mathcal{V}}\Psi_\alpha^*$ and $a_0 \to \sqrt{\mathcal{V}}\Psi_\alpha$, where Ψ_α is called the order parameter or the condensate wave function. The above *c*-number replacement is associated with U(1) symmetry breaking and can be validated in the framework of quasiaverage concept attracting the principle of the spatial weakening of correlations [45, 48]. It has also been proved to be exact in the thermodynamic limit [57]. Within the Bogoliubov approach, the Hamiltonian is truncated by the *c*-number terms and quadratic terms in creation and annihilation operators with non-zero momentum (the higher order terms are neglected since their contribution is considered to be small; they are associated with the quasiparticle interaction). Therefore, the Hamiltonian given by Eq. (47) becomes

$$\mathcal{H}(\Psi) \approx \mathcal{H}^{(0)}(\Psi) + \mathcal{H}^{(2)}(\Psi), \tag{48}$$

where

$$\frac{1}{\mathcal{V}}\mathcal{H}^{(0)}(\Psi) = \frac{U(0)}{2}(\Psi^*\Psi)^2 + \frac{J(0)}{2}(\Psi^* S^i \Psi)^2 + \\ + \frac{K(0)}{2}(\Psi^* q^b \Psi)^2 - h(\Psi^* S^z \Psi) - \mu(\Psi^*\Psi) \tag{49}$$

and

$$\mathcal{H}^{(2)}(\Psi) = \sum_{\mathbf{p}\neq 0} a_{\mathbf{p}\alpha}^\dagger \left[(\varepsilon_{\mathbf{p}} - \mu)\delta_{\alpha\beta} - hS_{\alpha\beta}^z\right] a_{\mathbf{p}\beta} + U(0)\sum_{\mathbf{p}\neq 0}(\Psi^*\Psi)(a_{\mathbf{p}}^\dagger a_{\mathbf{p}}) + \frac{1}{2}\sum_{\mathbf{p}\neq 0} U(\mathbf{p})\left[(a_{\mathbf{p}}^\dagger\Psi)(\Psi^* a_{\mathbf{p}}) + (a_{\mathbf{p}}^\dagger\Psi)(a_{-\mathbf{p}}^\dagger\Psi) + \text{h.c.}\right] + \\ + J(0)\sum_{\mathbf{p}\neq 0}(\Psi^* S^i\Psi)(a_{\mathbf{p}}^\dagger S^i a_{\mathbf{p}}) + \frac{1}{2}\sum_{\mathbf{p}\neq 0} J(\mathbf{p})\left[(a_{\mathbf{p}}^\dagger S^i\Psi)(\Psi^* S^i a_{\mathbf{p}}) + (a_{\mathbf{p}}^\dagger S^i\Psi)(a_{-\mathbf{p}}^\dagger S^i\Psi) + \text{h.c.}\right] + \\ + K(0)\sum_{\mathbf{p}\neq 0}(\Psi^* q^b\Psi)(a_p^\dagger q^b a_p) + \frac{1}{2}\sum_{\mathbf{p}\neq 0} K(\mathbf{p})\left[(a_{\mathbf{p}}^\dagger q^b\Psi)(\Psi^* q^b a_{\mathbf{p}}) + (a_{\mathbf{p}}^\dagger q^b\Psi)(a_{-\mathbf{p}}^\dagger q^b\Psi) + \text{h.c.}\right]. \tag{50}$$

The Hamiltonian defined by Eq. (49) is expressed in terms of the condensate wave function and does not include the creation and annihilation operators of atoms, whereas the Hamiltonian $\mathcal{H}^{(2)}(\Psi)$ represents the quadratic form in creation and annihilation operators of atoms with non-zero momentum. Here and below we omit the summation over the repeated indices assuming matrix multiplication law, e.g., $(\Psi^*\Psi) \equiv \Psi_\alpha^*\Psi_\alpha$, $(a_{\mathbf{p}}^\dagger a_{\mathbf{p}}) \equiv a_{\mathbf{p}\alpha}^\dagger a_{\mathbf{p}\alpha}$, $(\Psi^*\lambda^a\Psi) \equiv \Psi_\alpha^*\lambda_{\alpha\beta}^a\Psi_\beta$, and so on. The Gibbs statistical operator determined by Eq. (11) is then replaced by

$$w(\Psi) \simeq \exp\left[\Omega - \beta\left(\mathcal{H}^{(0)}(\Psi) + \mathcal{H}^{(2)}(\Psi)\right)\right]. \tag{51}$$

According to Eq. (13) the grand thermodynamic potential is found to be

$$\Omega(\Psi) = \beta\mathcal{H}^{(0)}(\Psi) - \ln \mathrm{Tr}\left[\exp\left(-\beta\mathcal{H}^{(2)}(\Psi)\right)\right]. \tag{52}$$

Following the Bogoliubov approach [45], in the main approximation (low temperatures and weak interatomic interaction), $\Omega(\Psi) \approx \beta\mathcal{H}^{(0)}(\Psi)$. This approximation guarantees the gapless structure of the single-particle excitation spectrum. Next, it is convenient to introduce the density of the thermodynamic potential $\varpi = \Omega/\beta\mathcal{V}$, which, up to a sign, coincides with pressure P, $\varpi = -P$. Then, the minimization of

$$\varpi \approx \frac{\mathcal{H}^{(0)}(\Psi)}{V} = \frac{U(0)}{2}(\Psi^*\Psi)^2 + \frac{J(0)}{2}(\Psi^* S^i\Psi)^2 + \\ + \frac{K(0)}{2}(\Psi^* q^b\Psi)^2 - h(\Psi^* S^z\Psi) - \mu(\Psi^*\Psi), \tag{53}$$

over Ψ_α^* results in the following equation for determining the condensate wave function Ψ_α as a function of chemical potential and interaction parameters:

$$\mu\Psi_\alpha - U(0)(\Psi^*\Psi)\Psi_\alpha - J(0)(\Psi^* S^i\Psi)S_{\alpha\beta}^i\Psi_\beta - \\ - K(0)(\Psi^* q^b\Psi)q_{\alpha\beta}^b\Psi_\beta + hS_{\alpha\beta}^z\Psi_\beta = 0. \tag{54}$$

To study the possible solutions of Eq. (54), it is convenient to introduce the condensate density n_0,

$$\Psi_\alpha = \sqrt{n_0}\zeta_\alpha, \quad \zeta_\alpha^*\zeta_\alpha \equiv (\zeta^*\zeta) = 1, \tag{55}$$

where ζ_α is the normalized state vector. Then Eq. (54) can be recast as

$$\mu\zeta_\alpha - n_0U(0)\zeta_\alpha - n_0J(0)(\zeta^* S^i\zeta)S_{\alpha\beta}^i\zeta_\beta - \\ - n_0K(0)(\zeta^* q^b\zeta)q_{\alpha\beta}^b\zeta_\beta + hS_{\alpha\beta}^z\zeta_\beta = 0. \tag{56}$$

Equation (56) determines the ground-state structure of a weakly interacting Bose gas of spin-1 atoms with condensate and quadrupole degrees of freedom. It has three solutions corresponding to the different magnetic phases [58].

(1) The first solution of Eq. (56) is of the form

$$\zeta = (0, 0, 1) \quad \text{with} \quad \mu = n_0U(0) + \frac{4}{3}n_0K(0). \tag{57}$$

Such a state vector vanishes the magnetization $\langle S^i\rangle = (\Psi^* S^i\Psi) = 0$ and breaks the spin-rotation symmetry since $\langle (S^z)^2\rangle = 0$, whereas $\langle (S^x)^2\rangle = \langle (S^y)^2\rangle = n_0$. This shows that the spin vector fluctuates in the *xy* plane. Therefore,

the state determined by Eq. (57) describes the *quadrupolar phase* [10]. For the expectation value of the quadrupole matrix, one obtains

$$\langle Q\rangle = (\Psi^* Q\Psi) = n_0\left(\frac{2}{3}\delta_{ik} - 2e_i e_k\right),$$

where $e_z = \pm 1$ is a unit vector perpendicular to the plane of fluctuations called a director. Taking into account Eqs. (53), (55), and (57), one finds the density of the thermodynamic potential,

$$\varpi = -\frac{1}{2}\frac{\mu^2}{U(0) + 4/3K(0)}. \tag{58}$$

For the stability of the state under study, the density of the thermodynamic potential must be negative (the pressure must be positive, $\varpi = -P$). This requirement gives the following stability condition:

$$U(0) + \frac{4}{3}K(0) > 0. \tag{59}$$

Now we obtain the single-particle excitation spectrum for the quadrupolar ground state. To this end, we turn to Eq. (50) for the quadratic part (in creation and annihilation operators) of the truncated Hamiltonian. Using Eq. (57) to eliminate the chemical potential and performing some algebraic transformations with the entering 3×3 matrices, we come to the Hamiltonian consisting of two commuting parts,

$$\mathcal{H}^{(2)}(n_0) = \mathcal{H}_1^{(2)}(n_0) + \mathcal{H}_2^{(2)}(n_0), \tag{60}$$

where

$$\mathcal{H}_1^{(2)}(n_0) = \sum_{\mathbf{p}\neq 0}\alpha_{\mathbf{p}z} a_{\mathbf{p}z}^\dagger a_{\mathbf{p}z} + \frac{1}{2}\sum_{\mathbf{p}\neq 0}\beta_{\mathbf{p}z}\left[a_{\mathbf{p}z}^\dagger a_{-\mathbf{p}z}^\dagger + a_{\mathbf{p}z}a_{-\mathbf{p}z}\right] \tag{61}$$

with

$$\alpha_{\mathbf{p}z} = \varepsilon_{\mathbf{p}} + \beta_{\mathbf{p}z}, \quad \beta_{\mathbf{p}z} = n_0\left(U(\mathbf{p}) + \frac{4}{3}K(\mathbf{p})\right).$$

As for the second part $\mathcal{H}_2^{(2)}(n_0)$, it can be written as the general quadratic form in creation and annihilation operators [45],

$$\mathcal{H}_2^{(2)}(n_0) = \sum_{\mathbf{p}\neq 0} a_{\mathbf{p}\alpha}^\dagger A_{\alpha\beta} a_{\mathbf{p}\beta} + \frac{1}{2}\sum_{\mathbf{p}\neq 0} a_{\mathbf{p}\alpha}^\dagger B_{\alpha\beta} a_{-\mathbf{p}\beta}^\dagger +$$

$$+ \frac{1}{2}\sum_{\mathbf{p}\neq 0} a_{\mathbf{p}\alpha} B_{\alpha\beta}^* a_{-\mathbf{p}\beta}, \quad \alpha,\beta = x,y. \tag{62}$$

In our case, the Hermitian ($A = A^\dagger$) and symmetric ($B = B^T$) matrices are specified by the following matrix elements:

$$A_{xx} = A_{yy} = \varepsilon_{\mathbf{p}} + n_0 J(\mathbf{p}) - 2n_0 K(0) + n_0 K(\mathbf{p}),$$

$$A_{xy} = A_{yx}^* = ih$$

and

$$B_{xx} = B_{yy} = n_0 K(\mathbf{p}) - n_0 J(\mathbf{p}), \quad B_{xy} = B_{yx} = 0.$$

It is clear that since both parts of the Hamiltonian $\mathcal{H}_1^{(2)}(n_0)$ and $\mathcal{H}_2^{(2)}(n_0)$ commute, they can be diagonalized separately. The Hamiltonian $\mathcal{H}_1^{(2)}(n_0)$ has the same form as in the original Bogoliubov theory for spinless atoms. Its standard diagonalization by the canonical unitary transformation gives the following dispersion law of quasiparticles (see, e.g., [48]):

$$\omega_{\mathbf{p}z} = (\alpha_{\mathbf{p}z}^2 - \beta_{\mathbf{p}z}^2)^{1/2} = \left[\varepsilon_{\mathbf{p}}^2 + 2\varepsilon_{\mathbf{p}} n_0\left(U(\mathbf{p}) + \frac{4}{3}K(\mathbf{p})\right)\right]^{1/2}. \tag{63}$$

It is clear that here and below the quasiparticle energies must be real. This imposes a corresponding restriction on the Fourier transforms of the interaction energies. The second part of the Hamiltonian $\mathcal{H}_2^{(2)}(n_0)$ can be also reduced to the diagonal form by the canonical unitary transformation U ($UU^\dagger = 1$)

$$U\mathcal{H}_2^{(2)}(n_0)U^\dagger = \sum_{\mathbf{p}\neq 0}\sum_{\gamma=x,y}\omega_{\mathbf{p}\gamma} a_{\mathbf{p}\gamma}^\dagger a_{\mathbf{p}\gamma} + \mathcal{E}_0, \tag{64}$$

where $\omega_{\mathbf{p}\gamma}$ are the energies of the single-particle excitations and $\mathcal{E}_0$ determines the ground state energy or the grand thermodynamic potential up to the contribution from the quadratic terms in the second quantized operators. The above unitary transformation "mixes" the creation and annihilation operators of atoms as follows:

$$Ua_{\mathbf{p}\alpha}U^\dagger = \sum_{\gamma=x,y}\left[u_{\alpha\gamma}(\mathbf{p})a_{\mathbf{p}\gamma} + v_{\alpha\gamma}^*(\mathbf{p})a_{-\mathbf{p}\gamma}^\dagger\right],$$

$$Ua_{\mathbf{p}\alpha}^\dagger U^\dagger = \sum_{\gamma=x,y}\left[u_{\alpha\gamma}^*(\mathbf{p})a_{\mathbf{p}\gamma}^\dagger + v_{\alpha\gamma}(\mathbf{p})a_{-\mathbf{p}\gamma}\right].$$

The requirement for the operators $Ua_{\mathbf{p}\alpha}^\dagger U^\dagger$ and $Ua_{\mathbf{p}\alpha}U^\dagger$ to meet the bosonic commutation relations gives the normalization and orthogonality conditions for the parameters $u_{\alpha\gamma}(\mathbf{p})$ and $v_{\alpha\gamma}(\mathbf{p})$:

$$\sum_{\gamma=x,y}\left[u_{\alpha\gamma}(p)u_{\beta\gamma}^*(\mathbf{p}) - v_{\alpha\gamma}^*(\mathbf{p})v_{\beta\gamma}(\mathbf{p})\right] = \delta_{\alpha\beta},$$

$$\sum_{\gamma=x,y}\left[u_{\alpha\gamma}(\mathbf{p})v_{\beta\gamma}^*(\mathbf{p}) - v_{\alpha\gamma}^*(\mathbf{p})u_{\beta\gamma}(\mathbf{p})\right] = 0.$$

The energies of the single-particle excitations $\omega_{\mathbf{p}\gamma}$ entering Eq. (64) satisfy the following eigenvalue equations [45]:

$$\sum_{\gamma=x,y}\left[A_{\alpha\gamma}(\mathbf{p})u_{\gamma\sigma}(\mathbf{p}) + B_{\alpha\gamma}(\mathbf{p})v_{\gamma\sigma}(\mathbf{p})\right] = \omega_{\mathbf{p}\sigma}u_{\alpha\sigma}(\mathbf{p}),$$

$$\sum_{\gamma=x,y}\left[A_{\alpha\gamma}^*(\mathbf{p})v_{\gamma\sigma}(\mathbf{p}) + B_{\alpha\gamma}^*(\mathbf{p})u_{\gamma\sigma}(\mathbf{p})\right] = -\omega_{\mathbf{p}\sigma}v_{\alpha\sigma}(\mathbf{p}).$$

This system of homogeneous liner equations has non-zero solution when the corresponding determinant turns to zero. This yields,

$$\omega_{\mathbf{p}x,y} = \Big[\Big(\varepsilon_{\mathbf{p}} + n_0 J(\mathbf{p}) + n_0 K(\mathbf{p}) - 2n_0 K(0)\Big)^2 - \Big(n_0 J(\mathbf{p}) - n_0 K(\mathbf{p})\Big)^2\Big]^{1/2} \pm h. \quad (65)$$

The obtained two modes of excitations $\omega_{\mathbf{p}x,y}$ differ only in the sign of the magnetic field and do not depend on the interaction amplitude $U(\mathbf{p})$. They describe the spin-quadrupole waves. In the absence of a magnetic field, they become degenerate and gapless. The third branch of excitations, given by Eq. (63), is independent of the external magnetic field and represents the Bogoliubov mode modified by the interaction of quadrupole degrees of freedom. It is always gapless and becomes a phonon (sound-like) mode for small momenta, $\omega_{\mathbf{p}z} \approx sp$, where the speed of sound is of the form

$$s = \sqrt{\frac{n_0}{m}\left(U(0) + \frac{4}{3}K(0)\right)}. \quad (66)$$

The requirement for the speed of sound to be real leads to the stability condition given by Eq. (59). Finally note that the obtained expression for the speed of sound corresponds to its hydrodynamic definition, $s = \sqrt{\partial P / \partial \rho_0}$, where $\rho_0 = mn_0$ is the mass density and $P = -\varpi$ (see. Eq. (58) for ϖ).

(2) The second solution of Eq. (56) has the form

$$\zeta = \frac{1}{\sqrt{2}}(1,\, i,\, 0),$$

$$\text{with} \quad \mu = n_0 U(0) + n_0 J(0) + \frac{1}{3} n_0 K(0) - h. \quad (67)$$

This solution describes the *ferromagnetic state* of a weakly interacting Bose gas with condensate because it generate the magnetization independent of the external magnetic field,

$$\langle S^i \rangle = (\Psi^* S^i \Psi) = n_0 \delta_{iz}.$$

Note that the emergence of BEC due to U(1) (or global phase) symmetry breaking leads to the spin anisotropy. The expectation value for the quadrupole matrix [see Eq. (22)] is

$$\langle \mathcal{Q} \rangle = (\Psi^* \mathcal{Q} \Psi) = n_0 \begin{pmatrix} -1/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 2/3 \end{pmatrix}.$$

Here, $\langle \mathcal{Q}^{xx} \rangle = \langle \mathcal{Q}^{yy} \rangle$ indicates that the order parameter has rotational symmetry about the z axis. The density for the thermodynamic potential, according to Eqs. (53), (55), and (67), reads

$$\varpi = -\frac{1}{2}\frac{(\mu + h)^2}{U(0) + J(0) + (1/3)K(0)}. \quad (68)$$

Therefore, the ferromagnetic state is thermodynamically stable under the following condition:

$$U(0) + J(0) + \frac{1}{3}K(0) > 0. \quad (69)$$

In order to find the single-particle excitation spectrum for the ferromagnetic phase, we turn to the quadratic Hamiltonian given by Eq. (50). Using Eqs. (67), it can be again represented as the sum of two commuting operators, which can be diagonalized independently of each other. The first one, $\mathcal{H}_1^{(2)}(n_0)$, now reads,

$$\mathcal{H}_1^{(2)}(n_0) = \sum_{\mathbf{p}\neq 0} \Big(\varepsilon_{\mathbf{p}} + h + n_0\big[J(\mathbf{p}) - J(0)\big] + n_0\big[K(\mathbf{p}) - K(0)\big]\Big) a^\dagger_{\mathbf{p}z} a_{\mathbf{p}z}. \quad (70)$$

The second operator, $\mathcal{H}_2^{(2)}(n_0)$, is formally determined by Eq. (62); however, the 2×2 matrices in it have the following matrix elements:

$$A_{xx} = A_{yy} = \varepsilon_{\mathbf{p}} + h + \frac{1}{2}n_0 U(\mathbf{p}) - n_0 J(0) + \frac{1}{2}n_0 J(\mathbf{p}) + \frac{7}{6}n_0 K(\mathbf{p}),$$

$$A_{xy} = A^*_{yx} = i\left[h - \frac{1}{2}n_0 U(\mathbf{p}) - n_0 J(0) - \frac{1}{2}n_0 J(\mathbf{p}) + \frac{5}{6}n_0 K(\mathbf{p})\right],$$

and

$$B_{xx} = -B_{yy} = \frac{1}{2}n_0 U(\mathbf{p}) - \frac{1}{2}n_0 J(\mathbf{p}) + \frac{1}{6}n_0 K(\mathbf{p}),$$

$$B_{xy} = B_{yx} = iB_{xx}.$$

While $\mathcal{H}_1^{(2)}(n_0)$ is diagonal in creation and annihilation operators with the following quasiparticle energy:

$$\omega_{\mathbf{p}z} = \varepsilon_{\mathbf{p}} + h + n_0\big[J(\mathbf{p}) - J(0)\big] + n_0\big[K(\mathbf{p}) - K(0)\big], \quad (71)$$

the second operator, $\mathcal{H}_2^{(2)}(n_0)$, must be diagonalized by applying to it the general method, briefly described above. As a result, we get two other types of excitations characterized by the following dispersion laws:

$$\omega_{\mathbf{p}x} = \varepsilon_{\mathbf{p}} + 2h + 2n_0\big[K(\mathbf{p}) - J(0)\big] \quad (72)$$

and

$$\omega_{\mathbf{p}y} = \left[\varepsilon^2_{\mathbf{p}} + 2\varepsilon_{\mathbf{p}} n_0 \left(U(\mathbf{p}) + J(\mathbf{p}) + \frac{1}{3}K(\mathbf{p})\right)\right]^{1/2}. \quad (73)$$

Similar to the quadrupolar phase, the single-particle excitation spectrum of the ferromagnetic state has a three-branch structure. Two gapful modes determined by Eqs. (71) and (72) describe the spin-quadrupole waves. The gapless mode given by Eq. (73) represents the generalization of the well-known Bogoliubov mode to the case of involving the spin-spin and quadrupole-quadrupole interactions. It has a phonon character at low momenta,

$$\omega_{\mathbf{p}y} = sp, \quad s = \sqrt{\frac{n_0}{m}\left(U(0)+J(0)+\frac{1}{3}K(0)\right)}. \quad (74)$$

As in previuos case, the speed of sound agrees with its hydrodynamic expression, $s = \sqrt{\partial P/\partial \rho_0}$ and the requirement for it to be real leads to the stability condition determined by Eq. (69).

(3) Finally, the third solution of Eq. (56) is of the form

$$\zeta = \frac{1}{2}(a,\, ib,\, 0) \quad \text{with} \quad \mu = n_0 U(0) + \frac{4}{3} n_0 K(0), \quad (75)$$

where

$$a = \exp(i\varphi_+)\sqrt{1+\frac{h}{c}} + \exp(i\varphi_-)\sqrt{1-\frac{h}{c}},$$

$$b = \exp(i\varphi_+)\sqrt{1+\frac{h}{c}} - \exp(i\varphi_-)\sqrt{1-\frac{h}{c}}. \quad (76)$$

Here $c = n_0(J(0)-K(0))$ and $\phi_\pm$ are the arbitrary real numbers. The state vector in the form of Eq. (75) describes the *paramagnetic phase* of a weakly interacting Bose gas with BEC. The magnetization of such a phase occurs only in the presence of an external magnetic field,

$$\langle S^i \rangle = (\Psi^* S^i \Psi) = \frac{h}{J(0)-K(0)}\delta_{iz}.$$

The expectation value of the quadrupole matrix, according Eq. (22), is found to be

$$\langle \mathcal{Q} \rangle = (\Psi^* \mathcal{Q} \Psi) =$$

$$= n_0 \begin{pmatrix} -1/3 - \gamma\cos(\phi_+ - \phi_-) & \gamma\sin(\phi_+ - \phi_-) & 0 \\ \gamma\sin(\phi_+ - \phi_-) & -1/3 + \gamma\cos(\phi_+ - \phi_-) & 0 \\ 0 & 0 & 2/3 \end{pmatrix},$$

where $\gamma = \sqrt{1-(h/c)^2}$. The arbitrary phases $\phi_\pm$ can be turn to zero without loss of generality (all physical quantities including pressure, magnetization, excitation energies do not depend on them). In this case, the non-diagonal matrix elements vanish and the structure of the quadrupole matrix shows that the spin fluctuations are anisotropic in the xy plane because $\langle \mathcal{Q}^{xx} \rangle \neq \langle \mathcal{Q}^{yy} \rangle$. In accordance with Eqs. (53), (55), and (75), the density of the thermodynamic potential is given by

$$\varpi = -\frac{1}{2}\left(\frac{h^2}{J(0)-K(0)} + \frac{\mu^2}{U(0)+(4/3)K(0)}\right). \quad (77)$$

It is easy to see that for the thermodynamic stability of the paramagnetic phase, at least one of the conditions below must be satisfied,

$$J(0) > K(0), \quad U(0) + (4/3)K(0) > 0. \quad (78)$$

The third condition involving a magnetic field follows from Eq. (76),

$$h \le n_0 \,|\, J(0) - K(0) \,|\,. \quad (79)$$

The three branches of the single-particle excitation spectrum are obtained in the same way as described above. The result is

$$\omega_{\mathbf{p}z} = \Big[\left(\varepsilon_{\mathbf{p}} + n_0 J(\mathbf{p}) + n_0 K(\mathbf{p}) - 2n_0 K(0)\right)^2 -$$

$$-\gamma^2 \left(n_0 J(\mathbf{p}) - n_0 K(\mathbf{p})\right)^2\Big]^{1/2}. \quad (80)$$

and

$$\omega_{\mathbf{p}x,y} = \left(\varepsilon_{\mathbf{p}}^2 + D\varepsilon_{\mathbf{p}} + F \pm \sqrt{G\varepsilon_{\mathbf{p}}^2 + L\varepsilon_{\mathbf{p}} + F^2}\right)^{1/2}. \quad (81)$$

The coefficients in Eq. (81) are determined by

$$D = n_0\left(U(\mathbf{p}) + J(\mathbf{p}) + \frac{7}{3}K(\mathbf{p}) - 2K(0)\right),$$

$$F = 2n_0^2\left(K(\mathbf{p}) - K(0)\right)^2\left(\gamma^2\frac{J(\mathbf{p})-K(\mathbf{p})}{K(\mathbf{p})-K(0)} + 1\right),$$

$$G = n_0^2\left(U(\mathbf{p}) - J(\mathbf{p}) + \frac{1}{3}K(\mathbf{p}) + 2K(0)\right)^2 +$$

$$+ 4n_0^2\frac{h^2}{c^2}\left(J(\mathbf{p}) - K(\mathbf{p})\right)\left(U(\mathbf{p}) - \frac{2}{3}K(\mathbf{p}) + 2K(0)\right),$$

$$L = -4n_0^3\left(K(\mathbf{p}) - K(0)\right)^2\Big[U(\mathbf{p}) + J(\mathbf{p}) - \frac{5}{3}K(\mathbf{p}) + 2K(0) +$$

$$+\gamma^2\frac{J(\mathbf{p})-K(\mathbf{p})}{K(\mathbf{p})-K(0)}\left(U(\mathbf{p}) - J(\mathbf{p}) - \frac{5}{3}K(\mathbf{p}) + 4K(0)\right)\Big].$$

The density and spin-quadrupole excitations are hybridized in the modes given by Eqs. (81). This becomes clear from the fact that in the linear approximation in momentum, the corresponding modes do not reproduce the coefficient consistent with the hydrodynamic speed of sound $s = \sqrt{\partial P/\partial \rho_0}$, where $P = -\varpi$. Another type of excitations that does not contain the interaction amplitude $U(\mathbf{p})$ [see Eq. (80)] is gapful in the presence of the external field.

5. Discussion of results

We have demonstrated that quantum atomic gases of interacting high-spin atoms represent a physical system in which the multipole degrees of freedom are manifested. They emerge in the description when the interatomic interaction is of non-local type. For a local interaction described by the s-wave scattering length, the multipole degrees of freedom do not reveal themselves. To illustrate our findings, we theoretically examine the phenomenon of Bose–Einstein condensation in an interacting gas of spin-1 atoms in an external magnetic field. This study is based on the SU(2) invariant Hamiltonian, which has a bilinear structure in the spin and quadrupole operators along with the scalar term. It was shown that depending on the conditions imposed on the interaction amplitudes (stability con-

ditions), the ground state may exhibit three different phases: quadrupolar, ferromagnetic, and paramagnetic. The basic thermodynamic characteristics such as ground state thermodynamic potential, pressure, magnetization, single-particle excitation energies are analyzed for all phases. For SU(3) invariant interaction Hamiltonian, $(J(\mathbf{p})=K(\mathbf{p}))$, the computed physical quantities reproduce the results of Ref. 36. It is worth noting that in this case, Eq. (56) has no solution corresponding to the paramagnetic phase. If the interaction Hamiltonian is SU(2) invariant but does not involve the quadrupole operators $(K(\mathbf{p})=0)$, then our results agree with the corresponding studies for non-local interaction [20, 22]. For local interaction,

$$U(\mathbf{p})=U(0)=\frac{4\pi\hbar^2}{m}\frac{(a_0+2a_2)}{3},$$

$$J(\mathbf{p})=J(0)=\frac{4\pi\hbar^2}{m}\frac{(a_2-a_0)}{3},$$

where a_0 and a_2 are the s-wave scattering lengths in the total spin $\mathcal{S}=0$ and $\mathcal{S}=2$ channels, respectively [see the explanation below Eqs. (28)], our findings cover the results of Refs. 19, 21, and 23.

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Мультипольні ступені свободи у фізиці високоспінових квантових атомних газів

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Наведено загальні аргументи на користь того, що квантові атомні гази взаємодійних високоспінових атомів є фізичною системою, в якій можуть проявлятися мультипольні (приховані) ступені свободи. Їх прояв відбувається при нелокальній міжатомній взаємодії. Для локальної взаємодії, що описується завдовжки розсіяння *s*-хвилі, мультипольні ступені свободи не проявляються. Щоб проілюструвати наші результати, теоретично досліджено явище конденсації Бозе–Ейнштейна у взаємодійному газі атомів зі спіном-1 у зовнішньому магнітному полі. Це дослідження засновано на інваріантному гамільтоніані SU (2), який має білінійну структуру в спінових та квадрупольних операторах разом зі скалярним членом. Показано, що залежно від умов, що накладаються на амплітуди взаємодії (умов стійкості), основний стан системи може мати три різні фази: квадрупольну, феромагнітну та парамагнітну. Основні термодинамічні характеристики, на які впливає прихований ступінь свободи, знайдено для всіх фаз.

Ключові слова: високоспінові атоми, квантові атомні гази, конденсація Бозе–Ейнштейна.