Many-Body Theory of Dilute Bose-Einstein Condensates with Internal Degrees of Freedom

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The Bogoliubov theory of weakly interacting bosons is generalized to Bose-Einstein condensates with internal degrees of freedom so that a single effective Hamiltonian produces various many-body ground states or metastable spin domains and the corresponding collective modes on an equal footing.

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The internal degrees of freedom of alkali Bose-Einstein condensates (BECs) arise primarily from electronic spin and are hence by far more amenable to manipulation than those of superfluid $^3$He. The realization of “spinor” BECs has motivated many researchers to study the magnetism of superfluid vapors and by Machida and Ho using mean-field theory. The many-body ground states were investigated by Law et al. and by Koashi and Ueda and Ho and Yip in the absence and presence, respectively, of a magnetic field; in the latter case, it is predicted that the magnetic sublevel $m = 0$ of a spin-1 antiferromagnetic BEC becomes populated as the magnetic field decreases.

The main aim of this Letter is to present a unified theory that derives the various many-body states of BEC and the corresponding excitation spectra of spinor BECs have been examined by Ohmi and by c-numbers. After some algebraic manipulation, we obtain

$$
\hat{H}_{\text{eff}} = \frac{c_0 + c_1}{2V} N(N - 1) - \frac{3c_1}{2V} \hat{A}^\dagger \hat{A} - p(\hat{n}_{01} - \hat{n}_{00})
+ \sum_{k \neq 0} \sum_{\alpha = 0, \pm 1} \left( \epsilon_k - po - \frac{(1 + |\alpha|)c_1}{V} \hat{n}_{\alpha \alpha} - \frac{c_0 c_1}{2V} \hat{n}_{\alpha \alpha} \right) \hat{n}_{\alpha \alpha}
+ \frac{1}{V} \sum_{k \neq 0} \left\{ \frac{c_0}{2} \left( \hat{D}_k \hat{D}_k^\dagger - \hat{D}_k^\dagger \hat{D}_k \right) + \frac{c_1}{2} \left( \hat{S}_k \hat{S}_k - \hat{S}_k^\dagger \hat{S}_k \right) \right.
+ \sum_{\alpha = 0, 1} c_1 \hat{a}_{\alpha \alpha}^\dagger \hat{a}_{\alpha \alpha}^\dagger \hat{a}_{\alpha 1 - \alpha \alpha} \hat{a}_{\alpha 1 - \alpha \alpha} - \hat{a}_{\alpha \alpha}^\dagger \hat{a}_{\alpha \alpha} \hat{a}_{\alpha 1 - \alpha \alpha} + \hat{a}_{\alpha \alpha}^\dagger \hat{a}_{\alpha \alpha} \hat{a}_{\alpha 1 - \alpha \alpha} \hat{a}_{\alpha 1 - \alpha \alpha} + h.c. \right\}
$$

where $\hat{D}_k = \sum_{\alpha = 0, \pm 1} \hat{D}_k^\alpha \hat{D}^\dagger_{\alpha \alpha}$, $\hat{S}_k = \sum_{\alpha = 0, \pm 1} \hat{S}_k^\alpha \hat{S}_k^\dagger_{\alpha \alpha}$, and $\hat{a}_{\alpha \alpha}^\dagger \hat{a}_{\alpha \alpha}$ describe density-wave and spin-wave operators, respectively. The first three terms on the right-hand side of Eq. (3) were studied in Refs. [4–6]; the remaining terms show how the internal and spatial degrees of freedom couple to one another.

To set a reference frame for later discussions, let us recapitulate the main results of Refs. [4–6]. The Hamiltonian discussed in these references reads essentially...
When \( c_1 < 0 \), the energy minimum is obtained by putting all particles in the state with \( k = 0 \) and \( \alpha = 1 \):

\[
|N_2 = 0, F = N, F_z = N\rangle = \frac{(\hat{a}_{01}^\dagger)^N}{\sqrt{N!}}|\text{vac}\rangle,
\]

(5)

where \( F \) and \( F_z \) denote the total spin and its projection on the \( z \) axis, and \( N_2 \) is given in terms of \( F \) and the total number of atoms \( N \) by \( N_2 = (N - F)/2 \). Because all spins are aligned in the same direction, the system is ferromagnetic. When \( c_1 > 0 \), the first term on the right-hand side of Eq. (4) energetically favors the spin-singlet (or antiferromagnetic) correlation, whereas the second one favors the parallel-spin configurations. For a given external magnetic field \((\propto p)\), the energy minimum is attained for the state \[|N_2 = (N - F)/2, F, F_z = F\rangle_0 \]

\( \propto (\hat{A}^\dagger)^{N/2} (\hat{F}_-)^{F - F_z} (\hat{a}_{01}^\dagger)^F |\text{vac}\rangle \),

(6)

where \( F \) denotes an integer that satisfies \( F - 1/2 < p/c_1 < F + 3/2 \), and \( \hat{F}_- \equiv (f^- - i f^+)_{\alpha\beta}\hat{a}_{0\alpha}^\dagger\hat{a}_{0\beta}^\dagger \). In both Eqs. (3) and (5), the depletion of the condensate due to interactions is not taken into account.

When the components with \( k = 0 \) are macroscopically occupied, we may replace \( \hat{a}_{0\alpha} \) in Eq. (3) with the c-numbers \( \sqrt{N}\zeta_\alpha \). To find the correct excitation spectra, it is crucial to take the depletion of the condensate into account. This is done by setting

\[
\sum_{k} |\zeta_{\alpha}|^2 = 1 - \frac{1}{N} \sum_{k \neq 0, \alpha} \hat{n}_{k\alpha},
\]

(7)

where the last term describes the fraction of the depletion. The energy of the condensate is given by

\[
E_0 = -\frac{c_1 N^2}{2N} \zeta_1^2 - 2\zeta_1 \zeta_\alpha \hat{n}_{k\alpha}^2 - \frac{pN}{\sqrt{N}}(|\zeta_1|^2 - |\zeta_\alpha|^2),
\]

(8)

where \( \zeta_\alpha \) are determined by requiring that \( E_0 \) be minimized subject to constraint (3).

For \( c_1 < 0 \), the minimum of \( E_0 \) is reached when

\[
\zeta_{\alpha} = \zeta_{-1} = 0, \quad |\zeta_1|^2 = 1 - \frac{1}{N} \sum_{k \neq 0, \alpha} \hat{n}_{k\alpha}.
\]

(9)

The Hamiltonian (3) then reduces to

\[
\hat{H}^F = \frac{c_0 + c_1}{2N} N(N - 1) - pN \left[ \sum_{k \neq 0} \left[ e_k \hat{n}_{k1} + \frac{(c_0 + c_1)N}{2N} (\hat{n}_{k1}^\dagger \hat{n}_{k1} + \hat{n}_{k1} + \text{h.c.}) \right] \right.

+ (\epsilon + p) \hat{n}_{k0} + \left. (\epsilon + 2p - \frac{2c_1 N}{N}) \hat{n}_{k-1} \right].
\]

(10)

Diagonalizing this Hamiltonian, we find the excitation spectra as

\[
E_{k,1}^F = \sqrt{e_k^2 + 2(c_0 + c_1)n},
\]

\[
E_{k,0}^F = e_0 + p,
\]

\[
E_{k,-1}^F = e_0 + 2p - 2c_1 n,
\]

(11)

in agreement with Ref. [2]. We may gain some insight into the nature of the many-body correlation by writing the many-body wave function in the coordinate representation:

\[
\Psi(r_1, \alpha_1, \ldots, r_N, \alpha_N) = \langle \text{vac} | \hat{\Psi}_{\alpha_1}(r_1) \cdots \hat{\Psi}_{\alpha_1}(r_1) | \Phi \rangle.
\]

(12)

Here \( |\Phi\rangle \) is given in the Bogoliubov approximation by

\[
|\Phi\rangle \sim \exp \left( \phi_0 \hat{a}_{01} - \sum_{k \neq 0} \nu_k \hat{a}_{k1}^\dagger \hat{a}_{k-1}^\dagger \right) |\text{vac}\rangle,
\]

(13)

where \( \phi_0^2 = N[1 - (8/3\sqrt{\alpha_0^2 + \pi})] \) and \( \nu_k = 1 + c_k - \sqrt{c_k(c_k + 2)} \) with \( c_k \equiv k^2/(8\pi a_0 n) \). In the dilute limit, the many-body wave function becomes very small unless all \( \alpha_0 \)'s are equal 1, and we find that

\[
\Psi(r_1, \cdots, r_N) \approx \exp \left( - \sum_{i < j} \frac{\alpha_i}{r_{ij}} e^{-r_{ij}/\xi} \right),
\]

(14)

where \( r_{ij} \equiv |r_i - r_j| \) and the terms that are of the order of 1/\( N \) are ignored. This result clearly shows that two bosons strongly repel each other when their distance becomes smaller than the healing length \( \xi \equiv (8\pi a_0 n)^{-1/2} \).

For \( c_1 > 0 \), minimizing \( E = E_0 - \delta \sum_\alpha |\zeta_\alpha|^2 \), where \( \delta \) is a Lagrange multiplier, yields

\[
|\zeta_\alpha| \left( e^{i(\phi_1 + \phi_{-1} - 2\phi_0)} + \frac{\delta}{\sqrt{\delta^2 - \gamma^2}} \right) = 0,
\]

(15)

where \( \phi_\alpha \equiv \text{arg}\zeta_\alpha \) and \( \gamma \equiv 2p/(c_1) \). In the presence of the external magnetic field (i.e., \( \gamma \neq 0 \)), the minimum of \( F \) is attained when

\[
\zeta_0 = 0, \quad |\zeta_{\pm 1}|^2 = \frac{1}{2} \pm \frac{\gamma}{4} - \frac{1}{2N} \sum_{k \neq 0, \alpha} \hat{n}_{k\alpha},
\]

(16)

and the corresponding Hamiltonian reads

\[
\hat{H}_{AF} = \frac{c_0 + c_1}{2N} N(N - 1) + \frac{c_1}{2N} \left( \frac{c_0 N^2}{4} - 1 \right) - p\gamma N \sum_{k \neq 0, \alpha} (\epsilon_k + c_1 n\delta_{\alpha,0}) \hat{n}_{k\alpha} + \frac{1}{2N} \sum_{k \neq 0} \left\{ c_0 (\hat{D}_k \hat{D}_{-k} + \hat{D}_{-k}^\dagger \hat{D}_k) \right. \\

+ c_1 (\hat{S}_{k\alpha}^\dagger \hat{S}_{-k} + \hat{S}_{k\alpha}^\dagger \hat{S}_{k} + n |\zeta_{-1}|^2 \hat{a}_{k0}^\dagger \hat{a}_{-k0} + \text{h.c.}) \left\}.
\]

(17)
The \( \alpha = 0 \) mode is decoupled and its dispersion relation is given by

\[
E_{k,0}^{\text{AF}} = \sqrt{\epsilon_k^2 + 2c_1n\epsilon_k + p^2}.
\]

(18)

The \( \alpha = \pm 1 \) modes are coupled, and the dispersion relations of the coupled modes are given by

\[
E_{k,\pm}^{\text{AF}} = \sqrt{\epsilon_k^2 + 2(c_0 + c_1)n\epsilon_k \pm \epsilon_k \sqrt{n^2(c_0 - c_1)^2 + \frac{4p^2c_0}{c_1}}}.
\]

(19)

again in agreement with Ref. [2]. Our theory thus reproduces all known collective modes that are derived using a different method.

An interesting situation arises in the absence of a magnetic field (i.e., \( \gamma = 0 \)), where condition (13) can be met if

\[
\phi_0 + \phi_0 - 2\phi_0 = \pi.
\]

(20)

This result is in accordance with a rule pointed out in Ref. [0], that is, when the interaction is attractive, the relative phase coherence, as implied by the constraint (21), will spontaneously emerge if more than two BECs coexist. In the present case, the attractive force applies among three spin components, as implied by the condition \( c_1 > 0 \) (see Eq. (6)).

When the relation (20) holds, Eq. (13) implies that \( |\zeta_0| \) is arbitrary, so we have \( |\zeta_1| = |\zeta_{-1}| \), \( |\zeta_0|^2 = 1 - 2|\zeta_1|^2 \). This, combined with Eq. (21), leads to a vectorial order parameter as \( \zeta = (\zeta_1, \zeta_0, \zeta_{-1}) = e^{i\phi_0} (-e^{i(\phi_0 - \phi_1)} \sin \beta/\sqrt{2}, \cos \beta, e^{-i(\phi_0 - \phi_1)} \sin \beta/\sqrt{2}) \).

This result agrees with Eq. (5) of Ref. [3] and implies that the spin components can change under spatial rotation. It is surprising that the many-body ground state predicts otherwise: from Eq. (8), we find that at zero magnetic field (hence \( F = 0 \)) spin components cannot change under spatial rotation but must always be the same [6] and is given by \( \hat{n}_{k,\alpha} = (N - \sum_{k'} \hat{n}_{k'}) / 3 \) for \( \alpha = 0, \pm 1 \), where we take into account the depletion of the condensate \( \sum_{k'} \hat{n}_{k'} \) due to interactions. This is a consequence of the fact that the true ground state is composed of spin-singlet “pairs” and is therefore invariant under rotation.

The above result for \( \hat{n}_{k,\alpha} \) and the relative phase relation (21) may be used to drastically simplify the Hamiltonian (8), giving

\[
\hat{H}_{\gamma = 0}^{\text{AF}} = \frac{c_0}{2V}N(N - 1) - \frac{c_1N}{2V} + \sum_{k \neq 0} \left[ (\epsilon_k + c_0n)\hat{d}_{k}^{\dagger}\hat{d}_{k} + (\epsilon_k + c_1n)(\hat{s}_{k}^{\dagger}\hat{s}_{k} + \hat{q}_{k}^{\dagger}\hat{q}_{k}) + \frac{n}{2}c_0\hat{d}_{k}^{\dagger}\hat{d}_{-k} + c_1(\hat{s}_{k}^{\dagger}\hat{s}_{-k} + \hat{q}_{k}^{\dagger}\hat{q}_{-k} + \text{h.c.}) \right],
\]

(21)

where

\[
\begin{align*}
\dot{\hat{c}}_k &= \frac{1}{\sqrt{3}}(\hat{a}_{k1}e^{-i\phi_0} + \hat{a}_{k0}e^{-i\phi_0} + \hat{a}_{k-1}e^{-i\phi_1}), \\
\dot{\hat{s}}_k &= \frac{1}{\sqrt{2}}(\hat{a}_{k1}e^{-i\phi_0} - \hat{a}_{k-1}e^{-i\phi_1}), \\
\dot{\hat{q}}_k &= \frac{1}{\sqrt{6}}(\hat{a}_{k1}e^{-i\phi_0} - 2\hat{a}_{k0}e^{-i\phi_0} + \hat{a}_{k-1}e^{-i\phi_1}).
\end{align*}
\]

(22)

We thus find that the density, spin, and quadrupolar fluctuations provide independent excitations. The novelty of these modes is that they are phase-locked to the spin components of the condensate. Diagonalizing the Hamiltonian (21), we obtain the following excitation spectra:

\[
E_{\alpha,k}^{\text{AF}} = \sqrt{\epsilon_k[\epsilon_k + 2c_0n]}, \quad E_{\alpha,k}^{\text{AF}} = \sqrt{\epsilon_k[\epsilon_k + 2c_1n]}.
\]

(23)

In the thermodynamic limit, these collective modes survive only at exactly zero magnetic field, and may be viewed as singular. However, in mesoscopic situations, e.g., when the system is confined in a quasi-one-dimensional torus (to which the present theory applies with minor modifications), these modes survive at small magnetic fields, provided the \( k = 0, \alpha = 0 \) mode is macroscopically occupied (for a more precise definition of “small” magnetic fields, see Ref. [3]).

Recently, an MIT group has observed the formation of metastable spin domains [14]. They first prepared all atoms in the \( \alpha = 1 \) state and then placed half of them in the \( \alpha = 0 \) state by irradiating the rf field. Letting the system evolve freely while using the quadratic Zeeman effect to prevent the \( \alpha = -1 \) component from appearing, they found that spin domains formed with the two components alternatively aligned. It was discussed [10] [12] that this phenomenon is due to the imaginary frequencies of the excitation modes. Here we use our theory to confirm this hypothesis and to derive a general expression for the dispersion relation. The experimental conditions in effect amount to setting

\[
|\zeta_1|^2 = |\zeta_0|^2 = \frac{1}{2} - \frac{1}{2N} \sum_{k \neq 0} (\hat{n}_{k1} + \hat{n}_{k0}), \quad \zeta_{-1} = 0.
\]

(24)

Our Hamiltonian (8) reduces to

\[
\hat{H} = \frac{c_0 + c_1}{2} n(N - 1) - \frac{c_1}{8} n N + \sum_{k \neq 0} \left[ \left( \epsilon_k + \frac{c_0n}{2} + \frac{3c_1n}{4} \right) \hat{n}_{k1} + \left( \epsilon_k + \frac{c_0n}{2} - \frac{c_1n}{4} \right) \hat{n}_{k0} + \frac{c_0}{8} \hat{a}_{k0} \hat{a}_{-k0} + \text{h.c.} \right] + \frac{c_0 + c_1}{8} n (\hat{a}_{k1} \hat{a}_{-k1} + \hat{a}_{k1} \hat{a}_{-k0} + \hat{a}_{k} \hat{a}_{-k} + \hat{a}_{k} \hat{a}_{-k} + \text{h.c.})].
\]

(25)

Diagonalizing the Hamiltonian, we find the dispersion relations as
\[(E_k)^2 = \xi_k^2 + (2u + v)\xi_k + \frac{3}{4}v^2 \pm \left[4(u^2 + 2uv + 2v^2)\xi_k^2 + 2u^2(2u + v)\xi_k - v^3 \left(u + \frac{3}{4}v\right)\right]^{\frac{1}{2}}, \quad (26)\]

where \(u \equiv c_0 n/2\) and \(v \equiv c_1 n/2\). For parameters of the MIT experiment \(n \sim 10^{14} \text{ cm}^{-3}\), \(a_t \sim 29\,\text{Å}\), and \(a_s \sim 26\,\text{Å}\) [13], we find that \(v/u \ll 1\). Ignoring in Eq. (26) higher-order powers of \(v/u\), we obtain

\[(E_k)^2 = \xi_k^2 + (2u + v)\xi_k \pm 2(u + v)\xi_k,\]

where the plus sign corresponds to the density wave, while the minus sign corresponds to the spin wave. We see that the energy of the spin wave becomes pure imaginary for \(\xi_k < v\), implying the formation of spin domains. The corresponding wavelength defines the characteristic length scale of the spin domains as

\[\lambda_c = \sqrt{\frac{3\pi}{(a_t - a_s)n}}. \quad (27)\]

This result agrees with that of Ref. [12] except for a numerical factor. Using the above parameters, we obtain \(\lambda \sim 18\,\mu\text{m}\), in reasonable agreement with the observed value of about 40\,\mu m [13].

In conclusion, we have presented a versatile many-body theory of spin-1 dilute bose gas. Depending on the parameters, a single effective Hamiltonian (3) describes various many-body ground states, metastable spin domains, and the corresponding excitation spectra. An extension to spin-2 BEC can be similarly carried out and will be reported elsewhere.

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