Coleman-Weinberg mechanism in spinor Bose-Einstein condensates

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received 7 May 2014; accepted in final form 17 July 2014
published online 1 August 2014

PACS 05.30.Jp – Boson systems
PACS 03.75.Hh – Static properties of condensates; thermodynamical, statistical, and structural properties
PACS 03.75.Mn – Multicomponent condensates; spinor condensates

Abstract – It is argued that a continuous quantum phase transition between different ordered phases in spinor Bose-Einstein condensates predicted by the mean-field theory is vulnerable to quantum fluctuations. By analyzing Lee-Huang-Yang corrections in the condensate, we demonstrate that the so-called Coleman-Weinberg mechanism takes place in such a transition, that is, the transition becomes of the first order by quantum fluctuations. A jump to be expected in this first-order transition is induced by a correction from density fluctuations despite a transition between different magnetic properties with keeping condensation. We exemplify this with an experimentally relevant case and show that a measurement of a condensate depletion can be utilized to confirm the first-order transition.

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Introduction. – A competition among different degrees of freedom changes the nature of phase transitions qualitatively. This has been first recognized in the elementary particle physics and is nowadays called Coleman-Weinberg mechanism [1] where the massless scalar field gains a mass due to quantum fluctuations on the gauge field. In the condensed-matter physics, a similar phenomenon has been rediscovered and is called fluctuation-induced first-order transitions where the thermal fluctuations on the gauge field and the director induce first-order transitions in the type-I superconductor and in the smectic-A liquid crystal, respectively [2], while a mean-field theory incorrectly predicts continuous phase transitions in both systems.

Recently, ultracold atomic gases have provided an ideal arena to explore classical and quantum phase transitions. If we focus our attention on a quantum phase transition being a particularly interesting class [3], superfluid-Mott insulator transition [4] and paramagnet-antiferromagnet transition in the quantum Ising model [5] have already been realized. In addition to the realizations of systems analogous to condensed-matter physics, a quantum phase transition in a new state of matter, which has yet to be discussed in other fields, can also be achieved.

Spinor Bose gas is one of such systems and has been studied because of the richness of the realized phases and a variety of quantum phase transitions among different ordered phases [6–8]. For example, in the system on a lattice [9–16], it has been shown that, contrary to the spinless case, the superfluid-Mott insulator transition is first order or continuous depending on the spin-dependent coupling and filling [11,12,15,16]. Even in the case with weak couplings where a Bose-Einstein condensate (BEC) is always present and the theory of weakly interacting BECs can be applied [17,18], interesting properties come out. One of the nontrivial predictions at the mean-field level is the emergence of continuous quantum phase transitions between different ordered phases while most of the transitions are first order [6,8,19]. Seemingly, this result is counterintuitive since it is thought that a phase transition between different ordered phases is first order [20] due to the observation that in many cases, order parameters at the phase boundary change abruptly [3,21]. At the same time, there exist situations in which the order parameter in each phase is smoothly connected at a boundary, which permits a continuous transition at the mean-field level and has motivated studies of quench dynamics [22–27] à la Kibble and Zurek [28,29].

In this letter, we show that the Coleman-Weinberg mechanism takes place in an experimentally verifiable spin-1 BEC. It is demonstrated that the continuous transition predicted at the mean field becomes first order, which
is driven by a correction from density fluctuations while a BEC is maintained during the transition in which a change of magnetic properties occurs. In this transition, the Bogoliubov modes from the transverse spin sector and charge sector play roles similar to the scalar and gauge fields in the model by Coleman and Weinberg [1], respectively. Our finding indicates that the nature of the transition is the itinerant property of particles and interplay between charge and spin sectors hidden at the mean-field level. Since the correction from the density fluctuations is dominant in spinor BECs with alkali species, this first-order phase transition may be experimentally detectable. We also reveal that a measurement of a condensate depletion is able to confirm our statement.

Hamiltonian and mean-field phase diagram. — We consider $N$ spin-1 identical bosons with an $s$-wave scattering in a three-dimensional box [30]. We assume that an external magnetic field is applied in the $z$-direction. Due to global spin conservation along the $z$-axis on time scales of experiments, the most dominant contribution comes from a quadratic Zeeman effect instead of a linear Zeeman effect [8,19]. Then, the low-energy Hamiltonian of a spin-1 BEC is given by

$$H = \int d\mathbf{x}(H_0 + H_{\text{int}}),$$

where

$$H_0 = \phi_m^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2M} + q_m^2 \right) \phi_m(x)$$

is the single-particle Hamiltonian with the quadratic Zeeman coupling $q$ and

$$H_{\text{int}} = \phi_m^\dagger \phi_{m'}^\dagger (c_0 \delta_{mn} \delta_{m'n'} + c_1 \mathbf{F}_{mn} \cdot \mathbf{F}_{m'n'}) \phi_n \phi_{n'}$$

is the interaction Hamiltonian. Here, $\mathbf{F}$ indicates spin-1 matrices, and $m$ gives the $z$ component of the hyperfine spin in each atom. As seen from eq. (3), $c_0$ and $c_1$ are spin-independent and spin-dependent coupling constants, respectively. Thus, $c_0 > 0$ is necessary for a stable BEC [31]. Essentially, an alkali species used in spinor BECs satisfies this condition along with an additional condition $c_0 \gg |c_1|$ [8].

In the mean-field theory, the field $\phi_m$ is treated as c-number $\psi_m$ with $\psi_m = \sqrt{n_c} \zeta_m$, where $n$ is the density of the atoms and variational parameters $\zeta_m$ are assumed to satisfy the normalization condition $\sum_m |\zeta_m|^2 = 1$. In the case of $c_1 < 0$, which is relevant to a spin-1 $^{87}$Rb condensate, the mean-field solutions are given by [19,32]

Ferromagnetic phase: $\zeta^F_m = (1, 0, 0)$, \hspace{1cm} (4)
Polar phase: $\zeta^P_m = (0, 1, 0)$, \hspace{1cm} (5)
Broken-axisymmetry phase:

$$\zeta^BA_m = \left( \frac{1}{4} + \frac{q}{8nc_1}, \frac{1}{2} - \frac{q}{4nc_1}, \frac{1}{4} + \frac{q}{8nc_1} \right).$$

The corresponding mean-field phase diagram is shown in fig. 1. We point out that each phase may be characterized by different magnetic orders whose basic properties have been confirmed experimentally [33–35]. In the ferromagnetic phase, the magnetization along the $z$-axis emerges, while in the broken-axisymmetry phase, the emergent magnetization is perpendicular to the magnetic-field direction. In relatively large positive $q$, the polar phase emerges where there is nematicity [36] but no magnetization. Here, we focus on the order of phase transitions: the transition between the ferromagnetic and broken-axisymmetry phases is first order while that between the polar and broken-axisymmetry phases is continuous [19,32]. They can easily be checked by the usual way, namely, taking the derivative of the mean-field ground-state energies with respect to the couplings [21,37]. Intuitively, they can be understood by the fact that the order parameter abruptly changes at the boundary between the ferromagnetic and broken-axisymmetry phases while a smooth change occurs between the broken-axisymmetry and polar phases. Therefore, the smooth transition between the broken-axisymmetry and polar phases is possible while the abrupt (first-order) transition is expected in the transition between the ferromagnetic and broken-axisymmetry phases due to the level crossing argument [8]. In addition, from the analysis of the lowest-order effective theory, this continuous transition is alleged to lie in the universality class of the (3 + 1)-dimensional $O(2)$ model due to the absence of the linear Zeeman effect, which induces the Berry phase term [22,38]. We note that the model discussed by Coleman and Weinberg [1] also belongs to this universality class at the mean-field level.

Quantum corrections of ground-state energies. — Along the lines of the argument by Coleman and Weinberg [1,39], we consider quantum fluctuation effects at the 1-loop level in the broken-axisymmetry and polar phases. In the case of the BEC systems [40], this corresponds to considering up to the Beliaev [41] or the Lee-Huang-Yang (LHY) [42,43] theory. To this end, we employ the Bogoliubov prescription [31] in each phase. This is achieved by considering the fluctuations of $\phi_m$ from the c-number $\psi_m$ up to the second order at the Hamiltonian level, and the resultant quantum correction to the ground-state energy is nothing but the LHY (1-loop) correction.
The ground-state energy in the polar phase is given by [44]

\[
E^P = E^P_{MF} - \frac{1}{2} \sum_\mathbf{k} \left[ (\epsilon_\mathbf{k} + nc_0 - E^P_{\mathbf{k},d}) + 2(\epsilon_\mathbf{k} + q + nc_1 - E^P_{\mathbf{k},f}) \right] - \frac{1}{2} \frac{(nc_0)^2 + 2(nc_1)^2}{2\epsilon_\mathbf{k}},
\]

(7)

where \( \epsilon_\mathbf{k} = \hbar^2 k^2/(2M) \), and

\[
E^P_{\mathbf{k},d} = \frac{\epsilon_\mathbf{k}(\epsilon_\mathbf{k} + 2nc_0)}{2},
\]

(8)

\[
E^P_{\mathbf{k},f} = \frac{\epsilon_\mathbf{k}(\epsilon_\mathbf{k} + q)(\epsilon_\mathbf{k} + q + 2nc_1)}{2},
\]

(9)

are Bogoliubov modes, which originate from density and spin fluctuations, respectively [32,44]. Here, \( E^P_{MF} = N\epsilon_0/2 \) with the total particle number \( N \) is the mean-field energy, and the remaining terms describe the LHY correction. As can be seen from eq. (7), while each term in the LHY correction has an ultraviolet divergence, these divergences are mutually cancelled out. Thus, a finite ground-state energy can be obtained. This is the consequence of the renormalization. On the other hand, the ground-state energy in the broken-axisymmetry phase is given by [44]

\[
E^{BA} = E^{BA}_{MF} - \frac{1}{2} \sum_\mathbf{k} \left[ (\epsilon_\mathbf{k} + q/2 - E^{BA}_{\mathbf{k},f}) + (2\epsilon_\mathbf{k} + nc_0 - nc_1 - E^{BA}_{\mathbf{k},d} - E^{BA}_{\mathbf{k},f}) \right] - \frac{1}{2\epsilon_\mathbf{k}} \left\{ \frac{(nc_1 - 2nc_0)q^2}{2nc_1} + (nc_0 + nc_1)^2 \right\},
\]

(10)

where \( E^{BA}_{MF} = N\epsilon_0(c_0 + c_1 + q)/2 + Nq^2/(8nc_1) \) is the mean-field energy and the others are LHY correction in the broken-axisymmetry phase. The Bogoliubov modes describing density and spin fluctuations are [44]

\[
E^{BA}_{\mathbf{k},d} = \sqrt{\epsilon_\mathbf{k}^2 + n(c_0 + c_1)\epsilon_\mathbf{k} + 2n^2c_1(c_1 - c_0) - E_1(k)},
\]

(11)

\[
E^{BA}_{\mathbf{k},f} = \sqrt{\epsilon_\mathbf{k}^2 + n(c_0 + c_1)\epsilon_\mathbf{k} + 2n^2c_1(c_1 - c_0) + E_1(k)},
\]

(12)

\[
E^{BA}_{\mathbf{k},f} = \sqrt{\epsilon_\mathbf{k}(\epsilon_\mathbf{k} + q)},
\]

(13)

with \( c_q = \frac{\hbar^2}{4n^2c_1} \) and

\[
E_1(k) = \left\{ (nc_0 + 3nc_1)^2 - 4n^2c_q(c_0 + 2c_1) \right\}^{1/2}
- 4n^3c_1(c_0 + 3c_1)(c_1 - c_0)\epsilon_\mathbf{k} + \left\{ 2n^2c_1(c_1 - c_0) \right\}^{1/2}. \tag{14}
\]

Here, the transverse spin mode \( E^{BA}_{\mathbf{k},f} \) is dependent on the spin-independent coupling \( c_0 \) except at the boundary. This is in contrast with the polar phase where such a mode depends only on the spin-dependent couplings, \( c_1 \) and \( q \).

**Fluctuation-induced first-order transition.** As far as the mean-field theory is concerned, the first derivative of the ground-state energy with respect to the coupling constants has no discontinuity at the boundary between the polar and broken-axisymmetry phases, which suggests the continuous transition. We now consider what happens when the quantum fluctuation effect is taken into account. To see this, we first point out that the phase boundary does not move in the presence of the LHY corrections, namely, \( E^P|_{q=-2nc_1} = E^{BA}|_{q=-2nc_1} \). This property originates from the fact that the Bogoliubov modes in the polar phase coincide with those in the broken-axisymmetry phase at the boundary.

We then consider its derivative with respect to \( q \) at the boundary. The derivative from the polar phase is found to be

\[
\frac{\partial E^P}{\partial q} \bigg|_{q=-2nc_1} = \frac{2N\sqrt{M^3}}{3\pi^2\hbar^4} \sqrt{n|c_1|^2},
\]

(15)

and that from the broken-axisymmetry phase is found to be

\[
\frac{\partial E^{BA}}{\partial q} \bigg|_{q=-2nc_1} = \frac{N\sqrt{M^3}}{3\pi^2\hbar^4} \left[ 2\sqrt{n|c_1|^2 + \sqrt{nc_0^4f(y)}} \right],
\]

(16)

where \( y = c_1/c_0 \) and

\[
f(y) = \frac{2 + (y)^{3/2} - 2(-y)^{5/2} + 4y + 3y^2}{(1 + y)}. \tag{17}
\]

Here, to obtain the above, we replaced the summation over \( \mathbf{k} \) in eqs. (7) and (10) by the integral. Since \( f(y) \) takes positive values for \( c_1 < 0 \) (or equally \( y < 0 \)), there is a jump in the first derivative at the boundary. We note that such a jump is characterized by the LHY correction to be small considering a weakly interacting BEC. This is consistent with the initial assumption, and the result should be valid [1,39].

We thus conclude that the fluctuation-induced first-order quantum phase transition occurs. While the transition between the polar and broken-axisymmetry phases is thought to be a magnetic one, such a jump is proportional to \( \sqrt{nc_0^3} \), that is, the LHY correction from density fluctuations. In the broken-axisymmetry phase, however, the order parameter (6) is the so-called noninert state [6,8], which even at the lowest-order level causes an admixture between the spin-independent and spin-dependent couplings in the excitation spectra in a complicated way. As a result, the transverse spin mode is dependent on \( c_0 \), which reflects the derivative of the ground-state energy and eventually leads to the nontrivial first-order quantum phase transition. This result would be reasonable once we recall the fact that each particle in a spinor BEC is itinerant, which is essentially different from spin systems and allows to deviate from the continuous transition. Finally, we point out that while the transition becomes of

\[\text{In addition to the smallness of the jump, the high rate of condensation and dimensionality are important to apply the Bogoliubov theory. Since the fluctuations around the 4-dimensional } O(2) \text{ model with the weakly interacting BEC are concerned, the Bogoliubov theory can be applied.}\]
the first order, the change in the expectation value of the transverse spin \( \langle F^\perp \rangle \) is still continuous even at the quantum level. Although this result can be easily checked by using the Bogoliubov theory, it may be interpreted as indicating that the first-order transition is induced by the density fluctuations, which does not break the spin rotational symmetry.

**Measuring the first-order transition.** – In the above, the jump in the first derivative is proportional to the LHY correction from density fluctuations, \( \sqrt{n c_0} \). Since the spin-independent coupling \( c_0 \) is dominant in a spinor BEC with alkali atoms, this effect may be detectable. Here, we relate such a jump to a physical observable. By using the Hellmann-Feynman theorem \([45,46]\) at finite temperature, we obtain

\[
\frac{\partial F}{\partial q} = \frac{1}{Z} \text{Tr} \left( e^{-H/(k_B T)} \frac{\partial H}{\partial q} \right) = \langle (N_1 + N_{-1}) \rangle_T, \tag{18}
\]

where \( Z \) is the partition function and the above is correct even at \( T = 0 \). Namely, the first derivative on \( q \) corresponds to the number of particles with hyperfine state \( m = \pm 1 \). By adding a magnetic-field gradient, which causes the Stern-Gerlach separation, the number of the particles in each hyperfine state is routinely measured \([8]\), which can also be utilized to confirm the first-order phase transition between the polar and broken-axisymmetry phases. At the mean-field level, we expect the smooth change of \( N_1 + N_{-1} \) where it takes a nonzero value in the broken-axisymmetry phase and takes zero in the polar phase and at the boundary. However, at the quantum level, while such a smooth change can be continued in each phase, \( N_1 + N_{-1} \) has a jump at the boundary due to the quantum fluctuations. By taking parameters of spin-1 \(^{87}\)Rb condensates \( y = 4.56 \times 10^{-3}, \ c_0/(4\pi \hbar^2 a_B/M) = 100.86 \) with the Bohr radius \( a_B \), we find that such a jump is about a few \% of the total number of particles with a typical value of the density in cold atoms of the order of \( 10^{14} \text{ cm}^{-3} \).

We briefly discuss the thermal fluctuation effects in the first-order quantum phase transition by means of the finite-temperature Bogoliubov theory \([31]\). The free energy in the polar phase is expressed as

\[
F^P = E^P + k_B T \sum_k \ln(1 - e^{-E^P_{k,a}/(k_B T)}) + 2 \ln(1 - e^{-E^P_{1},i/(k_B T)}) \tag{19}
\]

and that in the broken-axisymmetry phase is calculated as

\[
F^{BA} = E^{BA} + k_B T \sum_k \ln(1 - e^{-E^{BA}_{k,a}/(k_B T)}) + \ln(1 - e^{-E^{BA}_{1},i/(k_B T)}) + \ln(1 - e^{-E^{BA}_{-1},i/(k_B T)}). \tag{20}
\]

Although it is difficult to obtain analytic expressions of the free energies except for low and high temperatures, we can numerically evaluate it and its derivative. As shown in fig. 2, the difference of the first derivatives on the free energies at the boundary between the polar and broken-axisymmetry phases gets lower as the temperature increases, and the first-order phase transition is weakened. At the same time, if we look at the quantum regime in the transition where the finite-temperature Bogoliubov theory is valid, we can clearly see the first-order transition.

We now point out that the jump in the first derivative is enhanced on an optical lattice while such a jump is expected to be small under the typical current experimental condition in a continuum space. Unless we consider a too large lattice depth such that a Mott insulator comes out, the same treatment as we did in the continuum space can be performed \([47,48]\). This is due to the fact that the Bogoliubov Hamiltonian on the lattice is reduced to that in a continuum space by substitutions \( c_k \rightarrow 6t - 2t \sum_{j=1}^{3} \cos(k_j) \) and \( c_i \rightarrow U_i \) \((i = 0, 1)\), where \( t \) and \( U_i \) are the nearest-neighbor hopping matrix and Hubbard interaction, respectively. We also note that in addition to the Bogoliubov Hamiltonian, a similar form can be obtained for the condensate depletion on the lattice. It has been experimentally tested in a spinless BEC that such an analysis provides a semi-quantitative description for the condensate depletion \([49]\). In the case of spinor BECs, the total condensate depletion (sum of the condensate depletion in each component) on the lattice has been analyzed in \([50]\), which numerically estimates that the total condensate depletion scales as \( U_0/t \) with a positive exponent and is of the order of 10\% around the ten recoil energies. This result indicates that the jump in the first derivative is also expected to be around 10\% since the condensate depletion in the polar phase takes a large value for the \( m = 0 \) component rather than for the \( m = \pm 1 \) components and therefore \( N_1 + N_{-1} \) on the lattice is still around zero in the polar phase, which is in contrast with the case in the broken-axisymmetry phase where the large condensate depletion occurs for the \( m = \pm 1 \) components.
Thus, by shifting the magnetic field, we may clearly see the jump of $N_{1} + N_{-1}$ on the lattice such that the first-order effect cannot be blurred by the fluctuation of the magnetic field in experiments.

In conclusion, we have examined fluctuation effects of a would-be continuous quantum phase transition between polar and broken-axisymmetry phases in a spinor BEC. We have shown that an interplay between the spin and charge sectors hidden at the mean-field level leads to the first-order transition by the Coleman-Weinberg mechanism. This first-order transition is characterized by a correction from density fluctuations, which may pave the way to measure our finding. We have pointed out that a condensate depletion can be used to confirm the first-order transition by the Coleman-Weinberg mechanism. This first-order transition is realized in the phase transition between the polar and broken-axisymmetry phases: the ground-state energies and Bogoliubov modes coincide at the phase boundaries. At the same time, since the forms of the Bogoliubov modes are different in each phase except for the boundaries, we can naturally expect that the first derivative of the Bogoliubov modes on the coupling constants should be different even at the boundaries. Therefore, such continuum transitions may also become first order.

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The author thanks T. Giamarchi, M. Nitta, D. Takahashi, A. Tokuno, and M. Ueda for fruitful conversations. This work is supported by the Swiss National Science Foundation under MaNEP and division II.

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