Cyclic phase in $F=2$ spinor condensate: Long-range order, kinks, and roughening transition

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We study the effect of thermal fluctuations on homogeneous infinite Bose-Einstein condensate with spin $F = 2$ in the cyclic state, when atoms occupy three hyperfine states with $m_F = 0, \pm 2$. We use both the approach of small-amplitude oscillations and mapping of our model on the sine-Gordon model. We show that thermal fluctuations lead to the existence of the rough phase in one- and two-dimensional systems, when presence of kinks is favorable. The structure and energy of a single kink are found. We also discuss the effect of thermal fluctuations on spin degrees of freedom in $F = 1$ condensate.

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I. INTRODUCTION

Recent progress in the experimental physics of cold atoms allows for the creating of quasi-two-dimensional atomic gas either using one-dimensional optical lattices or applying tight axial trapping [1, 2, 3, 4]. Many properties of low-dimensional systems differ from that for the three dimensional ones. For instance, it is well-known that Bose-Einstein condensation is impossible in two-dimensional (2D) situation at any nonzero temperature, since long wavelength thermal fluctuations destroy a phase coherence. However, at low temperatures, there is still a quasi-long-range order, which disappears at the temperature of Berezinskii-Kosterlitz-Thouless (BKT) transition. Low temperature phase is often called quasicondensate, and this conception was introduced to the context of physics of alkali atoms gases in Refs. [5, 6], see also Ref. [7]. In was shown in those works that, in finite low-dimensional systems, there is still a long range order at low temperatures, and one has a true condensate, but at higher temperatures, coherence is again lost, and we have a quasicondensate.

The aim of the present paper is to study thermal fluctuations in homogeneous spinor condensates. We are mainly interested in the cyclic phase of $F = 2$ condensate, since it has unusual properties like phase locking and kinks, which are absent in other phases of $F = 2$ condensate. In the recent experiments [8, 9, 10, 11, 12], $F = 2$ spinor Bose-Einstein condensates have been created and studied. The order parameter in $F = 2$ system has five components; and, in the cyclic phase, all the particles populate three hyperfine states with $m_F = 0, \pm 2$. The characteristic feature of the cyclic phase is the fact that the ground state energy depends on the relative angle $\chi$ among the phases $S_j$ of different components of the order parameter, $\chi = 2S_0 - S_2 - S_{-2}$, through the spin-mixing term. This leads to the peculiar phase locking phenomena, since the energy has a term proportional to $\cos \chi$. In this paper we concentrate on thermal fluctuations of phases $S_j$ of different components of the order parameter as well as of $\chi$. First, we solve the Bogoliubov-de Gennes equations and calculate the mean square fluctuations of $S_j$. Each individual phase $S_j$ in this case behaves in the way similar to the case of scalar system. Namely, there is no long-range order for $S_j$ in one and two dimensions, whereas this order is kept for 3D situation. At the same time, the long-range order is still preserved for $\chi$. After this, we note that the Bogoliubov-de Gennes equations can be insufficient for the analysis of thermal fluctuations in the cyclic state, since this approach uses an expansion of the energy in the vicinity of one of the infinite number of equivalent minima at $\chi = 2\pi l$, $l$ being an integer number, and does not take into account a global periodic structure of the energy in functional space. In other words, $\cos \chi$ contribution to the energy is changed by the quadratic potential well with the infinite height. One of the possible solutions of the Gross-Pitaevskii equations for the cyclic phase is a kink, which separates two spatial domains with $\chi$ different by $2\pi$ from each other. At zero temperature, kink is energetically unfavorable. However, at finite temperature formation of kinks can become favorable due to entropic reasons. We determine analytically the structure and energy of a single kink. Also we note that our model can be mapped on the well-known sine-Gordon model. For this model, it was established before that, in low dimensions, a so called roughening transition can occur, when the system becomes unlocked from one of the minima of $\chi$. In 1D situation, a long range order for $\chi$ is absent for any nonzero temperature due to thermally-excited kinks, and the system is rough. If the system has a finite length, a nonzero temperature appears, below which still there is a long range order for $\chi$. We estimate this temperature from simple entropic arguments. In two dimensions, a roughening transition occurs at some finite nonzero temperature. From known results for the sine-Gordon model and some simple qualitative considerations we show that the temperature of the roughening transition is close to the BKT critical temperature and possibly coincides with it. We also discuss briefly the case of ferromagnetic $F = 1$ condensate. Based on the solutions of the Bogoliubov-de Gennes equations, we find that there is no long-range order in the one- and two-dimensional systems for the direction of spin. In finite systems, the order still exists...
at low temperatures, similarly to the phase coherence in scalar condensates.

The paper is organized as follows. In Section II we solve the Bogoliubov-de Gennes equations for \( F = 2 \) cyclic phase and find correlation functions. In Section III we determine the structure and energy of a single atom. In Section IV we study the order-disorder transition due to the proliferation of kinks. In Section V we study the case of ferromagnetic \( F = 1 \) condensate. We conclude in Section VI.

II. CYCLIC PHASE: SMALL AMPLITUDE OSCILLATIONS

We consider infinite homogeneous \( F = 2 \) condensate with a given density of particles \( n \) in zero magnetic field. The energy of the system depends on three interaction parameters \( \alpha, \beta, \) and \( \gamma \), which can be defined as \( 14, 15 \):

\[
\alpha = \frac{1}{4} (3g_2 + 3g_4),
\]

\[
\beta = -\frac{1}{7} (g_2 - g_4),
\]

\[
\gamma = \frac{1}{5} (g_0 - g_4 - \frac{2}{7} (g_2 - g_4)),
\]

where \( (q = 0, 2, 4) \)

\[
g_q = \frac{4\pi \hbar^2}{m} a_q
\]

and \( a_q \) is the scattering length characterizing collisions between atoms with the total spin 0, 2, and 4. In real atomic condensates, \( \alpha \gg \beta, \gamma \).

The order parameter in \( F = 2 \) case has five components \( \Psi_i (i = -2, -1, 0, 1, 2) \). The energy of the system is given by \( 13, 10 \):

\[
F = \int dr \left[ -\frac{\hbar^2}{2m} \Psi_j^* \Delta \Psi_j + \frac{\alpha}{2} \Psi_j^* \Psi^*_j \Psi_j \Psi_k + \frac{\beta}{2} \Psi_j^* (F_a)_{jk} (F_a)_{lm} \Psi_k \Psi_m + \frac{\gamma}{2} \Psi_j^* \Psi^*_k \Psi_{-j} \Psi_{-k} (-1)^j (-1)^k \right],
\]

where integration is performed over the system volume, repeated indices are summed, \( F_0, (a = x, y, z) \) is the angular momentum operator, which can be expressed in a usual matrix form.

In the absence of magnetic field and rotation, condensate can be in three different states \( 13 \), as seen from Eq. (5). These states are called ferromagnetic, cyclic and polar \( 13 \). In cyclic phase, \( \Psi_{\pm 1} = 0 \) and \( \Psi_{-2} = \frac{2}{\sqrt{3}} e^{i\theta} \), \( \Psi_0 = \frac{1}{\sqrt{2}} \), \( \Psi_2 = -\frac{1}{\sqrt{2}} e^{-i\theta} \), where \( \theta \) is an arbitrary phase (energy of the system is degenerate with respect to \( \theta \)). The ground state value of \( \chi \) in these notations is zero. Depending on values of scattering lengths \( a_q \) ferromagnetic, cyclic or polar phase has the lowest energy \( 13 \).

Extended Gross-Pitaevskii equations can be obtained as usually from the condition of minimum of free energy of the system Eq. (5). In the cyclic state, the last term in the right-hand side of Eq. (5) contains a spin-mixing contribution:

\[
F_{sm} = \gamma |\Psi_0|^2 |\Psi_2| |\Psi_{-2}| \cos \chi.
\]

Now we analyze small-amplitude oscillations of the order parameter in the cyclic phase. The fluctuations of phase of the given component of the order parameter can be expressed through the fluctuations of the order parameter itself as \( \delta S_j = Im(\delta \Psi_j)/|\Psi_j| \). For \( \delta \chi \), we have \( \delta \chi = 2\delta S_0 - \delta S_2 - \delta S_{-2} \).

The deviations of the five components of the order parameter from their equilibrium values \( \delta \Psi_j \) can be represented as

\[
\delta \Psi_j = \sum_k \left\{ c_k^{(j)} \exp(ikr + i\omega_k t) + d_k^{(j)*} \exp(-ikr - i\omega_k t) \right\},
\]

where \( c_k^{(j)} \) and \( d_k^{(j)} \) are constants to be found. Fluctuations of \( \Psi_{\pm 1} \) are decoupled from that for \( \Psi_0, \Psi_{\pm 2} \), as follows for the Bogoliubov-de Gennes equations for the cyclic phase. The spectrum for oscillations of \( \Psi_0, \Psi_{\pm 2} \) has three branches. For the first time, it was obtained in Ref. \( 17 \), and our results coincide with those results:

\[
\hbar \omega_k^{(1)} = \frac{\hbar^2 k^2}{2m} + 2\gamma n,
\]

\[
\hbar \omega_k^{(2)} = \sqrt{\frac{\hbar^2 k^2}{2m}} + 2\alpha n - \frac{\hbar^2 k^2}{2m},
\]

\[
\hbar \omega_k^{(3)} = \sqrt{\frac{\hbar^2 k^2}{2m}} + 4\beta n - \frac{\hbar^2 k^2}{2m}.
\]

The thermal distribution of quasiparticles is given by

\[
N_k^{(j)} = \frac{1}{\exp(\hbar \omega_k^{(j)}/k_B T) - 1}.
\]

One can also find eigenvectors corresponding to the branches (8)-(10). Eigenvectors for Eqs. (9) and (10) give no contribution to \( \delta \chi \), as it can be seen from the solutions of the Bogoliubov-de Gennes equations. This is the first branch (8), which is responsible for the fluctuations of \( \chi \). Physically, this is due to the fact that only branch (8) depends on the value of \( \gamma \), which yields the potential well for \( \chi \) via the spin-mixing term (6). Finally, we obtain simple expression for \( \delta \chi \):

\[
\delta \chi = \frac{1}{2i \sqrt{N} \sqrt{n}} \sum_k \{ \exp(ikr + i\omega_k t) - \exp(-ikr - i\omega_k t) \}.
\]

(12)
Next we can determine the behavior of the mean square fluctuations of $\chi$ at large distances. We found that this quantity in all dimensions tends to a constant, when the distance tends to infinity. This means that there is a long-range order for $\chi$. The reason is the presence of the gap in the excitation energy $8$). As an example, we present below the derivation and results for the 2D situation. From Eq. (12) we have

\[(\delta \chi(r) - \delta \chi(0))^2 = -\frac{1}{4Vn} \sum_{k_1,k_2} A_{k_1} A_{k_2}, \quad (13)\]

where

\[A_k = \exp(i\omega_k^{(1)}t) (\exp(ikr)-1) - \exp(-i\omega_k^{(1)}t) (\exp(-ikr)-1). \]

After averaging over the time, only terms with $k_1 = k_2$ survive in the expansion (13) and for the correlator we have

\[\langle [\delta \chi(r) - \delta \chi(0)]^2 \rangle_T = \begin{cases} \frac{T}{T_d} \exp(-2\gamma n/k_B T), & k_B T \ll \gamma n, \\ \frac{T}{T_d} \ln(k_B T/2\gamma n), & k_B T \gg \gamma n, \end{cases} \quad (16)\]

where $T_d = 2\pi h^2 n/k_B m$ is the temperature of quantum degeneracy.

The second and third branches of the spectrum, given by Eqs. (9) and (10), are responsible for the fluctuations of phases of individual components of the order parameter, $S_0$, $S_{\pm2}$. Our calculations of the mean square fluctuations of these phases revealed the behavior, which is similar to the scalar condensate. The long-range order is absent in one- and two-dimensional situations. It is interesting to note that, at the same time, the long-range order exists for the linear combination of these phases, $\chi$. Fluctuations of populations of different hyperfine states are small at $T \ll T_d$.

### III. KINK: STRUCTURE AND ENERGY

In the previous Section we have studied small-amplitude oscillations in the vicinity of homogeneous solution to the extended Gross-Pitaevskii equations. However, these equations have also a nonhomogeneous solution corresponding to the kink or domain wall between two spatial regions with values of $\chi$ different by $2\pi l$ from each other, since the energy of the system is degenerate with respect to $l$. Kinks are known to play an important role in the physics of low-dimensional systems, see e.g. the textbook [13]. Now we find the structure and energy of the one-dimensional kink in the cyclic phase for the most important case, when $l = 1$. We assume that all the quantities depend only on one coordinate $x$. For $\chi$ we have a boundary conditions $\chi(\infty) = 2\pi$, $\chi(-\infty) = 0$. The phase-dependent part of the energy consists of two contributions, one is the kinetic energy, and another one is the spin-mixing term (6):

\[ F_{ph} = \int_{-\infty}^{+\infty} dx \left[ \frac{\hbar^2}{2m} \sum_{j=-1}^{1} |\Psi_{2j}|^2 (\nabla S_{2j})^2 + \gamma |\Psi_0|^2 |\Psi_2| |\Psi_{-2}| \cos \chi \right]. \quad (17) \]
We can rewrite this expression in the diagonal form as

\[ F_{ph} = \int_{-\infty}^{+\infty} dx \left[ \frac{\hbar^2 n}{8m} \left( \frac{\hbar^2}{2m} \chi' \right)^2 + \frac{\gamma n^2}{4} \cos \chi + \frac{\hbar^2 n}{8m} \left( \frac{1}{2} \left( \nabla S_2 - \nabla S_{-2} \right)^2 + \frac{1}{4} \left( \nabla S_2 + \nabla S_{-2} + 2 \nabla S_0 \right)^2 \right) \right]. \quad (18) \]

One can easily see from Eq. (18) that the minimum energy solution for the kink corresponds to the conditions \( \nabla S_2 - \nabla S_{-2} = 0 \) and \( \nabla S_2 + \nabla S_{-2} + 2 \nabla S_0 = 0 \). In this case, the energy (18) can be mapped on the sine-Gordon energy functional. The function \( \chi(x) \) is found from the condition of minimum of \( F_{ph} \): \( \delta F_{ph} / \delta \chi = 0 \) and boundary conditions. Finally, we have

\[ \chi(x) = 2\pi - 4 \tan^{-1} \exp(-x/\xi_x), \quad (19) \]

\[ S_2(x) = S_{-2}(x) = -S_0(x) = -\frac{1}{4} \chi(x), \quad (20) \]

where

\[ \xi_x = \sqrt{\frac{\hbar^2}{2m} \frac{1}{4\gamma n}}. \quad (21) \]

is the healing length for \( \chi \). It also gives a characteristic length of the kink. The spatial structure of a single kink is presented in Fig. 1, where we have plotted \( x \)-dependences of \( \chi, S_{\pm 2}, \) and \( S_0 \). A single kink moving in the space is a soliton. As seen from Eq. (18), the energy of the kink \( F_{kink} \) scales as \( \gamma \xi_x \sim \sqrt{\gamma} \). More accurate calculation based on Eq. (19) yields

\[ F_{kink} = n^{3/2} \sqrt{\frac{\hbar^2}{m} \gamma}. \quad (22) \]

Note that in real atomic condensates \( \gamma \) has to be much smaller than \( \alpha \) and, therefore, \( \xi_x \) should far exceed the coherence length, which has a meaning of a length-scale for the density modulations.

The same structure of the kink can be obtained from the extended Gross-Pitaevskii equations supplemented by the boundary conditions for \( \chi \). These equations are rather cumbersome and we do not present them here (see e.g. our previous work \[18\]). It is easy to see by the direct substitution that Eqs. (19)-(21) with the constant populations of each magnetic sublevel yield the exact solution to these equations.

IV. ROUGHENING

At zero temperature, the sine-Gordon system in any dimension is locked in one of equivalent minima corresponding to \( \chi = 2\pi l \). At nonzero temperature, presence of kinks can be favorable due to their entropic contribution to the free energy \[18\]. Kinks destroy the long-range order and lead to the rough phase, in which height of fluctuations diverges with tending the system size to infinity. In one dimensional system of length \( L (L \gg \xi_x) \), the entropy corresponding to the single kink can be estimated as \( \ln L / \xi_x \), where \( L / \xi_x \) is just a number of places to put a kink. Therefore, a roughening temperature is

\[ T_R^{1D} \approx \frac{F_{kink}}{k_B \ln L / \xi_x}. \quad (23) \]

In the case of infinite 1D system (\( L \to \infty \)), \( T_R^{1D} = 0 \); and this result is very different from the result of small-amplitude oscillations approach, which shows a presence of long-range order for \( \chi \). Relation (23) is well-known for the sine-Gordon model and can be derived using more rigorous analysis, see e.g. Ref. \[20\] and references therein. Note that in 1D finite system, \( T_R^{1D} \to 0 \), as \( \gamma \to 0 \).

In two dimensions, a roughening temperature \( T_{R}^{2D} \) can be also estimated in a simple manner. In this case, \( F_{kink} \) given by Eq. (22) is the energy of a unit length of a kink. The ‘critical nucleus’ for the formation of the rough phase is represented by the step for \( \chi = 2\pi \) in a functional space with a perimeter \( \approx 2\pi \xi_x \). The total energy of such a nucleus is of the order of \( 2\pi F_{kink} \xi_x = \pi \hbar^2 n_s / 2m \), where we have changed density of atoms \( n \) by superfluid density \( n_s \) just below the roughening transition. It is interesting to note that this energy is independent on \( \gamma \). A roughening temperature \( T_{R}^{2D} \) can be estimated by equating the nucleus energy to the thermal one, \( T_{R}^{2D} \approx \pi \hbar^2 n_s / 2k_B m \). A more rigorous calculation for the 2D sine-Gordon model, based on renormalization group analysis \[18\], yields the same result:

\[ T_{R}^{2D} = \frac{\pi \hbar^2 n_s}{2k_B m}, \quad (24) \]

which is independent on \( \gamma \). The expression (24) for the roughening temperature coincides with the well-known result for the temperature of the BKT transition, see e.g. \[7\]. To describe properly the behavior of the system in this strongly fluctuative region at high temperatures, one needs more careful and detailed analysis. However, from the considerations presented here, we can conclude that a long range order for \( \chi \) in 2D systems survives up to quite high temperatures (of the order of the BKT critical temperature). Possibly, the roughening transition occurs simultaneously with the BKT transition, and both types of topological defects, kinks and vortices, proliferate together.

If the size of 1D or 2D finite system is less than \( \xi_x \) (which can be much larger than the coherence length), a formation of a kink is impossible, and, therefore, we...
expect that $\chi$ is nearly constant inside the cloud. At the same time, a value of $\chi$ can be different from $2\pi l$ due to thermal fluctuations. We have studied the similar situation before in Ref. [21], where the case of harmonically trapped quasi-two-dimensional $F = 1$ condensate was treated. An infinite homogeneous $F = 1$ condensate in zero magnetic field can be either in polar or ferromagnetic states, where atoms populate only one or two hyperfine states and the spin-mixing terms in the energy are zero in the equilibrium. However, in the case of a trapped rotated condensate containing vortices, there are some regions on the phase diagram, where all the three hyperfine states are populated, and the energy depends on the relative phase among them. This result was obtained before for the large class of disordered systems [14-16]. Namely, absence of long-range order in low dimensions. It is remarkable that, in this case, spin-mixing is important. An example of the systems, where spin-mixing is important, is independent on its value, but depends on the gradients of spin. The similar situation exists for the phase of the order parameter in scalar condensate (the energy of the magnetic state. The energy of the system is independent on the relative phase among them [22, 23, 24, 25, 26].

In the ground state and even in absence of rotation, applied magnetic fields and other external perturbations, as in $F = 1$ case. For the spin-mixing dynamics in $F = 1$ condensate, see Ref. [20]. Note that recently, a new experimental method for nondestructive study of internal degrees of freedom of spinor condensates was proposed [30].

VI. FERROMAGNETIC STATE IN $F = 1$ SPINOR CONDENSATE

In this Section we discuss thermal fluctuations in spinor $F = 1$ condensate. We concentrate on the ferromagnetic state. The energy of the system is independent on the direction of the spin but it depends on the gradients of spin. The similar situation exists for the phase of the order parameter in scalar condensate (the energy is independent on its value, but depends on the gradient), and therefore we can expect the similar behavior, namely, absence of long-range order in low dimensions. This result was obtained before for the large class of discrete and continuous spin models [13]. We assume that in the ground state all the atoms occupy the only one hyperfine state, $\Psi_{-1} = \Psi_0 = 0$, $\Psi_1 = \sqrt{n}$, and study small-amplitude oscillations induced by the temperature. In the ground state, spin is oriented along the $z$-direction, $S_z = 1$, $S_x = S_y = 0$. Perturbations of $\Psi_0$ lead to that of $S_x$ and $S_y$:

\[ \delta S_x = \frac{1}{\sqrt{2n}} (\delta \Psi_0 + \delta \Psi_0^*) , \]
\[ \delta S_y = \frac{i}{\sqrt{2n}} (\delta \Psi_0 - \delta \Psi_0^*) . \]

Using Eqs. (25)-(27) we have calculated mean square fluctuations for $S_x$ and $S_y$ at large distances and found an absence of long-range order in $1D$ and $2D$ cases. As an example, we show here the correlator in the $2D$ situation:

\[ \left\langle [S_x(r) - S_x(0)]^2 \right\rangle_T = \frac{T}{\lambda_T} \ln \frac{r}{\lambda_T} , \]

where

\[ \lambda_T = \frac{\hbar}{\sqrt{2mk_BT}} \]

The derivation is similar to the case of cyclic phase in $F = 2$ condensate, presented in Section IV. The result for $S_y$ is the same. For $1D$ case, the correlators behave as $\sim r$. This implies that in low-dimensional systems there is no long-range order in the direction of spin. However, the $2D$ system can be divided into blocks of a characteristic size $L$, $\xi_s \ll L \ll \lambda_T \exp(T_d/T)$, with nearly the same direction of spin in each block ($\xi_s \sim \sqrt{\frac{k_BT}{2m\hbar^2}}$ is the spin healing length). Different blocks are uncorrelated with each other. At temperatures of the order of $2T_d/\ln(k_BT_d/\beta n)$, $\xi_s$ becomes comparable to $\lambda_T \exp(T_d/T)$. In this case, the size of each block becomes of the order of $\xi_s$. In the quasi-1$D$ and 2$D$ trapped condensates, which have finite sizes exceeding $\xi_s$, at low temperatures, one can expect the same orientation of spins throughout the system, and at higher temperatures, the cloud should consist of uncorrelated blocks. This is similar to the problem of fluctuating phase in quasi-1$D$ and 2$D$ scalar condensates [31-34]. Note that the case of ferromagnetic $F = 2$ condensate is similar to that of spin-1 system.

VI. CONCLUSIONS

We have studied the effect of thermal fluctuations on homogeneous infinite Bose-Einstein condensate with spin $F = 2$. We were interested in the cyclic state of this system, in which all the particles occupy three hyperfine states with $m_F = 0, \pm 2$, and the energy depends on the relative phase $\chi = 2S_0 - S_2 - S_2$ through the spin-mixing term. Using Bogoliubov-de Gennes equations, we have calculated mean square fluctuations of $S_0, S_\pm$ and found absence of long-range order in one- and two-dimensional situations, but presence of this order for $\chi$. Then, we went beyond the small-amplitude oscillation approach and mapped our problem on the sine-Gordon model. A
structure and energy of a single kink separating two topological sectors with different values of $\chi$ were found. In 1D and 2D situations, thermal proliferation of kinks can lead to the roughening transition destroying a long-range order for $\chi$. One-dimensional infinite system is always in a rough phase, and finite 1D system, as well as infinite 2D system, experience roughening transition at finite temperatures, whose values we have estimated. At the end, we have also discussed thermal fluctuations in ferromagnetic $F=1$ system and found an absence of long-range order in the direction of spin in low-dimensional situations, as it can be expected from the Mermin-Wagner-Berezinskii theorem. We defined the typical size of each block, within which still there is an order in spin degrees of freedom. We expect that finite systems should be in the ordered phase at low temperatures.

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VII. FIGURE CAPTIONS

Fig. 1. The structure of a single kink in the cyclic state. Solid curve denotes $\chi$, dashed one corresponds to $S_0$, and dotted curve shows $S_2 = S_{-2}$. 
