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Vortex structure in spinor $F=2$ Bose-Einstein condensates

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Extended Gross-Pitaevskii equations for the rotating $F=2$ condensate in a harmonic trap are solved both numerically and variationally using trial functions for each component of the wave function. Axially symmetric vortex solutions are analyzed and energies of polar and cyclic states are calculated. The equilibrium transitions between different phases with changing of the magnetization are studied. We show that at high magnetization the ground state of the system is determined by interaction in “density” channel, and at low magnetization spin interactions play a dominant role. Although there are five hyperfine states, all the particles are always condensed in one, two, or three states. Two interesting types of vortex structures are also discussed.

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I. INTRODUCTION

Properties of Bose-Einstein condensates (BEC's) of alkali-metal-atom gases attract a considerable current interest. Recently quantized vortices and lattices of vortices have been obtained experimentally in BEC clouds confined by magnetic traps [1–4]. BEC's can have internal degrees of freedom associated with the hyperfine spin. Such condensates are usually called spinor BEC's. Examples of these systems with hyperfine spin $F=1$ were found in optically trapped ^{23}Na [5]. In zero magnetic field, spin $F=1$ condensate can be in two different states, which are called ferromagnetic and polar [6,7]. Depending on the values of interaction parameters, which determine coupling between different hyperfine states, one of these states has a lowest energy. Vortex matter in spinor BEC's is represented by a rich variety of rather exotic topological excitations. These vortices were investigated in a large number of theoretical works for the case $F=1$ (see, e.g., Refs. [8–17]).

In the most recent experiments, $F=2$ spinor Bose-Einstein condensates have been created and studied [18–21]. However, superfluid phases in the $F=2$ BEC were analyzed only for the case of the absence of magnetic field and rotation [22] (see also Refs. [23,24]). Spinor $F=2$ BEC has one more interaction parameter as compared to the $F=1$ BEC because of the larger spin value. Therefore there are three possible phases in absence of magnetic field: polar, ferromagnetic, and cyclic states.

Due to the internal degree of freedom, a rich variety of exotic vortices have been proposed in $F=1$ spinor BEC's by a large number of authors [25]. For instance, $F=1$ spinor BEC's with the ferromagnetic spin interaction exhibit $\text{SO}(3)$ symmetry in spin space, which means that the local spins may sweep the whole or half the unit sphere. It has been found that this topological excitation, called the Mermin-Ho vortex, can be stabilized in the rotating system [8]. In the case of $F=2$ spinor BEC's, the possibility of such the coreless vortex state has been predicted by Zhang *et al.* [26]. However, in the possible kinds of atoms, such as ^{87}Rb and ^{23}Na , the estimated spin interactions are situated in the close vicinity of the phase boundary between polar and cyclic phases [22]; the detailed study on the rotating ground state

with the cyclic spin interaction is an unexplored region.

The aim of the present work is to study vortex structure in rotating spinor $F=2$ condensate having finite magnetization. The condensate wave function has five components. We solved the extended Gross-Pitaevskii equations both numerically and variationally using trial functions for each component of the wave function. There is a good agreement between the results of both methods. We restricted our consideration only to the case of axially symmetric solutions. Energies of polar, ferromagnetic, and cyclic states with various sets of winding numbers for different components of the order parameter were evaluated. The equilibrium transitions between different phases with changing of the magnetization were studied.

II. THEORETICAL FORMALISM

Consider two-dimensional $F=2$ condensate with N particles confined by the harmonic trapping potential

$$U(r) = \frac{m\omega_{\perp}^2 r^2}{2}, \quad (1)$$

where ω_{\perp} is a trapping frequency, m is the mass of the atom, and r is the radial coordinate. The system is rotated with the angular velocity Ω . The energy of the system depends on three interaction parameters α , β , and γ , which can be defined as [22]

$$\alpha = \frac{1}{7}(4g_2 + 3g_4), \quad (2)$$

$$\beta = -\frac{1}{7}(g_2 - g_4), \quad (3)$$

$$\gamma = \frac{1}{5}(g_0 - g_4) - \frac{2}{7}(g_2 - g_4), \quad (4)$$

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

$$g_q = \frac{4\pi\hbar^2}{m} a_q \quad (5)$$

and a_q is the scattering lengths characterizing collisions between atoms with the total spin 0, 2, and 4.

The order parameter in $F=2$ case has five components Ψ_i ($i=-2, -1, 0, 1, 2$). The free energy of the system can be written as [6,7]

$$\begin{aligned} F = \int dS & \left(\Psi_j^* \hat{h} \Psi_j + \frac{\alpha}{2} \Psi_j^* \Psi_k^* \Psi_j \Psi_k \right. \\ & + \frac{\beta}{2} \Psi_j^* \Psi_l^* (F_a)_{jk} (F_a)_{lm} \Psi_k \Psi_m \\ & + \frac{\gamma}{2} \Psi_j^* \Psi_k^* \Psi_{-j} \Psi_{-k} (-1)^j (-1)^k \\ & \left. - B_z M - i\hbar \mathbf{\Omega} \cdot \Psi_j^* (\nabla \times \mathbf{r}) \Psi_j \right), \quad (6) \end{aligned}$$

where integration is performed over the system area, repeated indices are summed, B_z is the magnetic field, which is treated as a Lagrange multiplier, \hat{h} and M are the one-body Hamiltonian and magnetization, which are given by

$$\hat{h} = -\frac{\hbar^2 \nabla^2}{2m} + U(r), \quad (7)$$

$$M = \int dS |\Psi_i|^2 i. \quad (8)$$

Here F_a ($a=x, y, z$) is the angular momentum operator and it can be expressed in a matrix form as

$$F_x = \frac{1}{2} \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & \sqrt{6} & 0 & 0 \\ 0 & \sqrt{6} & 0 & \sqrt{6} & 0 \\ 0 & 0 & \sqrt{6} & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}, \quad (9)$$

$$F_y = \frac{i}{2} \begin{pmatrix} 0 & -2 & 0 & 0 & 0 \\ 2 & 0 & -\sqrt{6} & 0 & 0 \\ 0 & \sqrt{6} & 0 & -\sqrt{6} & 0 \\ 0 & 0 & \sqrt{6} & 0 & -2 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}, \quad (10)$$

$$F_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}. \quad (11)$$

It is convenient to introduce two additional order parameters $\langle \mathbf{f} \rangle = \Psi_j^* \mathbf{F}_{jk} \Psi_k / |\Psi|^2$ and $\Theta = (-1)^j \Psi_j^* \Psi_{-j} / |\Psi|^2$ characterizing ferromagnetic ordering and formation of singlet pairs, respectively [22]. In the absence of magnetic field and rota-

tion, BEC's can be in three different states [22] that is easily seen from Eq. (6). These states are called ferromagnetic, cyclic, and polar [22]. In ferromagnetic phase, only one component of the order parameter is nonzero: $\Psi_{-2}=1$. In cyclic phase, $\Psi_{-1}, \Psi_1=0$ and $\Psi_{-2}=\frac{1}{2}e^{i\theta}$, $\Psi_0=1/\sqrt{2}$, $\Psi_2=\frac{1}{2}e^{-i\theta}$, where θ is an arbitrary phase (energy of the system is degenerate with respect to θ). In the polar phase, there are three possibilities: in the first case $\Psi_{-2}=(1/\sqrt{2})e^{i\vartheta}$, $\Psi_{-1}, \Psi_0, \Psi_1=0$, $\Psi_2=(1/\sqrt{2})e^{i\nu}$, in the second case $\Psi_{-1}=(1/\sqrt{2})e^{i\vartheta}$, $\Psi_{-2}, \Psi_0, \Psi_2=0$, $\Psi_1=(1/\sqrt{2})e^{i\nu}$, and in the third case $\Psi_0=1$ and all other components are equal to zero. Here values of ϑ and ν are arbitrary and the energy is degenerate with respect to them. Depending on values of scattering lengths a_q ferromagnetic, cyclic, or polar phase has the lowest energy [22]. In the ferromagnetic phase, $\Theta=0$, $|\langle \mathbf{f} \rangle|=2$; in cyclic phase, $\Theta=0$, $\langle \mathbf{f} \rangle=0$; in polar phase, $|\Theta|=1$, $\langle \mathbf{f} \rangle=0$.

Extended Gross-Pitaevskii equations can be obtained in a standard way from the condition of minimum of free energy of the system Eq. (6):

$$\begin{aligned} \{ \hat{h} - \mu + \alpha \Psi_k^* \Psi_k \} \Psi_j + \beta \{ (F_a)_{lm} (F_a)_{jk} \} \Psi_l^* \Psi_m \Psi_k \\ + \gamma (-1)^j (-1)^k \Psi_k^* \Psi_k \Psi_j - i\hbar \mathbf{\Omega} \cdot \nabla \times \mathbf{r} \Psi_j - B_z j \Psi_j = 0, \quad (12) \end{aligned}$$

where a chemical potential μ is interpreted as the Lagrange multiplier. We use the total number of particles $N = \int dS \Psi_i^* \Psi_i$ and the magnetization M as independent variables.

III. VORTEX PHASES AND ENERGY

A. Classification of phases

Five nonlinear Gross-Pitaevskii equations, Eq. (12), are coupled and they can be solved numerically. However, some important consequences can be derived from the preliminary analysis of these equations. In this paper, we consider only axially symmetric solutions of the Gross-Pitaevskii equations. In this case, each component of the order parameter Ψ_j can be represented as

$$\Psi_j(r, \varphi) = f_j(r) \exp(-L_j \varphi), \quad (13)$$

where φ is a polar angle and L_j is a winding number. Axial symmetry of the solution implies that there are some constraints for the possible sets of L_j . It can be shown from Eq. (12) that L_j obeys the following equations:

$$L_2 + L_1 + L_{-1} + L_{-2} - 4L_0 = 0, \quad (14)$$

$$L_2 + L_{-2} - L_{-1} - L_1 = 0, \quad (15)$$

$$L_2 - 2L_{-2} - 2L_1 + 2L_{-1} = 0. \quad (16)$$

Equations (14)–(16) were obtained under the condition that all five components of the order parameter are nonzero. If some of these components are equal to zero identically then other possibilities appear for the L_j values. We list here all the possible phases different from ordinary vortex-free state: $(1, 1, 1, 1, 1)$, $(-1, \times, 0, \times, 1)$, $(1, \times, 0, \times, -1)$, $(\times, 0, \times, 1, \times)$,

$(\times, 1, \times, 0, \times)$, $(0, \times, 1, \times, 2)$, $(2, \times, 1, \times, 0)$, $(\times, 2, \times, 1, \times)$,
 $(\times, 1, \times, 2, \times)$, $(-2, -1, 0, 1, 2)$, $(2, 1, 0, -1, -2)$, $(-1, 0, 1, 2, 3)$,
 $(3, 2, 1, 0, -1)$, $(4, 3, 2, 1, 0)$, $(0, 1, 2, 3, 4)$. Here numbers denote
 values of L_j , “ \times ” denotes zero value of the corresponding
 component of the order parameter. We restricted ourselves
 only to the cases, when the largest winding number does not
 exceed 4, vortices with higher winding numbers are assumed
 to be nonstable.

B. Method

Now we can find the solutions of the Gross-Pitaevskii
 equations for each phase listed above. For the solution of Eq.
 (12), we apply a numerical method, which was used before
 in Ref. [27].

Besides the numerical solution, we also use a variational
 ansatz based on trial functions for each component of the
 order parameter. It follows from Eq. (12) that each compo-
 nent of the order parameter has an asymptotic $f_j(r) \sim r^{L_j}$
 at $r \rightarrow 0$ and that in the expansion of $f_j(r)$ in powers of r
 there are only terms proportional to r^{L_j+2n} , where $n \geq 0$ is an integer
 number. Superfluid density vanishes at infinite distances
 from the center of the potential well and $f_j(r) \rightarrow 0$ at $r \rightarrow \infty$.
 Therefore we have chosen the following trial function:

$$f_j(r) = C_j \left[\left(\frac{r}{R_j} \right)^{L_j} + a_j \left(\frac{r}{R_j} \right)^{L_j+2} \right] \exp\left(-\frac{r^2}{2R_j^2}\right), \quad (17)$$

where C_j , a_j , and R_j are variational parameters. Parameters
 C_j are not completely independent since they are related by
 one equation that is a condition of equality of number of
 atoms to the given number.

In the limit of noninteracting gas, Gross-Pitaevskii equa-
 tion becomes linear with respect to the order parameter. In
 this case, it is easy to see that $a_j=0$. In the Thomas-Fermi
 regime this is no longer valid and the system tries to mini-
 mize its energy by changing parameters a_j and R_j as com-
 pared to the limit of an ideal gas. According to our estimates,
 for the case of one-component order parameter, trial function
 (17) is able to give rather accurate results for the energy and
 for the rotation frequency of transition from the vortex-free
 to the vortex state even in the “moderate” Thomas-Fermi
 limit. Therefore in this paper we apply the method to the case
 of five-component order parameter. Note that variational ap-
 proaches were applied before for the analysis of vortex struc-
 tures in mesoscopic superconductors within the Ginzburg-
 Landau theory, see, e.g., Ref. [28], and for vortices in scalar
 and spinor BEC [29,30].

Using Eq. (6) and the normalization condition for the or-
 der parameter one can find the energy of the system analytically
 as a function of variational parameters for each set of
 L_j . However, final expression for the energy is rather cum-
 bersome and we do not present it here. Values of variational
 parameters can be calculated by a numerical minimization of
 the energy.

C. Results and discussion

We consider the situation, when the concentration of at-
 oms in the z direction is equal to $2000 \mu\text{m}^{-1}$, and the scat-

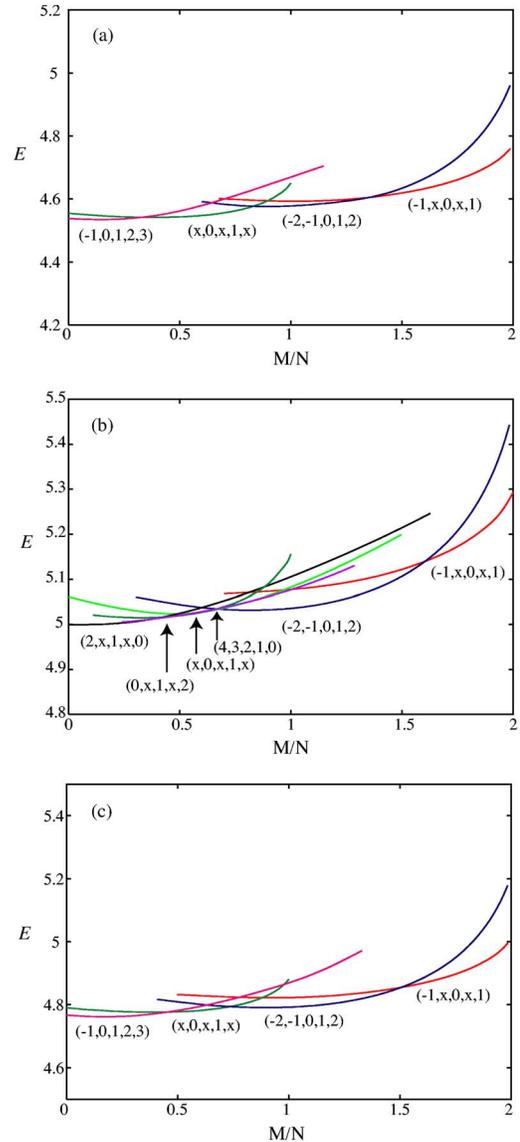


FIG. 1. (Color online) Dependences of energies of different vortex phases on the magnetization for cyclic (a), polar (b), and polar+cyclic (c) states. The energy is measured in units of $\hbar\omega_{\perp}$.

tering length a_0 equals 5.5 nm. According to the estimates
 made in Ref. [22], ^{23}Na , ^{83}Rb , ^{87}Rb , ^{85}Rb correspond to
 points on the phase diagram in the a_2 - a_4 vs the a_0 - a_4 plane
 (in absence of magnetic field and rotation), which are situ-
 ated in the close vicinity to the phase boundaries between
 ferromagnetic, polar, and cyclic states (see Fig. 1 in Ref.
 [22]). There are even some uncertainties in positions of these
 points on the phase diagram because of the error bars in a_q .
 It was assumed in Ref. [22] that ^{23}Na , ^{83}Rb , and ^{85}Rb BEC's
 are in polar, ferromagnetic, and cyclic states, respectively,
 and ^{87}Rb corresponds to the phase boundary between the
 polar and cyclic states. In this paper, we perform all the
 calculations for the polar state at $\beta=\alpha/50$, $\gamma=-\alpha/50$. For
 the cyclic state we put $\beta=\alpha/50$, $\gamma=\alpha/50$. And for the state
 situated on the phase boundary between cyclic and polar
 state, which we call cyclic+polar, we use $\beta=\alpha/50$, $\gamma=0$. We
 calculated the dependences of the energy of the system on

the magnetization for these three phases for different vortex states, when the system is rotated with the frequency $\Omega = 0.4\omega_{\perp}$. Our results obtained by the numerical solution to the Gross-Pitaevskii equations are presented in Fig. 1 for cyclic (a), polar (b), and cyclic+polar (c) states. In Table I we show numerically and variationally calculated values of the magnetization, at which the transitions occur between different phases for the case of cyclic state [Fig. 1(a)]. In this table, “a” denotes the transition between $(-1,0,1,2,3)$ and $(\times,0,\times,1,\times)$ states, “b” between $(\times,0,\times,1,\times)$ and $(-2,-1,0,1,2)$ states, and “c” between $(-2,-1,0,1,2)$ and $(-1,\times,0,\times,1)$ states. There is a good agreement between the numerical and variational results.

In general case, there can be phase differences between functions $f_j(r)$. Axial symmetry of the solution implies that there are some constraints on phases, which are similar for the constraints on winding numbers and can be also obtained from the GP equation (12). The energy of the system is then degenerate with respect to remaining phases, as in the non-rotating case, which was discussed above.

In all states under study, it also turns out that for the condensate it is energetically favorable to be distributed between one, two, or three hyperfine states and not between four or five.

It can be seen from Fig. 1 that, in all cases, at zero magnetization, states with nonzero winding numbers are energetically favorable due to the rotation of the system. By changing the magnetization it is possible to jump from one vortex phase to another one. The transitions between different phases are discontinuous. Note that in this paper we con-

TABLE I. Values of the magnetization corresponding to the transitions between different ground states for the case of cyclic phase [Fig. 1(a)], which were calculated numerically and variationally.

	<i>a</i>	<i>b</i>	<i>c</i>
Numerical	0.34	0.79	1.36
Variational	0.38	0.76	1.40

sider only the thermodynamical transitions between different states. Actual position of transition line between different vortex phases is controlled by local stability of states and therefore the prehistory of the system.

Which state has the lowest energy at given magnetization depends on many factors. For instance, at high magnetization, close to $M/N=2$, condensate has to be concentrated mostly in the state with $m_F=2$. Since our system is rotated with the frequency enough to create a vortex, for the condensate it is favorable energetically to have winding number 1 in this state. For other particles, which are not in $m_F=2$ state, it is energetically favorable to be in a superfluid phase with winding number 0 in order to occupy the inner part of the trap, where the trapping potential is small. That is why in all three phase diagrams presented in Fig. 1 vortex phase $(-1,\times,0,\times,1)$ has the lowest energy at high magnetization. The dependences of the density of particles in each hyperfine state on the distance from the potential well center is shown in Fig. 2(a) for the case of polar phase at $M/N=1.87$. Spatial

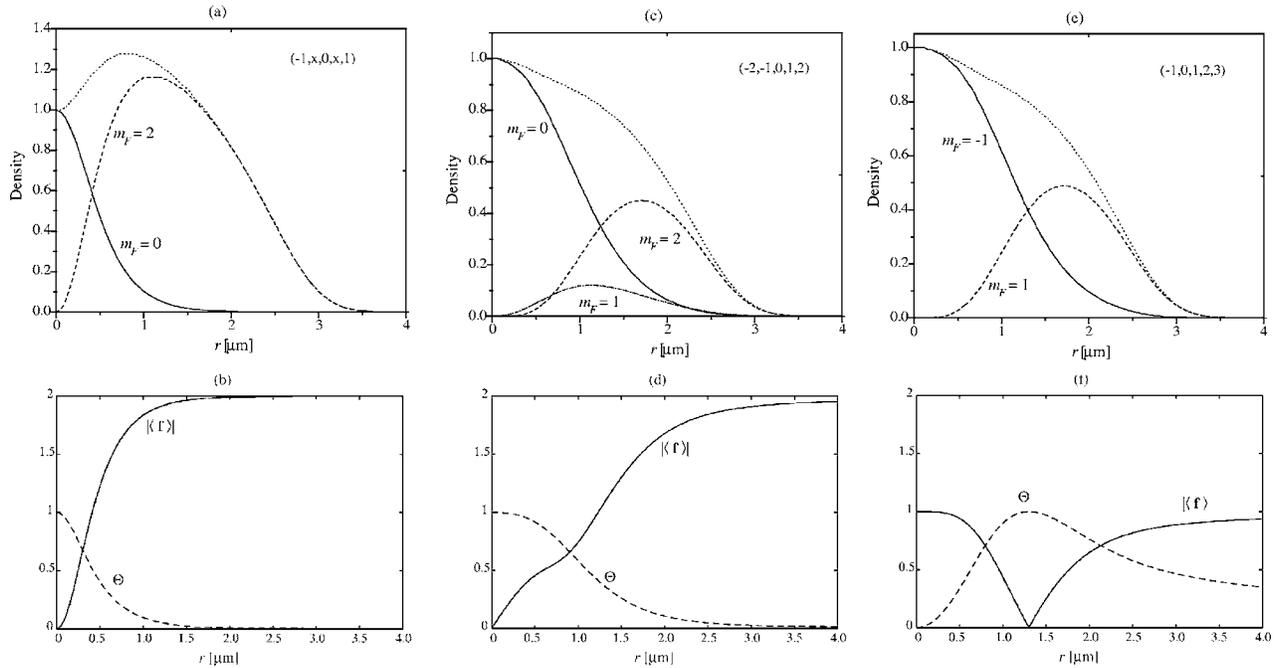


FIG. 2. The spatial variation of the density of particles in different hyperfine states normalized by the total density at the system axis and the order parameters Θ and $|\langle f \rangle|$ for different vortex phases. (a) and (b) correspond to the $(-1,\times,0,\times,1)$ polar phase at $M/N=1.87$; (c) and (d) to the $(-2,-1,0,1,2)$ phase at $M/N=1.21$; (e) and (f) to the cyclic+polar $(-1,0,1,2,3)$ state at $M/N=0.18$. Dotted lines show the total density of particles. The total number of particles is 10 000.

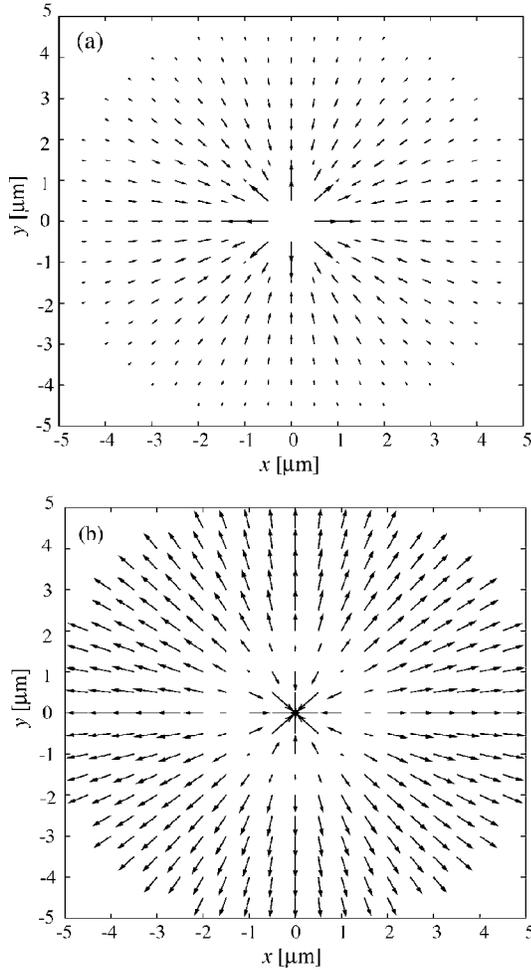


FIG. 3. Spin textures, $\langle f_x \rangle$ and $\langle f_y \rangle$, for the cyclic $(-1,0,1,2,3)$ phase at $M/N=0.16$ (a) and the cyclic $(-2,-1,0,1,2)$ phase at $M/N=1.21$ (b).

variations of the order parameters Θ and $|\langle \mathbf{f} \rangle|$ are presented in Fig. 2(b). It can be seen from Fig. 2(b) that Θ is maximum in the center of the potential well and vanishes at the infinity. At the same time, $|\langle \mathbf{f} \rangle|$ has a minimum at $r=0$ and tends to 2 at $r \rightarrow \infty$. This is because close to $r=0$ a component with $m_F=0$ has a maximum and all other components are small. Therefore Θ , which characterizes a formation of singlet pairs, has a maximum at $r=0$, and $|\langle \mathbf{f} \rangle|=0$. Far from the center of the cloud, the density of particles with $m_F=2$ is much larger than that for $m_F=0$ and the densities in all other hyperfine states are very small. For this reason, $\Theta=0$ and $|\langle \mathbf{f} \rangle|=2$ at $r \rightarrow \infty$.

For lower magnetization, condensate has to be distributed between the states with $m_F=0,1,2$. It turns out that again in all phase diagrams in Fig. 1 the ground state is represented by the phase $(-2,-1,0,1,2)$ in rather broad range of M . This is due to the fact that, in this case, it is favorable to put most of the particles in the state with winding number 0 in order to occupy the inner part of the trap. Most of remaining particles are condensed to the state with winding number 2 occupying the outer part of the trap and thus decreasing the energy of interaction (in “density” channel) of particles with $m_F=0$ and 2. Typical profiles of the particles densities in different hy-

perfine states for this vortex phase are shown in Fig. 2(c) for the cyclic state at $M/N=1.21$. Figure 2(d) indicates r dependences of the order parameters Θ and $|\langle \mathbf{f} \rangle|$, which physically are similar to that in the case of $(-1, \times, 0, \times, 1)$ state shown in Figs. 2(a) and 2(b).

At lower M particles have to be distributed between several states with different m_F . In this case, spin interactions become important and therefore the sequences of phase transitions for different phase diagrams in Fig. 1 are different. We can conclude that at high magnetizations $M \geq 1$ the state with lowest energy is mostly determined by interactions in the density channel, whereas at low magnetization $M \sim 0$, spin interactions play an important role. In Figs. 2(e) and 2(f) we present the r dependences of the superfluid density in different hyperfine states and order parameters Θ and $|\langle \mathbf{f} \rangle|$ for the cyclic+polar $(-1,0,1,2,3)$ state at $M/N=0.18$, where this phase has the lowest energy. In this case, particles are distributed between states $m_F=-1$ and $m_F=1$. The state with $m_F=-1$ has a winding number 0, and these particles occupy a space with minimal trapping potential. All other particles are condensed in the state with winding number 2 thus decreasing the interaction energy in the density channel. As a result, the order parameter Θ is nonzero everywhere except of the point $r=0$, since at any $r>0$ there are particles in the states with $m_F=\pm 1$, and the formation of singlet pairs is possible. The order parameter $|\langle \mathbf{f} \rangle|$ is nonzero at $r=0$ and $r \rightarrow \infty$, since in both cases there are particles condensed in the states with nonzero m_F . At the same time, at small values of r most of particles are condensed in the state with $m_F=-1$ and at larger r in the state with $m_F=1$. Therefore there is an abrupt change in the spin direction at intermediate values of r . This results in the vanishing of $|\langle \mathbf{f} \rangle|$ near the vortex core.

In Fig. 3 we show the spin texture, $\langle f_x \rangle$ and $\langle f_y \rangle$, for the phases $(-1,0,1,2,3)$ and $(-2,-1,0,1,2)$ in the cyclic state. In the first case, in the vortex-core region, the spins are polarized along the z direction. In the outer region the spin vanishes and Θ grows, where the spin amplitude has a node and the pure polar state forms. In the second case, in the outer region, the spins are polarized along the z direction. In the core region, the spins lean toward the origin. At the origin, the spin vanishes and the pure polar state forms ($\Theta=1$), because the spin texture exhibits the two-dimensional radial disgyration in the core region. Note that $(-2,-1,0,1,2)$ and $(-1,0,1,2,3)$ vortices were not described before in the literature.

IV. CONCLUSIONS

In summary, we analyzed the vortex structure in spinor $F=2$ condensate using extended Gross-Pitaevskii equations. We considered only axially symmetric vortices. Based on symmetric configurations, all possible vortex states were classified. The Gross-Pitaevskii equations were solved both numerically and by the variational method using trial functions for the order parameter. Spatial distribution of the particles density and the order parameters Θ and $|\langle \mathbf{f} \rangle|$ were obtained. Energies of different vortex phases were found as a function of magnetization, when the system is rotated with

the frequency $\Omega=0.4\omega_{\perp}$. We found that at high magnetization the energy of the system is mostly determined by the interaction in the density channel, whereas at low magnetization spin interaction plays an important role. Also, two different types of vortices were described.

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