Vortex Phase Diagram of $F = 1$ Spinor Bose-Einstein Condensates

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We have calculated the $F = 1$ ground state of a spinor Bose-Einstein condensate trapped harmonic potential with an applied Ioffe-Pitchard magnetic field. The vortex phase diagram is found in the plane spanned by perpendicular and longitudinal magnetic fields. The ferromagnetic condensate has two vortex phases which differ by winding number in the spinor components. The two vortices for the $F_z = -1$ antiferromagnetic condensate are separated in space. Moreover, we considered an average local spin $|\langle\vec{S}\rangle|$ to testify to what extent it is parallel to magnetic field (the nonadiabatic effects). We have shown that the effects are important at vortex cores.

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Introduction.—One of the recent developments in Bose-Einstein condensates (BEC) in atomic gases is the study of dilute Bose gases with spin degrees of freedom. The first realization of such a system is found in optically trapped ^{23}Na, which is a spin-1 Bose gas [1]. The nature of the spinor condensate depends on the magnetic interaction. In zero magnetic field the spinor condensate can be either ferromagnetic or antiferromagnetic ("polar"). Both have very different properties [2,3].

In this Letter we study the ground state structure of BEC described by a constituent atom with the hyperfine state $|F| = 1$ ($F_z = \pm 1, 0$) where the order parameter of the Bose condensate is characterized by three components: Ψ_α, $\alpha = \pm 1, 0$ similar to the spin part of superfluid ^{3}He. However, these degrees of freedom bring about a remarkable difference between the BEC of alkali atoms and that of ^{4}He. The hyperfine spin aligns along the direction of the local magnetic field when a BEC is magnetically trapped. Then, even though the alkali atoms carry spins, they behave like scalar particles. In contrast, the spin of the alkali atoms is an important degree of freedom in an optical trap formed by the optical dipole force which confines atoms in all hyperfine states $F_z = \pm 1, 0$ [4]. In order to manipulate by spin states we assume at the same time that the BEC is created in a magnetic Ioffe-Pitchard trap [5].

Following [6,7] we introduce the basis set $|x\rangle$, $|y\rangle$, $|z\rangle$ defined by $F_i|i\rangle = 0$, $i = x, y, z$. The order parameter is then expressed via a three-dimensional vector Ψ_i where

$$|\Psi\rangle = \Psi_x|x\rangle + \Psi_y|y\rangle + \Psi_z|z\rangle. \tag{1}$$

$\vec{\Psi}$ behaves as a vector under spin space rotation. In what follows, the Latin indexes define the XYZ basis (1) while the Greek indexes denote the z-quantized basis with $F_z = \pm 1, 0$.

In particular, a mean value of spin is equal to

$$\langle\vec{F}(\mathbf{r})\rangle = \Psi^*(\mathbf{r})_\alpha \vec{F}_{\alpha\beta}\Psi(\mathbf{r})_\beta, \tag{2}$$

where $\vec{F}_{\alpha\beta}$ are the matrix elements of the spin operators F_i in the basis (1). We write the order parameter via the Bose condensate density n

$$\Psi_i(\mathbf{r}) = \xi_i^*(\mathbf{r})\sqrt{n(\mathbf{r})}, \tag{3}$$

and the average local spin via normalized spinor ξ_α

$$\langle\vec{S}(\mathbf{r})\rangle = \xi_\alpha \vec{F}_{\alpha\beta}\xi_\beta. \tag{4}$$

In terms of the order parameter (1) the BEC free energy density has the form [6,8]

$$H = \Psi_i^*\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) - \mu\right)\Psi_i + \frac{1}{2}g_1(\Psi_i^*\Psi_i)^2 + \frac{1}{2}g_2(\Psi_i^*\Psi_i^*)(\Psi_j\Psi_j) + i\gamma_\mu\epsilon_{ijk}B_k\Psi_i^*\Psi_j, \tag{5}$$

where

$$U(\mathbf{r}) = m(\omega_z^2 z^2 + \omega r^2)/2 \tag{6}$$

is the potential of the optical trap, γ_μ is the gyromagnetic ratio, and $\mathbf{B(r)}$ is magnetic field of the Ioffe-Pitchard trap. The two interaction constants g_1 and g_2 are characteristics of the three-component order parameter which represent the spin degrees of freedom of the condensate. The two nonlinear terms in (5) originate from the interactions [6]

$$\tfrac{1}{2}g_n n^2 + \tfrac{1}{2}g_s\langle\mathbf{F}\rangle^2, \tag{7}$$

where $g_1 = g_s + g_n$, $g_2 = -g_s$. As shown by Klausen *et al.* [9], the spin interaction of ^{87}Rb is ferromagnetic ($g_s < 0$), while for ^{23}Na this interaction is antiferromagnetic ($g_s > 0$) [10].

When the system is uniform and infinitely large, the ground state is either ferromagnetic or antiferromagnetic [6,8]. However, a rich variety of topological defects have been predicted [6,8,11–14]. Ho and Shenoy [12] have shown that the spatial variations of the magnetic field $\mathbf{B}$ give rise to vortical ground state. In particular, these variations are necessary to produce the magnetic trapping. The basic assumption of Ho and Shenoy is that the spin state $\Psi_i(\mathbf{r}) = \xi_i(\mathbf{r})\Phi(\mathbf{r})$, defined by the normalized spinor ξ_i is aligned with the magnetic field. This approach has established locally a spin-gauge symmetry of the condensate. It means that a local gauge U(1) transformation is undone by a local spin rotation. Nodal points of the scalar field Φ define vortices. Yip [13] has considered composite vortices in the spin-1 BEC in a rotating trap. These vortices display interesting internal structure. They may have broken cylindrical symmetry with nodes of the order parameter of individual components appearing at positions other than the trap center.

Topological defects similar to composite vortices, called Skyrmions in general, have been proposed in the spinor BEC [11,14,15]. However, it was shown that in the ferromagnetic spin-1 BEC trapped in a harmonic potential, the Skyrmions or composite vortices are not thermodynamically stable without rotation [11,14]. The Skyrmions were shown to be favored over the singular vortices and other non-axis-symmetric vortices. Following [14] we introduce a specification of different vortex phase winding numbers as (m_1, m_0, m_{-1}) for the condensate wave function $(\Psi_1, \Psi_0, \Psi_{-1})$ with $m_\alpha = 0, \pm 1, \pm 2, \ldots$. We show that the vortices with different winding numbers are stable even without rotation in the Ioffe-Pitchard trap for the ground state.

Gross-Pitaevskii equations.—We consider the ground state of the spin-1 BEC which is uniform along the z axis. We introduce cylindrical coordinates $\mathbf{r} = (r, \varphi, z)$. Suppose that a Ioffe-Pitchard magnetic field

$$\mathbf{B} = [B_\perp(r)\cos\varphi, -B_\perp(r)\sin\varphi, B_z] \tag{8}$$

is applied to the system. The trapping potential (6) gives rise to a characteristic length $d = \sqrt{\hbar/2m\omega}$ and a characteristic energy $E_0 = \hbar\omega$ which allow one to write the dimensionless form of the free energy density (5),

$$\begin{aligned}\tilde{H} &= \frac{g_1}{E_0^2 d^3} H \\ &= \psi_i^*[-\nabla^2 + v(\rho) - \tilde{\mu}]\psi_i + \frac{1}{2}(\psi_i^*\psi_i)^2 \\ &\quad + \frac{\tilde{g}}{2}(\psi_i^*\psi_i^*)(\psi_j\psi_j) + i\epsilon_{ijk} b_k \psi_i^* \psi_j,\end{aligned} \tag{9}$$

where

$$\tilde{\mu} = \frac{\mu}{\hbar\omega}, \qquad \mathbf{b} = \frac{\gamma_\mu \mathbf{B}}{\hbar\omega}, \qquad \vec{\psi} = \sqrt{\frac{g_1}{\hbar\omega}}\vec{\Psi}, \qquad \tilde{g} = \frac{g_2}{g_1}. \tag{10}$$

Since the spin-1 BEC is uniform along the z axis, we fix the linear density of the Bose gas by condition

$$\int d^2\mathbf{r}|\Psi_j|^2 = \frac{N}{L}.$$

Substituting notations (10) and the coupling constants [8]

$$g_1 = \frac{4\pi\hbar^2}{m} a_2, \qquad g_2 = \frac{4\pi\hbar^2}{3m}(a_0 - a_2), \tag{11}$$

we obtain

$$\int d^2\vec{\rho}|\psi_i|^2 = 8\pi a_2 \frac{N}{L}, \tag{12}$$

where $\vec{\rho}$ is a dimensionless two-dimensional radius vector. For the case of ^{23}Na, $\tilde{g}$ is negative (≈ -0.1), and an external magnetic field is uniform, then the ground state is antiferromagnetic. For the case of ^{87}Rb $\tilde{g}$ is positive (≈ 0.03), and the ground state is ferromagnetic. For a strong magnetic field or small BEC density, it is reasonable to consider $\tilde{g} = 0$ as the first step. Then the Gross-Pitaevskii equation in the z-quantized basis ψ_α takes the following form:

$$[-\nabla^2 + v(\rho) - \tilde{\mu}]\psi_\alpha + n(\rho)\psi_\alpha - E_{\alpha\beta}\psi_\beta = 0, \tag{13}$$

where

$$E = \begin{pmatrix} b_z & \frac{b_\perp(\rho)}{\sqrt{2}} e^{i\varphi} & 0 \\ \frac{b_\perp(\rho)}{\sqrt{2}} e^{-i\varphi} & 0 & \frac{b_\perp(\rho)}{\sqrt{2}} e^{i\varphi} \\ 0 & \frac{b_\perp(\rho)}{\sqrt{2}} e^{-i\varphi} & -b_z \end{pmatrix}. \tag{14}$$

One can see that Eq. (13) gives rise to a separation of variables ρ and φ. Equations (13) and (14) imply that $\psi_\alpha = \psi_{\alpha-1} e^{i\varphi}$. This equality gives us the simple relation

$$m_\alpha = m_{\alpha-1} + 1 \tag{15}$$

between vortical winding numbers m_α of the spinor component ψ_α.

On the one hand, for the strong magnetic field b_z the spinor component ψ_1 is prevailing. On the other hand, the kinetic energy prevents this component from having nodes. Therefore, the solution for the ground state has the form

$$\begin{pmatrix} h_1(\rho) \\ h_0(\rho)e^{-i\varphi} \\ h_{-1}(\rho)e^{-2i\varphi} \end{pmatrix} \tag{16}$$

for which the Gross-Pitaevskii equation is

$$\begin{aligned}&\frac{d^2h_1}{d\rho^2} + \frac{1}{\rho}\frac{dh_1}{d\rho} - (v + n - \tilde{\mu})h_1 + b_z h_1 + \frac{b_\perp}{\sqrt{2}} h_0 = 0, \\ &\frac{d^2h_{-1}}{d\rho^2} + \frac{1}{\rho}\frac{dh_{-1}}{d\rho} - \left(v + n + \frac{4}{\rho^2} - \tilde{\mu}\right)h_{-1} - b_z h_{-1} + \frac{b_\perp}{\sqrt{2}} h_0 = 0, \\ &\frac{d^2h_0}{d\rho^2} + \frac{1}{\rho}\frac{dh_0}{d\rho} - \left(v + n + \frac{1}{\rho^2} - \tilde{\mu}\right)h_0 + \frac{b_\perp}{\sqrt{2}}(h_1 + h_{-1}) = 0.\end{aligned} \tag{17}$$

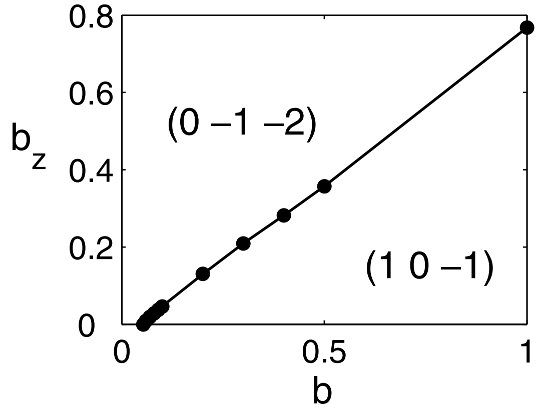

FIG. 1. Vortex phase diagram of the spin-1 BEC in the Ioffe-Pitchard trap for $\tilde{g} = 0$.

Here

$$v(\rho) = \frac{1}{4}\rho^2, \qquad b_\perp = b\rho, \tag{18}$$

with obvious normalization condition $n(\rho) = h_\alpha(\rho)^2$.

For small longitudinal magnetic field b_z a different solution of the Gross-Pitaevskii equation

$$\begin{pmatrix} f_1(\rho)e^{i\varphi} \\ f_0(\rho) \\ f_{-1}(\rho)e^{-i\varphi} \end{pmatrix} \tag{19}$$

could be favorable for the ground state. Substituting (19) into the Gross-Pitaevskii Eq. (13) we obtain

$$\begin{aligned} &\frac{d^2 f_1}{d\rho^2} + \frac{1}{\rho}\frac{df_1}{d\rho} - \left(v + n + \frac{1}{\rho^2} - \tilde{\mu}\right) f_1 + \\ &\qquad b_z f_1 + \frac{b_\perp}{\sqrt{2}} f_0 = 0, \\ &\frac{d^2 f_{-1}}{d\rho^2} + \frac{1}{\rho}\frac{df_{-1}}{d\rho} - \left(v + n + \frac{1}{\rho^2} - \tilde{\mu}\right) f_{-1} - \\ &\qquad b_z f_{-1} + \frac{b_\perp}{\sqrt{2}} f_0 = 0, \\ &\frac{d^2 f_0}{d\rho^2} + \frac{1}{\rho}\frac{df_0}{d\rho} - (v + n - \tilde{\mu}) f_0 + \frac{b_\perp}{\sqrt{2}}(f_1 + f_{-1}) = 0. \end{aligned} \tag{20}$$

Numerical results.—In order to find the ground state of the spin-1 BEC for $\tilde{g} = 0$ we numerically solved Eqs. (17) and (20). The ground states that correspond to solutions (16) and (19) were chosen by the minimum energy of the BEC. For computations, since in the magnetic field of the Ioffe-Pitchard trap magnetization is not conserved, we fixed the dimensionless linear density (12) but not magnetization similar to [7,8,12]. We took $N/L = 1000$ fitting the chemical potential $\tilde{\mu}$ in the Gross-Pitaevskii equations. The vortex phase diagram in the plane spanned by the perpendicular magnetic field b and longitudinal one b_z is shown in Fig. 1 for $\tilde{g} = 0$. As expected, the vortex phase $(0\ -1\ -2)$ is substituted by the vortex phase $(1\ 0\ -1)$ when the magnetic field b_z is decreased as shown in Fig. 1. One can see that the winding number rule (15) holds for each vortex phase. Figure 2 shows the radial behavior of the spinor components in the vortex phases presented in Fig. 1. We also performed a computation for the ground state of the ferromagnetic case $\tilde{g} = 0.03$ (^{87}Rb) using the Metropolis procedure with a total number of sites of the order 50 000. For this case the vortex phase diagram shown in Fig. 1 is slightly deformed. However, deviation of the effective constant $\tilde{g}$ from zero gives rise to a solution which violates rotational symmetry of the Bose condensate around the z axis.

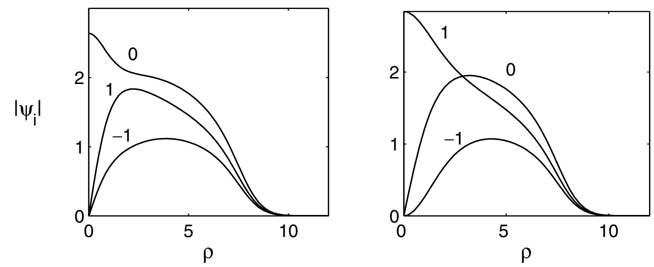

FIG. 2. The radial behavior of the $(1\ 0\ -1)$ vortex at $b_z = 0.7$, $b = 1$ and of the $(0\ -1\ -2)$ vortex at $b_z = 0.8$, $b = 1$.

For the antiferromagnetic case $\tilde{g} = -0.1$ (^{23}Na) the vortex phase diagram changes. The rule (15) still holds. However, a new vortex phase appears in which two modal points of the component ψ_{-1} are spacely separated as shown in Fig. 3. We denote this kind of vortices as two prime. At the solid line between vortex phases $(0\ -1\ -2')$ and $(0\ -1\ -2)$ shown in Fig. 4 the vortices of the component ψ_{-1} are joining together at $\rho = 0$. As the magnetic field b decreases, the distance between the vortices increases. For small b these vortices go to the region $\rho \gg 1$ where the wave function is exponentially small because of optical trapping. As a result the vortices become practically invisible. The dashed line in Fig. 4 shows where this happens.

The ground vortex phase $(1\ 0\ -1)$ is interesting because by that it has non-axis-symmetric vortices for the spinor components ψ_1 and ψ_{-1} as it was found by Mizushima *et al.* for rotating BEC [14].

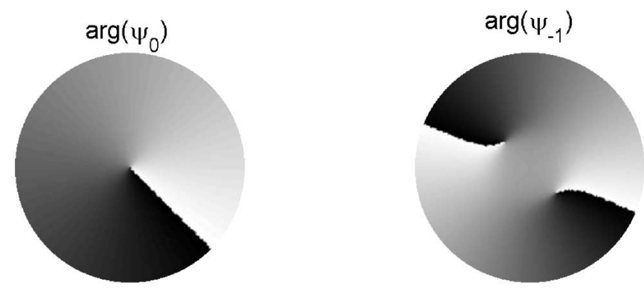

FIG. 3. Phase images $\arg(\psi_i)$ in the vortex phase $(0\ -1\ -2')$ for $\tilde{g} = -0.1$, $b_z = 0.9$, $b = 0.2$, $\tilde{\mu} = 11.44$.

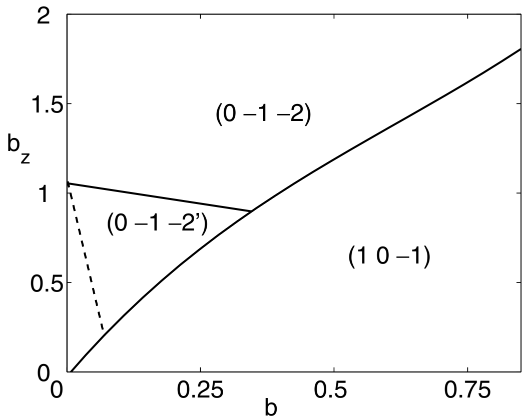

FIG. 4. Vortex phase diagram of the spin-1 BEC in the Ioffe-Pitchard trap for $\tilde{g} = -0.1$.

Next, we evaluated $|\langle \vec{S}(\rho)\rangle|$ in order to find out to what extent nonadiabatic effects are important [12]. It is well known that in quantum magnets with anisotropy these effects are important for the ground state. Quantitatively the nonadiabatic effects can be described by a quantum reduction of the spin $|\langle \vec{S}(\rho)\rangle| < 1$ and deviation of the direction of average local spin with respect to the magnetic field. In Fig. 5(a) we show the radial dependence of $|\langle \vec{S}(\rho)\rangle|$ in the vortex phases $(0\ -1\ -2)$ and $(1\ 0\ -1)$. As seen from Fig. 5(a) the quantum spin reduction is maximal for the vortex phase $(1\ 0\ -1)$. The value of the average local spin $|\langle \vec{S}(\rho)\rangle|$ substantially reduces at the vortex core. For the vortex phase $(0\ -1\ -2)$ the quantum spin reduction is almost absent [shown in Fig. 5(a) by the dashed line].

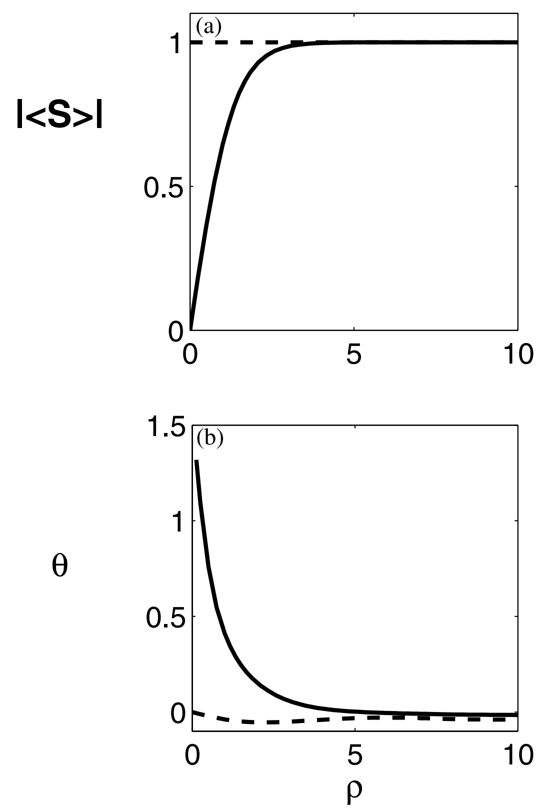

FIG. 5. The radial dependence of the average local spin $\langle \mathbf{S}(\rho)\rangle$ (a) and its projection onto the direction of local magnetic field $\mathbf{b}$ specified by the angle θ (b) for different vortex phases shown in Fig. 1. Solid line refers to the vortex phase $(1\ 0\ -1)$, $\tilde{g} = 0$, $b_z = 0.1$, $b = 0.2$, $\tilde{\mu} = 11.5$, and dashed line refers to the vortex phase $(0\ -1\ -2)$, $\tilde{g} = 0$, $b_z = 1.5$, $b = 0.5$, $\tilde{\mu} = 12$.

Moreover, we calculated the radial behavior of the deviation of the direction $\langle \vec{S}(\rho)\rangle$ relative to the direction of the local magnetic field $\vec{b}$. We found that in the plane perpendicular to the z axis the local spin completely follows the direction of the magnetic field. In the plane parallel to the z axis the situation is different. For the vortex phase $(1\ 0\ -1)$ shown in Fig. 5(b) the direction of the local spin (4) substantially differs from the direction of the magnetic field, while for the phase $(0\ -1\ -2)$ this is not so. Therefore, the adiabatic approximation is applicable only for the phase $(0\ -1\ -2)$.

Thus we conclude that the ground state of the spin-1 Bose-Einstein condensate trapped in the harmonic potential and subjected by the Ioffe-Pitchard magnetic field is given by a rich variety of winding numbers in different spinor components. At the vortex cores of the ground state the quantum spin reduction is substantially large and the direction of the average local spin can deviate from the magnetic field.

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