Uniaxial and Biaxial Spin Nematic Phases Induced by Quantum Fluctuations

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It is shown that zero point quantum fluctuations completely lift the accidental continuous degeneracy that is found in mean field analysis of quantum spin nematic phases of hyperfine spin-2 cold atoms. The result is two distinct ground states which have higher symmetries: a uniaxial spin nematic and a biaxial spin nematic with dihedral symmetry Dih_4. There is a novel first-order quantum phase transition between the two phases as atomic scattering lengths are varied. We find that the ground state of ^{87}Rb atoms should be a uniaxial spin nematic. We note that the energy barrier between the phases could be observable in dynamical experiments.

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Since the successful observation of magnetic ordering in condensates of sodium atoms in optical traps [1], the subject of spinor gases has attracted much attention [2–7]. The impressive efforts to measure spin-dependent interaction energies or two-body scattering lengths of cold atoms [8–12] and recent progress in cooling hyperfine spin $F = 3$ chromium atoms [13] have further stimulated extensive interest in spin-correlated many-body states of cold atoms.

In addition, in recent work, a much better understanding of spin collective phenomena of cold atoms in optical lattices has been achieved. Particularly among many other states in optical lattices [14], various quantum spin nematics have received much attention. Spin nematics have been suggested as ground states of $F = 1$ sodium atoms (^{23}Na), $F = 2$ rubidium atoms (^{87}Rb), and $F = 3$ chromium atoms (^{52}Cr) in optical lattices [15–19]; they are also proposed to be relevant to $F = 3/2$ cold atoms [20,21]. Quantum spin nematics are fascinating because of the rich topology of their ground state manifolds, which gives rise to exotic spin defects and unconventional vortices with noninteger circulation integrals. Spin nematics have not been successfully realized in conventional solid state systems, but it is widely believed that at least some of them are likely to be created and observed in cold atomic vapors. The spin nematics of bosonic cold atoms that have been discussed so far do not break the (lattice) translational symmetry but do break rotational symmetry. The absence of lattice translational symmetry breaking can be attributed to the relatively weak super exchange interaction between two bosons if they are spatially antisymmetric.

In fact, our mean field calculations show that, for cold atoms such as rubidium (^{87}Rb) in the $F = 2$ manifold, a one-parameter family of spin nematic ground states, including ones which are characterized by completely different symmetries, are degenerate in energy [see discussions after Eq. (3)]. In particular, uniaxial nematics that are invariant under any rotation around an easy axis are degenerate with biaxial nematics which are invariant only under a dihedral group (either Dih_2 or Dih_4 depending on eigenvalues of the nematic matrix; see below). The origin of this degeneracy is accidental due to the special form of energy in the dilute limit, very analogous to the highly degenerate family of solutions for d-wave pairing obtained by Mermin in the 1970s [22]. In this Letter, we shall study the effect of zero point quantum fluctuations (ZPQFs) on nematic order in cold atoms. ZPQFs are known to lead to a wide range of physical phenomena, including the Lamb shift in atomic physics [23], the Coleman-Weinberg mechanism of spontaneous symmetry breaking [24], fluctuation-induced first-order transitions in liquid crystals and superconductors [25], and *order from disorder* in magnetic systems [26,27]. For $F = 2$ cold atoms, we show that ZPQFs completely lift the accidental continuous degeneracy appearing in previous mean field calculations and result in two distinct states with higher symmetries: (a) the uniaxial spin nematic with Z_2 symmetry and (b) the biaxial spin nematic with Dih_4 symmetry.

We consider $F = 2$ atoms in optical lattices using the following Hamiltonian:

$$\mathcal{H} = \sum_k \frac{a_L}{2}(\hat{\rho}_k^2 - \hat{\rho}_k) + \frac{b_L}{2}(\hat{\mathcal{F}}_k^2 - 6\hat{\rho}_k) + 5c_L \mathcal{D}_k^\dagger \mathcal{D}_k - t_L \sum_{\langle kl\rangle} (\psi_{k,\alpha\beta}^\dagger \psi_{l,\beta\alpha} + \mathrm{H.c.}) - \sum_k \mu \hat{\rho}_k. \quad (1)$$

Here k is the lattice site index, $\langle kl\rangle$ are the nearest neighbor sites, μ is the chemical potential, and t_L is the one-particle hopping amplitude. $\psi^\dagger$ is a traceless symmetric tensor operator that has been introduced in a previous work [16]; a_L, b_L, c_L are three on-site coupling constants which are determined from three two-body scattering lengths a_F, $F = 0, 2, 4$, and on-site orbitals. Components $\psi_{\alpha\beta}^\dagger$, $\alpha, \beta = x, y, z$, are linear superpositions of five spin-2 creation operators $\psi_{m_F}^\dagger$, $m_F = 0, \pm 1, \pm 2$. The number operator $\hat{\rho}$, the dimer or singlet pair creation operator $\mathcal{D}^\dagger$, and the total spin operator $\hat{F}_\alpha$ are defined as $\hat{\rho} = \frac{1}{2}\,\mathrm{Tr}\psi^\dagger\psi$, $\mathcal{D}^\dagger = (1/\sqrt{40})\mathrm{Tr}\psi^\dagger\psi^\dagger$, and $\hat{F}_\alpha = -i\epsilon_{\alpha\beta\gamma}\psi_{\beta\eta}^\dagger\psi_{\eta\gamma}$, respectively.

The amplitude of a condensate is a traceless symmetric tensor $\tilde{\chi}_{\alpha\beta} = \langle \hat{\psi}_{k,\alpha\beta} \rangle$. In this condensate, atoms occupy a one-particle spin state $|\tilde{\chi}\rangle$ that is defined as a linear superposition of five $F = 2$ hyperfine states $|2, m_F\rangle$

$$|\tilde{\chi}\rangle = \sum_{\alpha\beta, m_F} \tilde{\chi}_{\alpha\beta} \mathcal{C}_{\alpha\beta, m_F} |2, m_F\rangle,$$
$$\mathcal{C}_{\alpha\beta, m_F} = \sqrt{\frac{15}{4\pi}} \int d\Omega \left(n_\alpha n_\beta - \frac{1}{3} \delta_{\alpha\beta} \right) Y^*_{2, m_F}(\theta, \phi). \tag{2}$$

Here n_α, $\alpha = x, y, z$, are components of a unit vector $\mathbf{n}(\theta, \phi)$; $n_x = \sin\theta\cos\phi$, $n_y = \sin\theta\sin\phi$, and $n_z = \cos\theta$. Y_{2, m_F}, $m_F = 0, \pm 1, \pm 2$, are five spherical harmonics with $l = 2$. The mean field energy per site as a function of $\tilde{\chi}$ can be obtained as

$$E_{\mathrm{MF}} = \frac{a_L}{8} \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}) \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}) + \frac{c_L}{8} \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}^*) \mathrm{Tr}(\tilde{\chi} \tilde{\chi}) + \frac{b_L}{4} \mathrm{Tr}[\tilde{\chi}^*, \tilde{\chi}]^2 - z t_L \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}) - \frac{\mu}{2} \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}), \tag{3}$$

where z ($= 6$) is the coordination number. Minimization of E with respect to the tensor $\tilde{\chi}$ yields nematic, cyclic, and ferromagnetic phases studied previously. Particularly when $c_L < 0$, $c_L < 4b_L$ [as for rubidium atoms (^{87}Rb)], minimization of energy in Eq. (3) requires that $\tilde{\chi}$ be a real symmetric tensor (up to a phase). An arbitrary solution $\tilde{\chi}$ can be obtained by applying an SO(3) rotation and a U(1) gauge transformation to a real diagonal matrix χ:

$$\tilde{\chi} = \sqrt{4M} e^{i\phi} \mathcal{R} \chi \mathcal{R}^{-1}; \tag{4}$$

$\mathcal{R}$ is an SO(3) rotation matrix, and χ is a normalized real diagonal traceless matrix [16]

$$\chi = \begin{pmatrix} \chi_{xx} & 0 & 0 \\ 0 & \chi_{yy} & 0 \\ 0 & 0 & \chi_{zz} \end{pmatrix}, \qquad \mathrm{Tr}(\chi\chi) = \frac{1}{2}. \tag{5}$$

Finally, the value of chemical potential μ is

$$\mu_L = \mu + 2 z t_L = (a_L + c_L) M, \qquad M = \tfrac{1}{2} \mathrm{Tr}(\tilde{\chi}^* \tilde{\chi}).$$

$M = \langle \hat{\rho}_k \rangle$ is the average number of atoms per lattice site. The shifted chemical potential $\mu_L = \mu + 2 z t_L$ measured from the bottom of the band depends on scattering lengths through its dependence on a_L, c_L.

In the mean field approximation, all of the quantum spin nematics specified by the different diagonal matrices equation (5) have the same energy, i.e., are exactly degenerate. For instance, when $2\chi_{xx} = 2\chi_{yy} = -\chi_{zz} = 1/\sqrt{3}$, up to an overall SO(3) rotation, all atoms are condensed in the hyperfine state $|2, 0\rangle$. This choice of χ represents a uniaxial spin nematic. When $\chi_{xx} = -\chi_{yy} = 1/2$ and $\chi_{zz} = 0$, the atoms are condensed in the state $(1/\sqrt{2})(|2, 2\rangle + |2, -2\rangle)$. In general, consider the parametrization of the matrix elements ($\xi \in [0, 2\pi]$):

$$\chi_{xx} = \frac{\sin(\xi - \frac{\pi}{6})}{\sqrt{3}}, \quad \chi_{yy} = \frac{\sin(\xi - \frac{5\pi}{6})}{\sqrt{3}}, \quad \chi_{zz} = \frac{\sin(\xi - \frac{9\pi}{6})}{\sqrt{3}}. \tag{6}$$

To study ZPQFs, we first examine the energy spectra of collective modes. For this, we expand $\psi^\dagger$ about the mean field $\tilde{\chi}$:

$$\hat{\psi}^\dagger_{k,\alpha\beta} = \sqrt{4M} \chi_{\alpha\beta}(\xi) + \sum_\nu L^\nu_{\alpha\beta}(\xi) \hat{\theta}^\dagger_{k,\nu}, \tag{7}$$

where the superscript $\nu = x, y, z, t, p$ labels zero point motions of χ along five orthogonal directions: three SO(3) spin modes (x, y, and z mode) for rotations about the x, y, and z axes, respectively, a spin mode (t mode) for the motion along the unit circle of ξ, and a phase mode (p mode) describing fluctuations of the condensate's overall phase. The corresponding matrices are

$$L^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L^y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad L^z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{8}$$

and $L^t = 2\chi(\xi + \frac{\pi}{2})$, $L^p = 2\chi(\xi)$. These matrices are mutually orthogonal, $\mathrm{Tr}(L^\mu L^\nu) = 2\delta_{\mu\nu}$. The five modes are decoupled, and the corresponding operators obey the bosonic commutation relations $[\theta_{k,\mu}, \theta^\dagger_{l,\nu}] = \delta_{kl}\delta_{\mu\nu}$.

We expand the Hamiltonian in Eq. (1) using Eq. (7) and keep the lowest-order nonvanishing terms. The result is a Hamiltonian for the fluctuations which is bilinear in $\theta^\dagger_{k,\nu}$, $\theta_{k,\nu}$. It can be diagonalized by a Bogoliubov transformation. The result can be expressed in terms of Boguliubov operators $\tilde{\theta}^\dagger_{\mathbf{q},\nu}$ and $\tilde{\theta}_{\mathbf{q},\nu}$:

$$\mathcal{H} = \sum_{\mathbf{q},\nu} \sqrt{\epsilon_{\mathbf{q}} (2 m_{\mathrm{BN}} v_\nu^2 + \epsilon_{\mathbf{q}})} \left(\tilde{\theta}^\dagger_{\mathbf{q},\nu} \tilde{\theta}_{\mathbf{q},\nu} + \frac{1}{2} \right). \tag{9}$$

Here $\epsilon_{\mathbf{q}} = 4 t_L \sum_\alpha (1 - \cos q_\alpha d_L)$ is the kinetic energy of an atom with crystal quasimomentum $\mathbf{q} = (q_x, q_y, q_z)$; d_L is the lattice constant. $m_{\mathrm{BN}} = 1/4 t_L d_L^2$ is the effective band mass. v_ν ($\nu = x, y, z, t, p$) is the sound velocity of the ν mode in the small-$|\mathbf{q}|$ limit; $v^2_{\alpha=x,y,z} = 4 M t_L d_L^2 (b_L G^{\alpha\alpha} - c_L)$, $v_t^2 = 4 M t_L d_L^2 (-c_L)$, $v_p^2 = 4 M t_L d_L^2 (a_L + c_L)$. The velocities of three spin modes depend on a $\tilde{\chi}$-dependent 3×3 symmetric matrix $G^{\alpha\beta}$, $G^{\alpha\beta} = -(1/2) \times \mathrm{Tr}([L^\alpha, L^p][L^\beta, L^p])$. More explicitly, $G^{\alpha\beta}$ is a diagonal matrix with elements: $G^{xx} = 4\sin^2(\xi - \frac{2\pi}{3})$, $G^{yy} = 4\sin^2(\xi + \frac{2\pi}{3})$, $G^{zz} = 4\sin^2\xi$. Notice that the velocity of the phase mode v_p can be written as $\sqrt{\mu_L / m_{\mathrm{BN}}}$, depending only on the band mass m_{BN} and the chemical potential μ_L; it is independent of ξ.

Unlike the mean field energy E_{MF} that is independent of ξ, the zero point energy of spin nematics per lattice site E is ξ-dependent (α summed over x, y, and z):

$$E(\xi) = \frac{1}{2N_T}\sum_{\mathbf{q},\alpha}\sqrt{\epsilon_{\mathbf{q}}[2m_{\mathrm{BN}}v_\alpha^2(\xi) + \epsilon_{\mathbf{q}}]}. \qquad (10)$$

Here N_T is the number of lattice sites. The main contribution to the ξ dependence of energy is from fluctuations of wave vector $|\mathbf{q}| \sim m_{\mathrm{BN}}v_\alpha(\xi)$; for condensates, this characteristic momentum is much smaller than $\hbar/d_L$. The ξ-dependent energy is proportional to $\sum_\alpha v_\alpha^5/(d_L^5 t_L^4)$; the amplitude of it can be expressed as $|Mc_L|^{5/2}/t_L^{3/2} g(b_L/c_L, |c_L|/t_L)$, where $g(x, y)$ is a dimensionless function that is studied numerically. In Fig. 1, we plot the energy as a function of ξ. We find that there are two distinct phases when the parameters occur in the region $c_L < 0$ and $b_L > c_L/4$. They are separated by the $b_L = 0$ line. When b_L is positive, $\xi = 0, \pi/3, 2\pi/3, \ldots$ are ground states. These are uniaxial nematic states which are rotationally invariant along an easy axis [see Fig. 2(a)]. When b_L is negative, the points of $\xi = \pi/6$, $\pi/2$, $5\pi/6$ ... are the stable ground states, while the uniaxial nematics are unstable.

The energy as a function of ξ has the following symmetries:

$$E(\xi) = E(-\xi), \qquad E\left(\frac{\pi}{3} + \xi\right) = E(\xi). \qquad (11)$$

These are a result of the rotation and gauge invariance of the energy function. They are found by examining the mean field solutions in Eqs. (4) and (6). A rotation $\mathcal{R}$ of 120° around the $x = y = z$ line effectively transforms a solution at ξ to $\xi + \pi/3$, or $\mathcal{R}^T\chi(\xi)\mathcal{R} = -\chi(\xi + \frac{\pi}{3})$. Also, because the energy is invariant under SO(3) rotations and is an even function of χ, one finds that $E(\xi) = E(\xi + \pi/3)$. In addition, a rotation of 180° around the $x + y = 0$ line in the xy plane transforms $\chi(\xi)$ to $\chi(-\xi)$, i.e. $\mathcal{R}^T\chi(\xi)\mathcal{R} = \chi(-\xi)$; so similarly one finds that $E(\xi) = E(-\xi)$. These symmetries depend only on rotational and gauge invariance and are exact. So the energy is an even and periodical function of ξ, with the period equal to $\pi/3$. For an analytical function with these symmetries, $\xi = 0$, $\pi/6$, and $\pi/3$ are always extrema. Our calculations of the zero point energy are consistent with this. The above observation also indicates that, up to an SO(3) rotation and a phase factor, states at ξ and at $\xi + \pi/3$ are equivalent.

We now examine the topology of the manifold of ZPQF-induced spin nematics. Without loss of generality, we first consider the uniaxial nematic state at $\xi = 0$, i.e., $\chi_{xx} = \chi_{yy} = -1/2\sqrt{3}$ and $\chi_{zz} = 1/\sqrt{3}$; in this case, the nematic easy axis specified by a unit vector $\mathbf{e}$ is pointing along the z direction [see Fig. 2(a)]. Such an uniaxial state is invariant under an arbitrary rotation around the nematic axis $\mathbf{e}$; it is further invariant under an inversion of the nematic axis $\mathbf{e} \rightarrow -\mathbf{e}$, which is evident in the plot for the wave function. The vacuum manifold for the uniaxial nematic is therefore simply $S^2/Z_2 \otimes S^1$; here S^2/Z_2 is where the nematic director lives, and S^1 is the unit circle of condensate phase variable. Unlike in uniaxial spin nematics of $F = 1$ atoms [28], here the spin orientation and condensate phase are not entangled.

For the biaxial nematic state at $\xi = \pi/2$, $\chi_{xx} = -\chi_{yy} = 1/2$ and $\chi_{zz} = 0$. The state is invariant under the

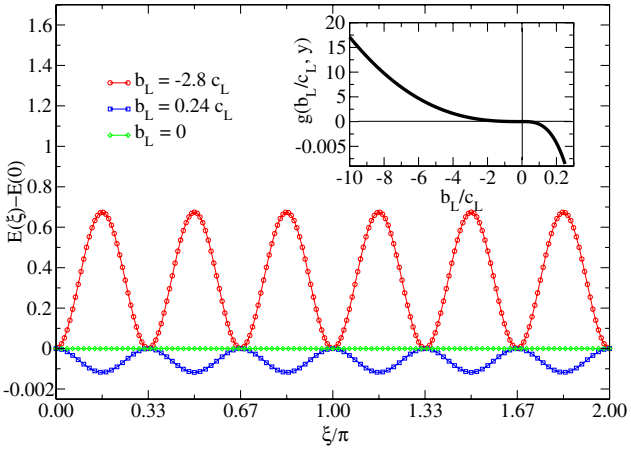

FIG. 1 (color online). The zero point energy of spin nematics per lattice site as a function of ξ (in units of $|Mc_L|^{5/2}/t_L^{3/2}$, $c_L < 0$). The inset is $g(x, y)$, the amplitude of $E(\xi = \frac{\pi}{6}) - E(0)$ as a function of $x(= b_L/c_L)$. $y(= |c_L|/t_L)$ has been set to be 8×10^{-3}. A quantum first-order phase transition occurs at $b_L = 0$ as a result of ZPQFs. For a positive b_L, the energy minima correspond to uniaxial spin nematics while the maxima to biaxial spin nematics with Dih_4 symmetries.

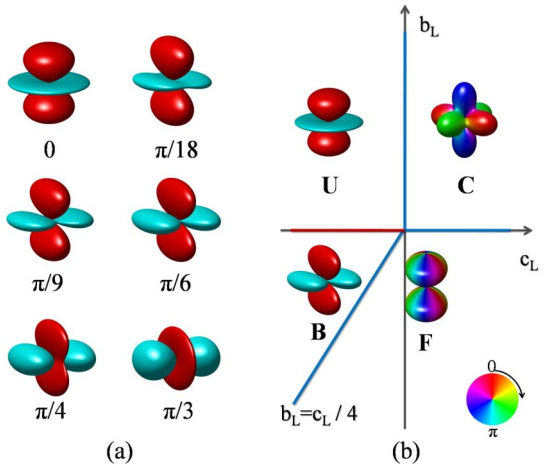

FIG. 2 (color online). (a) Wave functions of spin nematics at various ξ; (b) wave functions of uniaxial spin nematics (U), biaxial spin nematics with Dih_4 symmetries (B), ferromagnetic condensates (F), and cyclic condensates (C). Plotted here are spin wave functions Ψ_S (represented by the usual spherical harmonics) in spherical coordinates (ρ, θ, ϕ). $\rho = |\Psi_S(\theta, \phi)|$, and $\Psi_S = \sum_{\alpha\beta}\sqrt{(15/4\pi)}\chi_{\alpha\beta}n_\alpha n_\beta$. n_α, $\alpha = x, y, z$, are components of a unit vector $\mathbf{n}(\theta, \phi)$ [see also Eq. (2)]; colors indicate the phase of wave functions. The phase boundaries between U and C, C and F, and F and B are obtained by minimizing Eq. (3) (similar to the calculations in Ref. [16]); the phase boundary between U and B is obtained by taking into account ZPQFs.

eight element dihedral-four group Dih_4. The seven rotations that leave the state invariant (up to a phase shift) are 90°, 180°, and 270° rotations about the z axis and 180° rotations about the x and y axes and about the $x \pm y = 0$ lines in the xy plane. Four of these rotations—the 90° and 270° rotations around the z axis and the 180° rotation around the $x \pm y = 0$ lines—must be accompanied by a shift of the phase of the condensate by π. The manifold therefore is $[\mathrm{SO}(3) \times S^1]/\mathrm{Dih}_4$, where the dihedral elements in the denominator contain the rotations mentioned plus the π-phase shifts. These nematics contain half-vortices.

On the other hand, a generic biaxial spin nematic (with no accidental symmetries) is invariant only under a rotation of 180° around the x, y, or z axis, and the invariant subgroup is the Klein-four or dihedral-two group [29]; it has lower symmetries than either of the spin nematics selected by ZPQFs.

The perturbative calculation carried out in this Letter is valid when fluctuations of the order parameter χ are small. Here we estimate the fluctuations along each of the five directions $\nu = x, y, z, t, p$. Using Eq. (7), we evaluate the amplitude of local fluctuations in an orthogonal mode, $A_1(\nu) = \langle 0|\theta^\dagger_{k,\nu}\theta_{k,\nu}|0\rangle$. Taking into account the expression for υ_ν, we have the following estimate for the relative amplitude of fluctuations:

$$\frac{A_1(\nu)}{M} \sim M^{1/2}\left(\frac{\tilde{a}_\nu}{\tilde{a}_p}\frac{a_L + c_L}{t_L}\right)^{3/2}. \tag{12}$$

$\tilde{a}_\nu$ is the effective scattering length of each mode which is a linear combination of scattering lengths in $F = 0, 2, 4$ channels: $\tilde{a}_\alpha = [(2 - G^{\alpha\alpha})/7](a_2 - a_4) - \frac{1}{5}(a_0 - a_4)$, $\tilde{a}_t = \frac{2}{7}(a_2 - a_4) - \frac{1}{5}(a_0 - a_4)$, and $\tilde{a}_p = \frac{1}{7}(2a_2 + 5a_4) + \frac{1}{5}(a_0 - a_4)$. For ^{87}Rb atoms in optical lattices, $\tilde{a}_\alpha/\tilde{a}_p \sim 10^{-2}$ and $a_L \sim 50nk$, and when $t_L \sim 300nk$, the relative amplitude of fluctuations in the x, y, z, or t mode is typically less than 1%. Finally, we would like to point out that in nematic insulating states the properties spin modes are very similar to those discussed here.

In conclusion, we have found that ZPQFs lift a continuous degeneracy in spin nematics. Only uniaxial spin nematics or biaxial nematics with dihedral-four symmetries are selected as the true ground states. For Rb^{87} atoms in the hyperfine spin-2 manifold, b_L is between $-3c_L$ and $-10c_L$. According to the above analysis, the ground state should be a uniaxial spin nematic. The ZPQF-induced energy landscape can be experimentally mapped out by investigating the *macroscopic quantum dynamics* of condensates prepared in certain initial states. A condensate of rubidium atoms initially prepared at state $(1/\sqrt{2})(|2, 2\rangle + |2, -2\rangle)$ (corresponding to the $\xi = \pi/2$ point), because of the ZPQF-induced potential shown in Fig. 1, could evolve towards a condensate with atoms at state $\frac{1}{2}|2, 0\rangle + (\sqrt{3}/2\sqrt{2})(|2, 2\rangle + |2, -2\rangle)$ (corresponding to the $\xi = \pi/3$ point). This leads to a temporal oscillation of the population of atoms at state $|2, 0\rangle$, which can be studied in experiments. This study could yield information on the potential.

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Note added.—After the submission of this manuscript, we noticed that similar results were obtained in Ref. [30].

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