Fluctuations and correlations in rotating Bose-Einstein condensates

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We investigate the effects of correlations on the properties of the ground state of the rotating harmonically trapped Bose gas by adding Bogoliubov fluctuations to the mean-field ground state of an N-particle single-vortex system. We demonstrate that the fluctuation-induced correlations lower the energy compared to that of the mean-field ground state, that the vortex core is pushed slightly away from the center of the trap, and that an unstable mode with negative energy (for rotations slower than a critical frequency) emerges in the energy spectrum, thus pointing to a better state for slow rotation. We construct mean-field ground states of zero-, one-, and two-vortex states as a function of rotation rate and determine the critical frequencies for transitions between these states, as well as the critical frequency for appearance of a metastable state with an off-center vortex and its image vortex in the evanescent tail of the cloud.

I. INTRODUCTION

A rotating ultracold harmonically trapped Bose gas is predicted to pass through many exotic phases with increasing rotation rate (for a recent review, see Ref. [1]). The mean-field description, which omits all correlations, predicts the zero-temperature ground state for a large number of particles to be a vortex lattice [2,3], and is in good agreement with current experiments [4]. However, exact diagonalization of the many-body Hamiltonian [5] suggests the breakdown at very high rotation rates of the mean-field picture and a melting transition to strongly correlated ground states, bosonic analogs of quantum Hall states [6,7]. The onset of correlations and quantum fluctuations can be expected to play a significant role in this transition to a strongly correlated quantum liquid. However, a consistent theory of the zero-temperature melting of the vortex lattice does not exist so far [8–11] (for a theory of thermal melting of the lattice, see Ref. [12]). A crucial first step in constructing such a theory is to understand better how correlations affect the system.

With increasing rotation rate, the cloud expands in the transverse direction, and the particle density decreases. In each unit cell of the lattice, the vortex core occupies a larger fraction of the area of the cell [13], and the average displacement of the vortex from its equilibrium position increases [9] due to the zero-point motion of the Tkachenko mode [14,15]. Hence, the uncertainty in the position of vortices, which plays a leading role in the melting, increases at faster rotation rates [1]. This uncertainty is completely absent in the mean-field picture, in which the vortex positions are fixed and do not fluctuate.

The nature of the correlations between particles changes as the rotation rate increases. For angular momentum per particle less than or equal to unity (in units of $\hbar$ throughout), correlations in the exact ground state wave function [16] are described by polynomials in the relative distance of the particles from the center of mass, $\psi \sim \sum_{i_1 < i_2 < \cdots < i_L} (z_{i_1} - z_c)(z_{i_2} - z_c) \cdots (z_{i_L} - z_c)$, where $z \sim (x + iy)$ are the positions of the particles and z_c the center of mass in the complex plane. On the other hand, when the angular momentum per particle is of order the number of particles, correlations appear in the distances of particles from each other, as in the bosonic Laughlin wave function [17] $\psi \sim \prod_{i<j}(z_i - z_j)^2$.

The aim of the first part of this paper is to build relevant correlations on top of the mean-field many-body ground state and to investigate their effects on the energetics and physical properties of the ground state. Based on the inferred modifications of the ground state, the second part of this paper investigates, at the mean-field level, different ground states of the (zero-, one-, and two-vortex) Bose gas and their respective transitions as the external rotation rate increases.

Small-amplitude Bogoliubov fluctuations around the mean-field ground state induce correlations by allowing small numbers of excitations to appear in nearby single-particle states. In a condensate with a large number of vortices, the number of excited modes (single-particle harmonic oscillator eigenstates) involved is of order the number of vortices. Therefore, carrying out the general diagonalization is a mathematically challenging task for a many-vortex condensate. However, one can gain insight by working with a few-vortex system; for example, including the first three harmonic oscillator states is sufficient to describe systems with up to two vortices, as we show below. The simplest such system is a condensate with one singly quantized vortex at the center of the trap, rotating at the critical frequency Ω_c, at which the vortex becomes thermodynamically stable [2,18], and, hence, having unit angular momentum per particle.

We find, indeed, that the correlations induced by Bogoliubov fluctuations lead to a better ground state in the thermodynamic limit, lower in energy than the mean-field one. We also see that the fluctuations drive the vortex core away from the center of the trap by a fluctuating distance of $O(1/\sqrt{N})$ (in units of the characteristic length of the trap). Moreover, for rotations slower than the critical frequency Ω_c, we find excitations with negative eigenenergy in the spectrum [18] which remove one unit of angular momentum from the gas, indicating an instability toward a lower-energy nonrotating state for rotation rate $\Omega < \Omega_c$ and emphasizing the fact that the single-vortex mean-field ground state is not the best starting state.

Based on these results, we construct a more energetically favorable mean-field condensate which, as a function of Ω, is either nonrotating, a single-vortex state, or a two-vortex state. The phase diagram in Fig. 1 summarizes our results. At a certain frequency Ω_m (below Ω_c), there exists a metastable
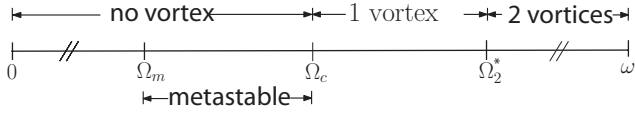
FIG. 1. Schematic phase diagram of the condensate.

state (a local minimum of the energy) with two off-center vortices in the cloud which are asymmetric about the origin; for a vortex close to the center of the trap, there exists an image vortex much farther away where the particle density is negligible, in agreement with Ref. [19]. We calculate the critical frequencies Ω_c and Ω_2^*, respectively, at which the first and second vortices enter the cloud. The former agrees with the numerical result of Ref. [2], while the latter is somewhat larger owing to our incorporating only a restricted number of single-particle eigenstates in the mean-field ground state.

In the next section, we outline the basic description of the rotating Bose gas in terms of Landau levels in the Coriolis force. In Sec. III, we determine the small-amplitude fluctuations about the mean-field condensate and their effect on the properties of the ground state, and then in Sec. V, we present the stable mean-field wave function that encapsulates the various phases of the rotating gas and their respective critical rotation frequencies. We set $\hbar = 1$ throughout.

II. BASIC MODEL

We consider a cloud of N bosons of mass m in a harmonic trap with frequencies ω in the x-y plane and ω_z in the z direction (with $\omega_z \gg \omega$ to tightly confine the gas in the axial direction), rotating around the z axis with angular velocity Ω. The characteristic oscillator lengths are $d = 1/\sqrt{m\omega}$ in the transverse direction and $d_z = 1/\sqrt{m\omega_z}$ in the axial direction. We assume weak two-body repulsive interactions of strength $g = 4\pi a/m$ where a is the s-wave scattering length. In the limit of fast rotation, $\Omega \lesssim \omega$, the gas becomes quasi-two-dimensional, and at zero temperature, it resides approximately in the ground state of the harmonic trap in the z direction. The many-body Hamiltonian in the rotating frame is $\mathcal{H}' = \sum_{i=1}^{N}(\mathfrak{h}_i^0 - \Omega\mathfrak{l}_i) + \sum_{i<j} g_{2D}\delta(\mathbf{r}_i - \mathbf{r}_j)$, with the noninteracting single-particle Hamiltonian and angular momentum

$$\mathfrak{h}_i^0 = \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}m\omega^2\mathbf{r}_i^2, \quad \mathfrak{l}_i = \hat{\mathbf{z}} \cdot (\mathbf{r}_i \times \mathbf{p}_i), \quad (1)$$

where $\mathbf{r}$ and $\mathbf{p}$ are the particle positions and momenta in the x-y plane, and $g_{2D} = g/\sqrt{2\pi}d_z$ is the effective interaction strength in two dimensions.

The eigenstates of $\mathfrak{h}^0$ are the Landau levels $|nm\rangle$, where the Landau level index n is the radial quantum number and $m \geqslant -n$ is the angular momentum along the rotation axis, with eigenvalues $\epsilon'_{nm} = (2n + |m| + 1)\omega - m\Omega$. The characteristic energy scale of the two-body interaction is $V_0 = g_{2D}/2\pi d^2$. The energy difference between two successive higher Landau levels ($n \neq 0$) is $O(2\omega)$ which, for $\Omega \to \omega$, is much larger than that $O(\omega - \Omega)$ between two states in a given Landau level. We assume the interactions to be sufficiently weak that $V_0 \ll 2\omega$; thus, we ignore the small higher Landau level components in the wave function and safely assume that the system resides in the manifold of the $n = 0$ lowest Landau level (LLL) states.

With this assumption, the only relevant quantum number is the angular momentum index m; from now on, we drop the Landau level index n from the eigenfunctions, operators, and occupation numbers for simplicity, unless otherwise noted.

The LLL eigenfunctions and eigenenergies are

$$\phi_m(z) = \langle \mathbf{r}|0m\rangle = \frac{1}{d\sqrt{\pi m!}}z^m e^{-|z|^2/2}, \quad (2a)$$

$$\epsilon'_m = \epsilon'_{0m} = \omega + (\omega - \Omega)m, \quad (2b)$$

where $z = (x + iy)/d$ is the position in the complex plane; we use $\mathbf{r}$ and z interchangeably. In terms of the corresponding creation and annihilation operators $a_m^\dagger$ and a_m, the second-quantized Hamiltonian in the rotating frame is

$$\mathcal{H}' = \sum_m \epsilon'_m a_m^\dagger a_m + \frac{1}{2}\sum_{\{m_i\}} V_{m_2 m_1}^{m_4 m_3} a_{m_4}^\dagger a_{m_3}^\dagger a_{m_2} a_{m_1}, \quad (3)$$

where the interaction matrix element in the LLL is

$$V_{m_2 m_1}^{m_4 m_3} = \int \phi_{m_4}^*(\mathbf{r})\phi_{m_3}^*(\mathbf{r}')g_{2D}\delta(\mathbf{r} - \mathbf{r}')\phi_{m_2}(\mathbf{r}')\phi_{m_1}(\mathbf{r})$$

$$= V_0 \frac{(m_1 + m_2)! \, \delta_{m_3 + m_4, m_1 + m_2}}{2^{m_1 + m_2}\sqrt{m_4!m_3!m_2!m_1!}}. \quad (4)$$

III. BOGOLIUBOV HAMILTONIAN IN THE LOWEST LANDAU LEVEL

We now turn to determining the effects of small-amplitude Bogoliubov fluctuations about the mean-field condensate on the properties of the system. We start with a condensate with a vortex at the center which rotates with angular frequency Ω_c, to be determined. We derive an effective LLL Hamiltonian along with its excitation spectrum (which includes an unstable normal mode) and show that its ground state has lower energy than the initial mean-field state in which *all* particles are condensed into the state $|01\rangle$. The initial condensate is

$$\psi(\mathbf{r}) = \sqrt{N_1}\,\phi_1(\mathbf{r}), \quad (5)$$

with N_1 particles in $|01\rangle$, describing a vortex at the center with winding number 1. For $N_1 \lesssim N$, we make the usual replacement of the operators $a_1^\dagger$ and a_1, corresponding to $|01\rangle$, by $\sqrt{N_1}$ in the limit of large N. Although the total number of particles is fixed, interactions cause the number of particles in the condensate to fluctuate; the number of condensed particles can, thus, be written in terms of the total and the noncondensed particle numbers as

$$N_1 = N - \sum_m' a_m^\dagger a_m, \quad (6)$$

where the prime indicates that $|01\rangle$ is excluded from the sum.

In the thermodynamic limit ($N \to \infty$ with NV_0 constant), interaction terms that represent scattering of only one condensate particle or no condensate particles are, respectively, $O(1/\sqrt{N})$ and $O(1/N)$ smaller than those that involve two particles from the condensate and, thus, can be ignored. Following the standard procedure to write the Hamiltonian up to quadratic order in the excitation operators and using

Eq. (6) to conserve the total number of particles, we derive the LLL Hamiltonian in the rotating frame,

$$\mathcal{H}' = \left[N(2\omega - \Omega) + \tfrac{1}{4}N^2 V_0\right] + \left[\tfrac{1}{2}N V_0 - (\omega - \Omega)\right]a_0^\dagger a_0$$
$$+ \left[\tfrac{1}{4}N V_0 + (\omega - \Omega)\right]a_2^\dagger a_2 + \tfrac{1}{\sqrt{8}}N V_0(a_0^\dagger a_2^\dagger + a_0 a_2). \tag{7}$$

The constant first term in square brackets is the energy of the mean-field state with all N particles condensed into $|01\rangle$ and no fluctuations present. The only two states in the LLL connected by the interactions in the presence of a condensate in $|01\rangle$ are $|00\rangle$ and $|02\rangle$, i.e., for a LLL system, the maximum angular momentum transferred in any scattering process is ± 1, whereas allowing higher Landau levels brings in and connects $|10\rangle$ and $|12\rangle$, $|20\rangle$ and $|22\rangle$, etc. Larger transfers of angular momentum take the system out of the LLL as well, e.g., $|03\rangle$ is connected to $|1, -1\rangle$ by a transfer of ± 2 units, $|2, -2\rangle$ to $|04\rangle$ by a transfer of ± 3 units, etc.

Conservation of angular momentum is reflected in the fact that any scattering process involves simultaneous transfers of $+m$ and $-m$ units of angular momentum (relative to the condensate). The same method presented here was previously used by Linn and Fetter [18] to include higher Landau levels perturbatively in the Bogoliubov excitation spectrum of this system. Also, Dodd *et al.* [20] have used a similar argument to describe angular momentum conservation in this system in the presence of an external perturbation. Later, Rokhsar reinterpreted their argument to show [21] the existence of a negative energy excitation (the anomalous mode) with vortex core properties similar to those we find in Sec. IV.

The canonical transformations to the bosonic quasiparticle operators

$$\alpha_{+1} = u\, a_2 + v\, a_0^\dagger$$
$$\alpha_{-1} = u\, a_0 + v\, a_2^\dagger \tag{8}$$

(with u and v real and positive) diagonalize the Hamiltonian, provided that $u^2 = 2$ and $v^2 = 1$. The new operators describe quasiparticles with ± 1 units of angular momentum relative to the condensate. Thus, the LLL Hamiltonian in the rotating frame becomes

$$\mathcal{H}' = \left[N(2\omega - \Omega) + \tfrac{1}{4}N^2 V_0 - \tfrac{1}{4}N V_0\right]$$
$$+ (\Omega - \Omega_c)\alpha_{-1}^\dagger \alpha_{-1} + (\omega - \Omega)\alpha_{+1}^\dagger \alpha_{+1}, \tag{9}$$

where

$$\Omega_c = \omega - \tfrac{1}{4}N V_0. \tag{10}$$

This equation shows that the Bogoliubov ground state (with no excited quasiparticles) has lower energy compared to the mean-field one by $-N V_0/4$. Also, the normal mode denoted by -1 has negative eigenenergy in the region $\Omega < \Omega_c$, indicating an instability in the system against being condensed into $|01\rangle$; this is the anomalous mode (see Ref. [22] and references therein). Its existence shows that $\psi(\mathbf{r})$ is not the correct condensate for $\Omega < \Omega_c$ and, therefore, the Hamiltonian in Eq. (9) is not the correct one for this regime. As the rotation rate increases beyond Ω_c, further LLL states beyond $\{|00\rangle, |01\rangle, |02\rangle\}$ come into play in the ground state, especially once two or more vortices enter the cloud (see Sec. V). Then,

one must include Bogoliubov fluctuations around this new ground state in order to find the Bogoliubov Hamiltonian and its normal modes. For simplicity, we limit the discussion here to $\Omega = \Omega_c$ which corresponds to our starting point, a system fully condensed in $|01\rangle$.

In the manifold of the first three lowest Landau levels, the field operator for removing a particle at position $\mathbf{r}$ is

$$\Psi(\mathbf{r}) = \phi_0(\mathbf{r})\, a_0 + \phi_1(\mathbf{r})\, a_1 + \phi_2(\mathbf{r})\, a_2. \tag{11}$$

Inverting Eq. (8) gives

$$a_0 = u\, \alpha_{-1} - v\, \alpha_{+1}^\dagger,$$
$$a_2 = u\, \alpha_{+1} - v\, \alpha_{-1}^\dagger, \tag{12}$$

and, thus, the expansion of $\Psi(\mathbf{r})$ in terms of the quasiparticles is

$$\Psi(\mathbf{r}) = \psi(\mathbf{r}) + [u\,\phi_2(\mathbf{r})\alpha_{+1} - v\,\phi_0(\mathbf{r})\alpha_{+1}^\dagger]$$
$$+ [u\,\phi_0(\mathbf{r})\alpha_{-1} - v\,\phi_2(\mathbf{r})\alpha_{-1}^\dagger]. \tag{13}$$

This is the mode expansion $\Psi(\mathbf{r}) = \psi(\mathbf{r}) + \sum_j [u_j(\mathbf{r})\alpha_j - v_j^*(\mathbf{r})\alpha_j^\dagger]$ in terms of the quasiparticles (see, e.g., Ref. [23]). Hence, the amplitudes for the -1 eigenmode are

$$u_{-1}(\mathbf{r}) = u\,\phi_0(\mathbf{r}),$$
$$v_{-1}(\mathbf{r}) = v\,\phi_2^*(\mathbf{r}). \tag{14}$$

This mode, although having a negative eigenenergy for $\Omega < \Omega_c$, has a positive norm, since

$$\int [|u_{-1}(\mathbf{r})|^2 - |v_{-1}(\mathbf{r})|^2]d^2r = u^2 - v^2 = 1, \tag{15}$$

and is thus physical. Since $\langle \mathbf{r}|02\rangle^* = \langle \mathbf{r}|2, -2\rangle$, we arrive at the same amplitudes as derived up to zeroth order in V_0 in Sec. III of Ref. [18]. We note, however, that the only two states that are mixed, in fact, are $|00\rangle$ and $|02\rangle$ which are in the LLL, and not $|2, -2\rangle$ which is a higher Landau level; up to the level of the approximation used in this article, the fluctuations reside solely in the LLL.

IV. PROPERTIES OF THE BOGOLIUBOV GROUND STATE

We now investigate the stable ground state of the Hamiltonian, Eq. (9), for $\Omega = \Omega_c$ and show that fluctuations drive the vortex away from the center of the trap and modify its velocity profile. The order parameter is $\psi(\mathbf{r}) = \langle\Psi(\mathbf{r})\rangle$ or, in terms of annihilation operators, $\langle a_1\rangle = \sqrt{N_1}$ for the macroscopic condensate with N_1 particles in $|01\rangle$. The condensed state $|N_1\rangle$ is a coherent state that satisfies the eigenvalue equation $a_1|N_1\rangle = \sqrt{N_1}|N_1\rangle$ with the normalized solution

$$|N_1\rangle = e^{-N_1/2}\, e^{\sqrt{N_1}a_1^\dagger}|\text{vac}\rangle, \tag{16}$$

where $|\text{vac}\rangle$ is the vacuum. This state does not conserve particle number.

The Bogoliubov ground state is determined by the condition that no quasiparticles be present, i.e.,

$$\alpha_{\pm 1}|G\rangle = 0. \tag{17}$$

Following the standard procedure (see, e.g., Ref. [24]), we find the normalized Bogoliubov ground state

$$|G\rangle = \frac{1}{\sqrt{2}} e^{-a_2^\dagger a_0^\dagger/\sqrt{2}} |N_1\rangle, \qquad (18)$$

which has an expectation value of the angular momentum operator $\mathcal{L} = \sum_m m\, a_m^\dagger a_m$ given by $\langle G|\mathcal{L}|G\rangle = N$.

We now compare the laboratory-frame energy of $|G\rangle$ with that of the mean-field and exact ground states. The exact non-normalized many-body ground state for $2 \leqslant L \leqslant N$ is [16]

$$\psi_x^L(z_1 \cdots z_N) = \sum_{i_1 < i_2 < \ldots < i_L} (z_{i_1} - z_c)(z_{i_2} - z_c) \cdots (z_{i_L} - z_c), \qquad (19)$$

where $z_c = \sum_{i=1}^N z_i/N$ is the center of mass coordinate; we suppress the factor $\exp[-\sum_{k=1}^N |z_k|^2/2]$ common to all N-particle LLL states from now on for brevity. This state has energy $E_x^L = (N+L)\omega + V_0 N(N-1-L/2)/2$ in the laboratory frame. The mean-field ground state for $L = N$ with a vortex at origin,

$$\psi_{\text{mf}}(z_1 \cdots z_N) = \prod_{i=1}^N \phi_1(z_i), \qquad (20)$$

has energy $E_{\text{mf}} = 2N\omega + V_0 N^2/4$ in the laboratory frame. Therefore, at $L = N$ (and, hence, at $\Omega = \Omega_c$), the Bogoliubov ground state lies exactly halfway in energy between the mean-field ground state and the exact one.

A diagnostic of the structure of the vortex is the circulation around a closed contour $\mathcal{C}$ encircling the center,

$$\Gamma = \oint_{\mathcal{C}} \mathbf{v}(\mathbf{r}) \cdot d\mathbf{r}, \qquad (21)$$

quantized in units of $2\pi\hbar/m$ for a quantum vortex. The velocity is $\mathbf{v}(\mathbf{r}) = \langle \mathbf{j}(\mathbf{r})\rangle/\langle\rho(\mathbf{r})\rangle$ where $\langle \mathbf{j}(\mathbf{r})\rangle = (\hbar/m)\text{Im}\langle\Psi^\dagger(\mathbf{r})\nabla\Psi(\mathbf{r})\rangle$ is the expectation value of the current operator and $\langle\rho(\mathbf{r})\rangle = \langle\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})\rangle$ is that of the density operator. In the mean-field state, Eq. (20),

$$\mathbf{v}_{\text{mf}}(\mathbf{r}) = \frac{\hbar}{m}\frac{\hat{\boldsymbol{\theta}}}{r}, \qquad (22)$$

which describes an irrotational superflow (except at the origin where the vortex is located) with circulation $\Gamma_{\text{mf}} = 2\pi\hbar/m$. However, the Bogoliubov ground state (18) gives

$$\langle \mathbf{j}(z)\rangle = \frac{\hbar}{m}\left[N\left(1 - \frac{2}{N} + \frac{3}{N^2}\right) + |z|^2\right]|z|\frac{e^{-|z|^2}}{\pi d^2}\hat{\boldsymbol{\theta}}, \qquad (23)$$

$$\langle\rho(z)\rangle = \left[1 + N\left(1 - \frac{2}{N} + \frac{3}{N^2}\right)|z|^2 + \frac{|z|^4}{2}\right]\frac{e^{-|z|^2}}{\pi d^2}. \qquad (24)$$

Thus, in the limit of large N, the velocity field is

$$\mathbf{v}_G(\mathbf{r}) = \frac{\hbar}{m}\frac{r\hat{\boldsymbol{\theta}}}{r^2 + \Delta(r)}, \qquad (25)$$

where $\Delta(r) = (1 - \frac{1}{2}r^4)/(N + r^2)$ is the correction due to quantum fluctuations. The circulation in $|G\rangle$ is then

$$\Gamma_G(\mathbf{r}) = \Gamma_{\text{mf}}\frac{r^4 + Nr^2}{\frac{1}{2}r^4 + Nr^2 + 1}. \qquad (26)$$
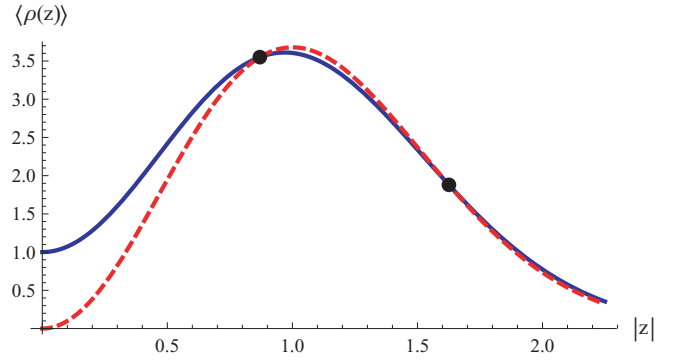

FIG. 2. (Color online) Density (in units of $1/\pi d^2$) of the Bogoliubov (solid line) and mean-field (dashed line) ground states for $N = 10$, showing a vortex at the center.

For large but finite N, we find $\Gamma_G/\Gamma_{\text{mf}} \sim 1$ (increasing from $1/2$ to $4/3$) for the large range $1/\sqrt{N} \lesssim r \lesssim \sqrt{N}$, while $\Gamma_G/\Gamma_{\text{mf}} \to 0$ as $r \to 0$ and $\Gamma_G/\Gamma_{\text{mf}} \to 2$ as $r \to \infty$. The vortex (at the center of the trap in mean-field) is now pushed off-center by quantum fluctuations, hence the vanishing circulation as the contour shrinks toward the origin. The off-center vortex fluctuates very close about the origin, as shown by the circulation approaching its mean-field value as the contour radius expands past $O(1/\sqrt{N})$. On the other hand, as the contour expands even farther toward infinity, the circulation grows to twice its mean-field value, indicating the presence of an image vortex much farther from the origin. These results agree with those of Sec. V. In the thermodynamic limit ($N \to \infty$), however, Γ_G equals the quantum of circulation everywhere except at the origin (where it is zero) and at infinity (where it is twice the quantum of circulation); therefore, increasing the number of particles suppresses quantum fluctuations of the vortex and leads to the vortex being driven less farther from the center of the trap and the image vortex being driven more outward to infinity.

Quantum fluctuations change the particle density of the ground state compared to its mean-field value, $\rho_{\text{mf}} = N|z|^2 e^{-|z|^2}/\pi d^2$. The average density is now non-zero at the center of the trap, $\langle\rho(0)\rangle = 1/\pi d^2$ (see Fig. 2). One can understand this finite density in terms of the vortex fluctuating about the origin, as discussed above. Snapshots of the cloud in the laboratory would reveal a vortex at random positions (varying from shot to shot due to Bogoliubov fluctuations); averaging over these density snapshots would lead to Eq. (24) for the average particle density of $|G\rangle$. One can also understand the finite density at the origin in terms of the single-particle quantum states, in particular, the nonzero occupation of $|00\rangle$ whose wave function does not vanish at the origin.

V. THE STABLE CONDENSATE

The anomalous mode, denoted by -1 in Eq. (9), suggests that a condensate with a singly quantized vortex at the center of the trap is not stable against fluctuations for $\Omega < \Omega_c$. However, Eqs. (13) and (14) indicate that a mean-field condensate wave function of the form

$$\psi(z) = \sqrt{N_1}\,\phi_1(z) + u\,\phi_0(z) - v\,\phi_2(z) \qquad (27)$$

can have lower energy and be stable, depending on the values of u and v (which can be taken to be real). We search for a better ground state by tuning the two extra degrees of freedom, u and v, as follows.

Normalizing $\psi(z)$ leads to $N = N_1 + u^2 + v^2$; hence, u and v are bounded by $u^2 + v^2 \leqslant N$. The energy in the rotating frame, then, becomes

$$
\begin{aligned}
E' = {} & \left[N(2\omega - \Omega) + \frac{1}{4}N^2 V_0 \right] + \left[\left(\Omega - \omega + \frac{NV_0}{2} \right) u^2 \right. \\
& + \left(\omega - \Omega + \frac{NV_0}{4} \right) v^2 - \frac{NV_0}{\sqrt{2}} uv \right] \\
& + V_0 \left(-\frac{1}{4}u^4 - \frac{5}{16}v^4 - \frac{3}{4}u^2 v^2 + \frac{1}{\sqrt{2}}u^3 v + \frac{1}{\sqrt{2}}uv^3 \right).
\end{aligned}
\tag{28}
$$

The constant term is the energy of a condensate with N particles in $|01\rangle$. Note that E' is invariant under the simultaneous transformation $u \to -u$ and $v \to -v$. We choose $0 \leqslant v \leqslant u$, because this sector of the u-v plane is energetically favorable.

We denote $\tilde{E}' = E' - [N(2\omega - \Omega) + N^2 V_0/4]$ as the energy contribution from the mixing of $|00\rangle$ and $|02\rangle$ with the condensate. Then, introducing the parametrization $u = \zeta \cosh(\theta/2)$ and $v = \zeta \sinh(\theta/2)$, we find

$$
\begin{aligned}
\tilde{E}' = {} & \zeta^2 \left[\left(\Omega - \omega_\perp + \frac{NV_0}{8} \right) + \frac{NV_0}{8}(3\cosh\theta - \sqrt{8}\sinh\theta) \right] \\
& + \zeta^4 \frac{V_0}{128} \left[-15 + 4\cosh\theta - 21\cosh(2\theta) \right. \\
& \left. + 16\sqrt{2}\sinh(2\theta) \right].
\end{aligned}
\tag{29}
$$

Ignoring the quartic part for now, i.e., assuming $u, v \ll \sqrt{N_1}$ or $N_1 \lesssim N$, we minimize the quadratic part with respect to θ and find $\tanh\theta_m = \sqrt{8}/3$, which is depicted by the straight dashed line in the u-v plane in Fig. 3. With this value of θ, we have

$$
\tilde{E}' = (\Omega - \Omega_c)\zeta^2 + \frac{3V_0}{16}\zeta^4.
\tag{30}
$$

The quadratic term shows that up to second order in the mixing due to interactions, the system is unstable for $\Omega < \Omega_c$, as in the quantum treatment.
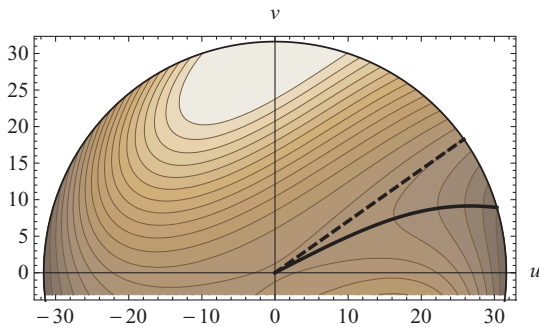

FIG. 3. (Color online) Contour plot of E' for $N = 10^3$, $NV_0 = 0.1$, and $\Omega = \omega - \frac{3}{8}NV_0$. Darker shades indicate lower energies. The straight dashed line represents the direction given by $\tanh\theta_m = \sqrt{8}/3$; the curved solid line is the solution of Eq. (47), discussed below.

For $\Omega > \Omega_c$, Eq. (30) is a monotonically increasing function of ζ with a minimum at $\zeta = 0$ or

$$
u_m^> = v_m^> = 0,
\tag{31}
$$

describing a system fully condensed into $|01\rangle$ with one vortex at the center of the trap. (The superscripts "$<$" or "$>$" denote rotations slower or faster than Ω_c.) The energy in the rotating frame becomes

$$
E_m'^> = \left(N\omega + \frac{1}{2}N^2 V_0 \right) + N(\Omega_c - \Omega),
\tag{32}
$$

where the first term is just the energy were all N particles condensed into $|00\rangle$. For $\Omega \leqslant \Omega_c$, though, minimizing Eq. (30) gives

$$
u_m^< = \sqrt{\frac{16(\Omega_c - \Omega)}{3V_0}}, \quad v_m^< = \sqrt{\frac{8(\Omega_c - \Omega)}{3V_0}},
\tag{33}
$$

so that $u_m^< = \sqrt{2}\, v_m^<$, and the rotating-frame energy becomes

$$
E_m'^< = \left(N\omega + \frac{1}{2}N^2 V_0 \right) + N(\Omega_c - \Omega) - \frac{4(\Omega_c - \Omega)^2}{3V_0}.
\tag{34}
$$

The boundedness of u and v implies $0 \leqslant \zeta_m^2 \cosh\theta_m \leqslant N$. Hence, the region of validity of Eqs. (33) and (34) is $\Omega_m \leqslant \Omega \leqslant \Omega_c$, where

$$
\Omega_m = \omega - \frac{3}{8}NV_0.
\tag{35}
$$

Then, for $\Omega < \Omega_m$, the point $(u_m^<, v_m^<)$ lies outside the circle defined by $u^2 + v^2 = N$ and does not represent a physical solution.

In order to check for the existence of lower-energy states on the edge of the circle, where $u^2 + v^2 = N$, we have to compare $E_m'^{\lessgtr}$ with the corresponding energy $E_e'^{\lessgtr}$ for points on the edge. Since $N_1 = 0$ on the edge, we find

$$
E_e' = \left(N\omega + \frac{1}{2}N^2 V_0 \right) + 2(\Omega_c - \Omega)v^2 + \frac{3V_0}{16}v^4.
\tag{36}
$$

For $\Omega \leqslant \Omega_c$, this energy increases monotonically with v, with the minimum at

$$
u_e^< = \sqrt{N}, \quad v_e^< = 0,
\tag{37}
$$

representing a system fully condensed into $|00\rangle$ (with no vortex) and the rotating-frame energy

$$
E_e'^< = N\omega + \frac{1}{2}N^2 V_0.
\tag{38}
$$

For $\Omega > \Omega_c$, however, the minimum is at

$$
u_e^> = \sqrt{N - \frac{16(\Omega - \Omega_c)}{3V_0}}, \quad v_e^> = \sqrt{\frac{16(\Omega - \Omega_c)}{3V_0}},
\tag{39}
$$

and the energy in the rotating frame is

$$
E_e'^> = \left(N\omega + \frac{1}{2}N^2 V_0 \right) - \frac{16(\Omega - \Omega_c)^2}{3V_0}.
\tag{40}
$$

Therefore, for $\Omega_m \leqslant \Omega \leqslant \Omega_c$, the difference between the two energies is

$$E_m'^< - E_e'^< = \frac{4}{3V_0}(\Omega_c - \Omega)(\Omega - \Omega_1^*), \qquad (41)$$

where $\Omega_1^* = \omega - NV_0$. Since $\Omega_1^* < \Omega_m$, we find that the point $(u = \sqrt{N}, v = 0)$ corresponds to the *global* minimum of the energy for the entire region $0 \leqslant \Omega \leqslant \Omega_c$, indicating that the system has fully condensed into $|00\rangle$ with no vortex, whereas a *local* minimum of the energy appears at $(u = u_m^<, v = v_m^<)$ for $\Omega_m \leqslant \Omega \leqslant \Omega_c$. This latter point corresponds to a metastable state which describes two vortices (asymmetric with respect to the origin) in the condensate; hence, the metastability frequency Ω_m is the rotation frequency at which a metastable state appears in the energy spectrum. On the other hand, for $\Omega > \Omega_c$, the difference between the two energies is

$$E_m'^> - E_e'^> = \frac{16}{3V_0}(\Omega - \Omega_c)(\Omega - \Omega_2^*), \qquad (42)$$

where $\Omega_2^* = \omega - \frac{1}{16}NV_0$. Thus, if $\Omega_c < \Omega \leqslant \Omega_2^*$, the point $(u = 0, v = 0)$, i.e., the center of the circle, corresponds to the *global* minimum of the energy, indicating that the system has fully condensed into $|01\rangle$ with one vortex at the center. For $\Omega > \Omega_2^*$, however, the *global* minimum of the energy is at $(u = u_e^>, v = v_e^>)$ on the edge of the circle, and the ground state is a coherent superposition of $|00\rangle$ and $|02\rangle$ with two vortices in a symmetric configuration with respect to the origin.

Hence, Ω_c is the critical frequency for creating a centered vortex, and Ω_2^* is the critical frequency at which two vortices nucleate in the condensate. Note that Ω_c agrees with the external rotation frequency derived in Refs. [2,18]; however, Ω_2^* is bigger than the two-vortex nucleation frequency, $\omega - 0.078NV_0$, calculated numerically in Ref. [2] due to the very limited Hilbert space used here with only $\{|00\rangle, |01\rangle, |02\rangle\}$ as opposed to a rather large one used in Ref. [2].

The metastable state, for which $u_m^< = \sqrt{2}\, v_m^<$, has two vortices at the zeros of $\psi(z)$, i.e.,

$$z_m^\pm(\Omega) = \frac{\sqrt{N - 3(v_m^<)^2} \pm \sqrt{N + (v_m^<)^2}}{\sqrt{2}\, v_m^<}, \qquad (43)$$

where Ω enters through $v_m^<$ on the right side. Using Eq. (33), we find $v_m^< = \sqrt{N/3}$ at $\Omega = \Omega_m$. Hence, $z_m^\pm(\Omega_m) = \pm\sqrt{2}$. However, as Ω increases toward Ω_c, we find for small $v_m^<$ that $z_m^\pm \to \pm\sqrt{2}(v_m^</\sqrt{N})^{\mp 1}$ or, in other words, $z_m^+ \to +\infty$ whereas $z_m^- \to 0$. As Ω increases from Ω_m to Ω_c, the vortex at $+\sqrt{2}$ moves to infinity, while the one at $-\sqrt{2}$ reaches the center and becomes stable there.

It is instructive to compare this result to that of Ref. [19], where the authors assume a condensate with an off-center vortex at position b close to the center, i.e., $\chi(z) \sim \sqrt{N}(z - b)$, and find perturbative corrections to the wave function using the Gross-Pitaevskii equation. The new non-normalized wave function in the LLL up to $O(b^2)$ is $\chi(z) \sim \sqrt{N}(z - b)(1 + bz/2 + \cdots)$ [see Eq. (15) of Ref. [19]] with the rotation frequency, to lowest order in b, being $\Omega \simeq \Omega_c$ [see Eq. (16) of

Ref. [19]]. This wave function represents two vortices at b and $-2/b$. Normalizing this wave function up to $O(b^2)$ leads to

$$\chi(z) \sim \sqrt{N}\left[\frac{b}{2}z^2 + \left(1 - \frac{3}{4}b^2\right)z - b\right]. \qquad (44)$$

We can repeat a similar procedure for the metastable state for which $u_m^< = \sqrt{2}\, v_m^<$. Then, the condensate wave function, Eq. (27), becomes

$$\psi(z) \sim \sqrt{N_1}\, z + u_m^< - \frac{u_m^<}{2}z^2. \qquad (45)$$

Expanding for small $u_m^<$ and defining $\mathfrak{b} = -u_m^</\sqrt{N}$, we have

$$\psi(z) \sim \sqrt{N}\left[\frac{\mathfrak{b}}{2}z^2 + \left(1 - \frac{3}{4}\mathfrak{b}^2\right)z - \mathfrak{b}\right]. \qquad (46)$$

Thus, $\chi(z)$ and $\psi(z)$ have the same form with $b \leftrightarrow \mathfrak{b}$. Since $\mathfrak{b}$ is small, $\psi(z)$ also represents two off-center vortices at $\mathfrak{b}$ (close to the origin) and $-2/\mathfrak{b}$ (much farther away in the evanescent tail of the cloud). Using Eq. (33), we find the rotation rate of this two-vortex configuration in the laboratory frame to be $\Omega = \Omega_c - (3/16)NV_0|\mathfrak{b}|^2$ which includes the next-order correction of $O(|\mathfrak{b}|^2)$ to the result of Ref. [19]. Note that while the calculations of Ref. [19] are limited to the fast rotating regime and are valid only in the vicinity of Ω_c (due to their perturbative nature in the small parameter $\Omega - \omega$), the method presented here covers the entire region $0 \leqslant \Omega \leqslant \omega$ and is only limited by the number of states included in the condensate wave function.

VI. THE VALLEY AND THE METASTABLE POINT

The derivation of the local minimum of the energy in the metastable regime, $\Omega_m \leqslant \Omega \leqslant \Omega_c$, has so far been restricted to small values of u and v, i.e., when $\Omega \to \Omega_c$ according to Eq. (33). Ignoring the quartic term in Eq. (29) leads to a constant θ_m, representing a straight line in the u-v plane which the local minimum traverses as Ω varies. Including the quartic terms causes the valley in the energy landscape to curve, as seen in Fig. 3. In this section, we rederive the metastable state and its onset frequency Ω_m for larger values of u and v, keeping the quartic terms in the energy.

We first determine the equation governing the valley. The valley is a set of points, denoted here by $v(u)$, at which the change in the energy is extremum. We define $u = R\cos\eta$ and $v = R\sin\eta$ and write $\delta E' = E'(u + \delta u, v + \delta v) - E'(u, v) \simeq (\delta u\, \partial_u E' + \delta v\, \partial_v E')$. We find the direction that extremizes the change in the energy by keeping R constant while varying η; thus, $\delta u = -R\sin\eta\, \delta\eta$ and $\delta v = R\cos\eta\, \delta\eta$. Then, $\delta E'/\delta\eta = R(-\sin\eta\, \partial_u E' + \cos\eta\, \partial_v E') = 0$ which gives $\partial_v E'/\partial_u E' = \tan\eta = \delta v/\delta u$, where the last equality is just the slope of the tangent to the curve $v(u)$. Therefore, the differential equation for the bottom of the valley is

$$\frac{dv}{du} = \frac{\partial_v E'}{\partial_u E'} \quad \text{with} \quad v(u = 0) = 0. \qquad (47)$$

Its solution for $\Omega = \omega - \frac{3}{8}NV_0$ is the solid line in Fig. 3.
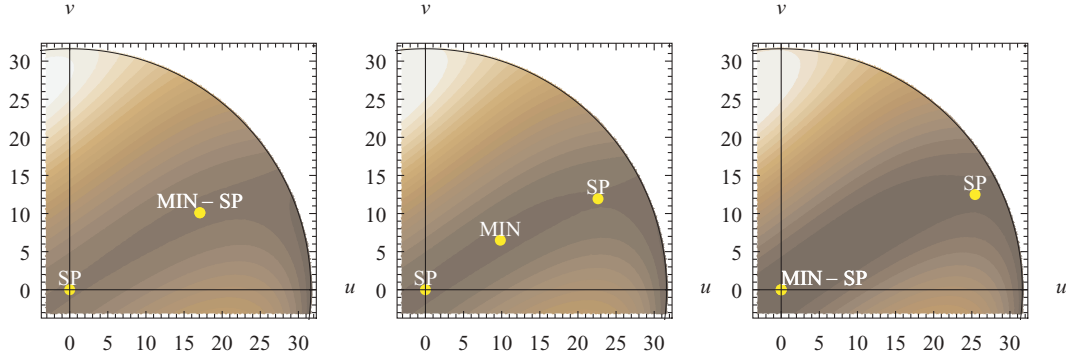
FIG. 4. (Color online) Energy landscapes for $\Omega = \omega - (2.1824/8)NV_0$, $\omega - (2.1094/8)NV_0$, and $\omega - (1/4)NV_0$ from left to right, for $N = 10^3$ and $NV_0 = 0.1$. The dots represent the critical points, with SP and MIN indicating the saddle-points and minima, respectively.

We rewrite $\tilde{E}'$ as $\zeta^2 A(\theta) + \zeta^4 B(\theta)$, where

$$A(\theta) = \frac{NV_0}{8}\big[\tilde{\Omega} + (3\cosh\theta - \sqrt{8}\sinh\theta)\big], \qquad (48)$$

$$B(\theta) = \frac{V_0}{128}\big[-15 + 4\cosh\theta - 21\cosh(2\theta) + 16\sqrt{2}\sinh(2\theta)\big], \qquad (49)$$

with $\tilde{\Omega} = (\Omega - \omega + \frac{1}{8}NV_0)/\frac{1}{8}NV_0$. At the critical points, $\partial_\zeta\tilde{E}' = \partial_\theta\tilde{E}' = 0$. The trivial solution, $\zeta = 0$, represents the center of the circle. Then, assuming $\zeta \neq 0$, we find

$$\frac{1}{A}\frac{\partial A}{\partial\theta} = \frac{1}{2B}\frac{\partial B}{\partial\theta}, \qquad (50)$$

which gives the critical points for all values of Ω.

For small Ω, the only critical point in the valley is at the origin. However, Fig. 4 shows that as Ω increases toward Ω_c, two other critical points (a saddle point and a minimum of the energy) appear in the valley. It is also evident that the minimum moves toward the center as Ω increases. Thus, there should be a rotation frequency, namely, the metastability frequency Ω_m, at which the saddle-point and the minimum lie on top of each other and, hence, the second derivative of the energy vanishes. Using Eq. (50), we find that at Ω_m,

$$\frac{1}{A}\frac{\partial^2 A}{\partial\theta^2} = \frac{1}{2B}\frac{\partial^2 B}{\partial\theta^2} - \left(\frac{1}{2B}\frac{\partial B}{\partial\theta}\right)^2. \qquad (51)$$

The single critical point (apart from the origin) at Ω_m satisfies both Eqs. (50) and (51). Dividing Eq. (51) by Eq. (50) leads to an equation for θ independent of any other variable, namely,

$$\frac{\partial^2 A/\partial\theta^2}{\partial A/\partial\theta} = \frac{\partial^2 B/\partial\theta^2}{\partial B/\partial\theta} - \frac{1}{2}\frac{\partial B/\partial\theta}{B}, \qquad (52)$$

with the solution $\cosh\theta_m \simeq 2.0776$ at Ω_m or, using Eq. (50), $\tilde{\Omega}_m \simeq -1.1824$. Therefore, the frequency at which the first metastable state appears is, in fact,

$$\Omega_m = \omega - \frac{2.1824}{8}NV_0, \qquad (53)$$

which is much closer to the critical frequency Ω_c compared to the frequency given by Eq. (35). Contour plots of energy for rotation frequencies Ω_m and Ω_c can be seen in the left and right panels of Fig. 4, showing that the saddle-point at

the origin (for $\Omega < \Omega_c$) turns into a minimum for $\Omega > \Omega_c$. Since the approximations of the previous section are valid for $\Omega \lesssim \Omega_c$, the minimum approaches the origin following the line $v = u/\sqrt{2}$, i.e., the slope of the valley at the origin is $1/\sqrt{2}$ near Ω_c.

The metastable state located at (u_m, v_m) represents two off-center vortices at the zeros of the condensate wave function $z_m^\pm$, where

$$\frac{v_m}{\sqrt{2}}z_m^{\pm 2} - \sqrt{N - (u_m^2 + v_m^2)}\,z_m^\pm - u_m = 0. \qquad (54)$$

The positions of the two roots of this equation as functions of Ω are plotted in Fig. 5 for the metastable regime, $\Omega_m \leqslant \Omega \leqslant \Omega_c$. Just as before, one vortex approaches the center of the trap while the other moves to infinity as Ω increases. However,
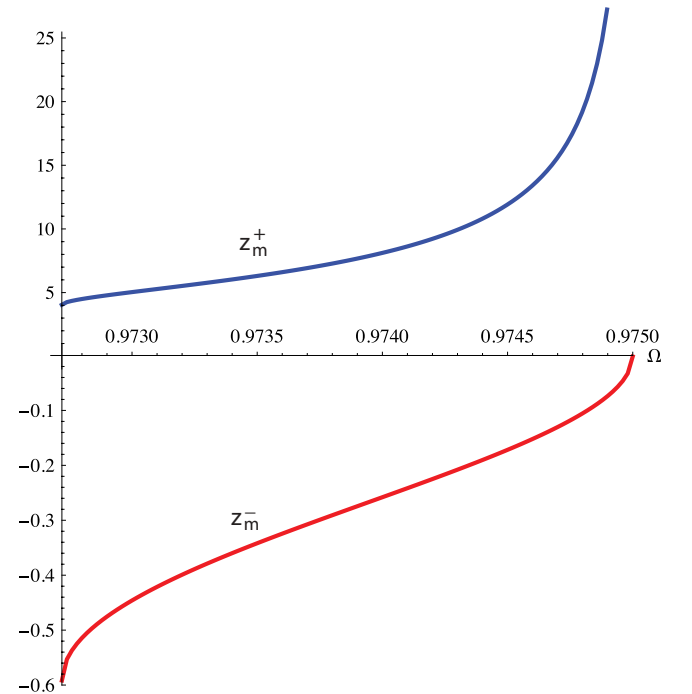

FIG. 5. (Color online) The position of the two off-center vortices for $N = 10^3$, $NV_0 = 0.1$, and $\Omega_m \leqslant \Omega \leqslant \Omega_c$. Note the different vertical scales for z_m^+ and z_m^-.

their initial positions are not symmetric with respect to the origin but are at $z_m^-(\Omega_m) = -0.5917$ and $z_m^+(\Omega_m) = +4.2506$ for the particular values of N and V_0 used in the figure. Since the vortices are stationary in the rotating frame, they precess around the origin with frequency Ω in the laboratory frame. Therefore, as seen in the laboratory frame, z_m^- spirals in toward the center of the trap, while z_m^+ spirals out to infinity as Ω increases.

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