Weakly interacting Bose-Einstein condensates under rotation

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We investigate the ground and low excited states of a rotating, weakly interacting Bose-Einstein condensed gas in a harmonic trap for a given angular momentum. Analytical results in various limits as well as numerical results are presented, and these are compared with those of previous studies. Within the mean-field approximation and for repulsive interaction between the atoms, we find that for very low values of the total angular momentum per particle, $L/N \to 0$, where $L\hbar$ is the angular momentum and N is the total number of particles, the angular momentum is carried by quadrupole ($|m|=2$) surface modes. For $L/N=1$, a vortexlike state is formed and all the atoms occupy the $m=1$ state. For small negative values of $L/N-1$, the states with $m=0$ and $m=2$ become populated, and for small positive values of $L/N-1$, atoms in the states with $m=5$ and $m=6$ carry the additional angular momentum. In the whole region $0 \leqslant L/N \leqslant 1$, we have strong analytic and numerical evidence that the interaction energy drops linearly as a function of L/N. We have also found that an array of singly quantized vortices is formed as L/N increases. Finally, we have gone beyond the mean-field approximation and have calculated the energy of the lowest state up to order N for small negative values of $L/N-1$, as well as the energy of the low-lying excited states.

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I. INTRODUCTION

One of the basic questions about Bose-Einstein condensates in trapped alkali-metal atom vapors [1] is how they behave under rotation. A lot of theoretical work has been done on this subject, both analytical and numerical [2–11], and the problem has been studied theoretically, both in the Thomas-Fermi limit of strong interactions [2–5] and in the limit of weak interactions [6–11], which we consider in this paper.

Wilkin *et al.* have considered [6] a weakly interacting Bose gas in a harmonic trap. For attractive interactions, they showed that in the lowest-energy state of a given angular momentum, the angular momentum is carried by the center-of-mass motion. For repulsive interactions, they studied especially the state with angular momentum per particle equal to $\hbar$ and, on the basis of numerical and other evidence, made a conjecture for the wave function. Butts and Rokhsar calculated numerically the moment of inertia of a weakly interacting trapped Bose gas with effective repulsive interactions [7]. One of us identified the elementary modes of excitation for small angular momentum and demonstrated in Ref. [8] that a system of rotating weakly interacting bosons exhibits two additional kinds of condensation associated with the nature of low-lying excitations. Bertsch and Papenbrock performed in Ref. [9] exact numerical diagonalization within the subspace of states with a given angular momentum that are degenerate in the absence of interactions, and they presented a conjecture for the wave functions and lowest eigenvalue for $2 \leqslant L \leqslant N$. Wilkin and Gunn [10] considered systems with $L > N$ and presented approximate structures for describing these wave functions. Finally, Linn and Fetter [11] examined the stability of a vortex in the limit of weak interactions. See also the note added in proof.

Experimentally, the detection of vortex states in a two-component system has been reported by Matthews *et al.* [12], while Madison *et al.* [13] have provided evidence for the formation of vortex states in a stirred one-component Bose-Einstein condensate.

Our basic goal in this study is to identify the lowest-energy states of a harmonically trapped, weakly interacting Bose gas for a given angular momentum L. As we show below, these states are selected by the interactions. In Sec. II, we describe the model and discuss the degeneracy of the many-body states for a given angular momentum in the absence of interactions. In Sec. III, we use the mean-field approximation to calculate the interaction energy, and derive numerical and analytical results under various conditions. In Sec. IV, we describe how one can go beyond the mean-field approximation and study as an example the specific case of small negative $L/N-1$. Finally, in Sec. V we give our conclusions.

II. THE MODEL

Our starting point is the Hamiltonian H, given by

$$H = H_0 + V. \tag{1}$$

Here

$$H_0 = \sum_i \left[-\frac{\hbar^2}{2M}\nabla_i^2 + \frac{1}{2}M\omega^2(x_i^2+y_i^2) + f(z_i) \right], \tag{2}$$

where M is the atomic mass, which includes the kinetic energy of the particles and their potential energy due to the trapping potential. The axis of rotation is taken to be the z axis, and the trapping potential is assumed to be that of an isotropic harmonic oscillator of frequency ω in the x-y plane. Our results do not depend on the trapping potential $f(z)$ in the z direction. The effective interaction V between atoms is assumed to be of zero range,

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$$V=\frac{1}{2}U_0\sum_{i\neq j}\delta(\mathbf{r}_i-\mathbf{r}_j), \tag{3}$$

where $U_0=4\pi\hbar^2a/M$ is the strength of the effective two-body interaction, with a being the scattering length for atom-atom collisions. We assume that the interaction is repulsive, $a>0$. Attractive interactions have been studied in Refs. [6] and [8].

Much theoretical work on rotating condensates has been done in the Thomas-Fermi limit of strong interactions, where the superfluid coherence length

$$\xi=(8\pi na)^{-1/2}, \tag{4}$$

n being the particle density, is much less than the size of the cloud. Under these conditions, the system is expected to exhibit properties much like those of liquid helium II [14]. Most experiments are performed in this regime. In this study, we examine the opposite limit of weak interactions, $nU_0 \ll \hbar\omega$ and $nU_0 \ll \Delta E_z$, where ΔE_z is the energy separation between the first excited state and the ground state for motion in the z direction. Under the above conditions,

$$\frac{\xi}{a_{\rm osc}}\sim\left(\frac{a_z}{Na}\right)^{1/2}, \tag{5}$$

where N is the number of atoms in the trap, $a_{\rm osc}=(\hbar/M\omega)^{1/2}$ is the oscillator length, and a_z is the characteristic length associated with the motion of the atoms in the z direction. Therefore, the coherence length is larger than the size of the cloud, and the situation is analogous to that for BCS pairing of nucleons in nuclei. In this regime, the interaction energy plays a dominant role in determining the character of eigenstates, whereas for strong coupling, the kinetic energy is important. This, together with the fact that the system is similar to ones encountered in other contexts, makes this regime an interesting one for theoretical studies.

Since we consider rotation around the z axis, the condition $nU_0 \ll \Delta E_z$ implies that the motion in this direction is frozen out and the problem is essentially two-dimensional. It is well known that for the harmonic-oscillator potential in two dimensions, the single-particle energies ϵ are given in the absence of interactions by

$$\epsilon=(2n_r+|m|+1)\hbar\omega, \tag{6}$$

where n_r is the radial quantum number and m is the quantum number corresponding to the angular momentum. In the lowest-energy state of the many-boson system, all particles are in states with $n_r=0$ and with m being zero or having the same sign as the total angular momentum. The energy of the lowest state of a system of noninteracting bosons with angular momentum L measured relative to that of the ground state is therefore

$$E=L\hbar\omega. \tag{7}$$

There is a huge degeneracy corresponding to the many different ways of distributing L quanta of angular momentum among N atoms. Interactions between the atoms lift the degeneracy. We incorporate the effect of the interactions in the mean-field approximation as well as by diagonalization within some appropriately chosen truncated space of degenerate states. We describe the two methods separately below.

III. MEAN-FIELD APPROXIMATION

We start with the mean-field Gross-Pitaevskii approach. Butts and Rokhsar have used this method to derive numerical results for the moment of inertia of a Bose gas [7]. In this scheme the many-body wave function with N particles and L units of angular momentum $\Psi_{L,N}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is taken to be the product of the single-particle states $\Psi(\mathbf{r}_i)$,

$$\Psi_{L,N}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\Psi(\mathbf{r}_1)\Psi(\mathbf{r}_2)\cdots\Psi(\mathbf{r}_N). \tag{8}$$

The single-particle state $\Psi(\mathbf{r}_i)$ can be expanded in terms of the harmonic-oscillator eigenstates $\Phi_m(\mathbf{r}_i)$:

$$\Psi(\mathbf{r}_i)=\sum_{m=0}^{\infty}c_m\Phi_m(\mathbf{r}_i), \tag{9}$$

where the c_m are variational parameters, which are complex in general and are functions of L. The summation in Eq. (9) is restricted to positive m, since states with negative m do not belong to the space of degenerate states. The quantity $|c_m|^2$ gives the occupation probability for state Φ_m. Also

$$\Phi_m(\mathbf{r})=\frac{1}{(m!\,\pi a_{\rm osc}^2)^{1/2}}g(z)\left(\frac{\rho}{a_{\rm osc}}\right)^{|m|}e^{im\phi}e^{-\rho^2/2a_{\rm osc}^2}. \tag{10}$$

Here ρ, z, and ϕ are cylindrical polar coordinates. In the above expression, we have assumed that the bosons are in the ground state $g(z)$ for motion in the z direction. The expectation value of the interaction energy V in the state given by Eq. (8) is

$$\langle V\rangle=\frac{1}{2}N(N-1)U_0\int|\Psi|^4d\mathbf{r}. \tag{11}$$

To find the lowest-energy state, we calculate $\langle V\rangle$ as a function of the variational parameters c_m, and minimize it with respect to them under the following two constraints: the normalization condition,

$$\sum_m|c_m^2|=1, \tag{12}$$

and the condition that the expectation value of the angular momentum per particle be fixed,

$$\sum_m m|c_m|^2=L/N. \tag{13}$$

The parameters c_m are complex in general, and therefore both their magnitudes and their phases need to be determined. However, Eqs. (12) and (13) impose two constraints on the magnitudes of the c_m. Furthermore, the overall phase of the wave function is arbitrary. Finally, the axial symmetry

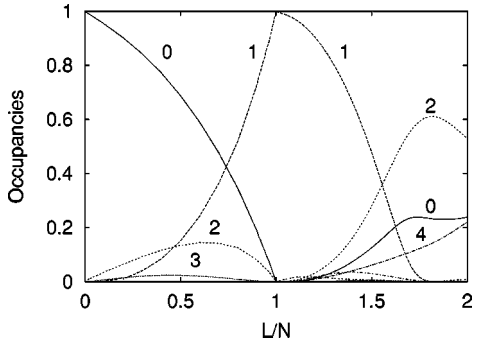

FIG. 1. The coefficients $|c_m|^2$ calculated numerically by minimizing the energy, as a function of L/N. The numbers refer to the corresponding states with angular momentum $m\hbar$. The two lowest curves in the region $L/N \approx 1.5$ give the occupancy of the $m=5$ (upper) and $m=6$ (lower) states.

of the confining potential implies that the origin of the angular coordinate is arbitrary, which corresponds to the condition for conservation of angular momentum, which holds even in the presence of interactions. Therefore, if the expansion (9) is truncated at a value $m_{\max}$, the number of independent real variables is $2\times(m_{\max}+1)-4=2(m_{\max}-1)$.

A. Numerical results

We have examined the problem numerically with $m_{\max}$ up to 9. The total number of terms in the expression for $\langle V\rangle$ is 125 in this case. The result of such a calculation with $m_{\max}=6$ is shown in Fig. 1 for $0\leqslant L/N\leqslant 2$.

We show the results with $m_{\max}=6$, since the occupancy of states with higher m is very low, and therefore including states with $m>6$ would not alter the results on this scale. Figure 2 shows the corresponding interaction energy and Fig. 3 shows lines of constant density, $|\Psi|^2=\text{const}$, for $L/N=0.1$, 0.6, 0.8, and 1.0. Figure 3 shows the gradual transition from mostly quadrupole, and to a lesser extent, octupole excitations, which are present at low angular momentum, to vortexlike structures as L approaches N. We should also mention that the structures in Fig. 3, as well as those in Fig. 4, rotate with an angular frequency Ω given by

$$\Omega=\frac{1}{\hbar}\frac{\partial E_{\text{tot}}}{\partial L}=\omega-\frac{1}{N\hbar}\frac{\partial\langle V\rangle}{\partial l}, \tag{14}$$

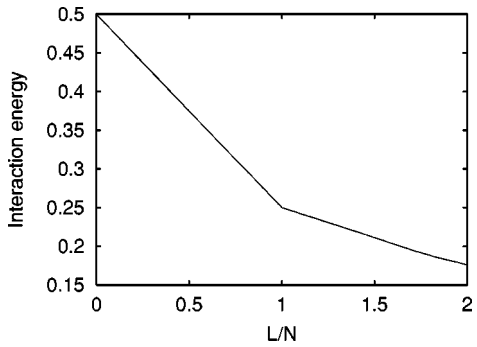

FIG. 2. The interaction energy, $\langle V\rangle$, in units of N^2v_0 as a function of L/N.

which is lower than the trap frequency ω. Here E_{tot} is the total energy of the system.

When L increases beyond N, the rotational invariance for $L/N=1$ is lost. Density contours for various values of L between N and $2.1N$ are shown in Fig. 4. These were calculated including states up to $m=6$. For $L\gtrsim 1.75N$, the optimal wave function has a twofold axis of symmetry, and the odd-m coefficients in the wave function vanish smoothly as the transition is approached, as shown in Fig. 1. There is a first-order transition from a state with twofold symmetry to one with threefold symmetry for $L\approx 2.03N$. The solution for $L/N=2.0$ with the states $m=0$, 2, 4, 6, and 8 considered has an energy $0.1757N^2v_0$, whereas the one with threefold symmetry, with $m=0$, 3, 6, and 9, has an energy $0.1761N^2v_0$. By contrast, for $L/N=2.1$ the state with threefold symmetry has an energy $0.1691N^2v_0$, which is lower than that of the solution with twofold symmetry, $0.1700N^2v_0$.

More generally, we have found that as L/N increases, the lowest-energy states are the ones where a vortex array is formed, in agreement with the results of Ref. [7].

B. Analytical results for $L/N\to 0$

We now turn to an analytic approach to the problem. One can systematically develop power-series expansions for the occupancies $|c_m|^2$ of the states, as well as for the energy in certain limits. We start with the case of very low angular momentum, $l=L/N\to 0$. Working in terms of quantum-mechanical states, one of us has calculated in Ref. [8] the difference in the energies of two states where in the one state all N particles have $m=0$ and in the other state a particle is promoted to the state with $m=\lambda$, and $N-1$ particles have $m=0$. If we denote the states by

$$|0^{N_0},1^{N_1},2^{N_2},\ldots\rangle, \tag{15}$$

where N_m is the number of particles with angular momentum $m\hbar$, the two states are $|0^N\rangle$ and $|0^{N-1},\lambda^1\rangle$. The difference ϵ_λ in the energy between these two states, which correspond to the energy of a 2^λ-pole excitation, is given by

$$\epsilon_\lambda=\lambda\hbar\omega-\left(1-\frac{1}{2^{\lambda-1}}\right)Nv_0+O(v_0), \tag{16}$$

where $v_0=U_0\int|\Phi_0|^4d\mathbf{r}$. One can easily see from Eq. (16) that at this level of approximation the excitations with the highest gain in interaction energy per unit of angular momentum are the ones with $\lambda=2$ or $\lambda=3$, i.e., quadrupole or octupole excitations.

We now calculate the interaction energy for low values of l. The calculation of the energies of elementary excitations indicates that one would expect quadrupole and octupole modes to be the most important ones for small l. To determine the most energetically favorable way of giving the system angular momentum, one has to identify the behavior of $|c_2|^2$ and $|c_3|^2$ as $l=L/N\to 0$, and then it is possible to build up a power-series expansion. Motivated by the fact that the $\lambda=2$ and 3 excitations are degenerate, and are the ones

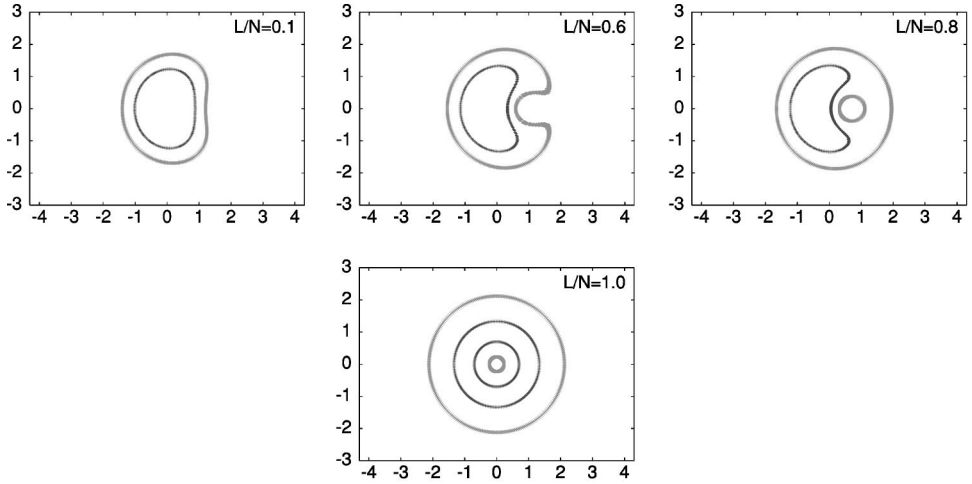

FIG. 3. Lines of constant density for $L/N=0.1$, 0.6, 0.8, and 1.0 in a plane perpendicular to the z axis. On the darker curves $|\Psi|^2=0.3n_0$, and on the lighter curves $|\Psi|^2=0.1n_0$, where $n_0=g(z)^2/\pi a_{\rm osc}^2$. The unit of length is the oscillator length $a_{\rm osc}$. These pictures show how a vortex enters the cloud of bosons as the angular momentum per particle increases.

which give the highest gain in energy per unit of angular momentum, we assume that both c_2 and c_3 are of order $l^{1/2}$. As we show below, the mode-mode interaction lifts this degeneracy, making the $\lambda=2$ mode dominant for low values of angular momentum.

It is instructive to give an explicit example, so let us examine the interaction energy up to order l^2. In order to minimize the interaction energy to this order, the states with $m=1$, 4, 5, and 6 need to be considered, in addition to those with $m=0$, 2, and 3, since the phases of off-diagonal terms, such as, for example, $|c_0||c_1||c_2||c_3|$, can be chosen to have a negative sign, and thus lower the energy as compared to the case where only c_0, c_2, and c_3 are nonzero. A useful formula for the matrix elements of the potential is

$$\int \Phi_k^*(\mathbf{r})\Phi_l^*(\mathbf{r})\Phi_m(\mathbf{r})\Phi_n(\mathbf{r})d\mathbf{r} = \delta_{k+l,m+n}\frac{(k+l)!}{2^{(k+l)}\sqrt{k!l!m!n!}}\int |\Phi_0(\mathbf{r})|^4 d\mathbf{r}. \quad (17)$$

As will become clear below, to calculate the energy up to order l^2 we must include the following terms:

$$\langle V\rangle = \left(\frac{1}{2}|c_0|^4+\frac{1}{2}|c_0|^2|c_2|^2+\frac{1}{4}|c_0|^2|c_3|^2+\frac{3}{16}|c_2|^4 + \frac{5}{32}|c_3|^4+\frac{5}{8}|c_2|^2|c_3|^2+|c_0|^2|c_1|^2 - \frac{\sqrt{3}}{2}|c_0||c_1||c_2||c_3|+\frac{1}{8}|c_0|^2|c_4|^2-\frac{\sqrt{6}}{8}|c_0||c_2|^2|c_4| + \frac{1}{16}|c_0|^2|c_5|^2-\frac{\sqrt{10}}{8}|c_0||c_2||c_3||c_5|+\frac{1}{32}|c_0|^2|c_6|^2 - \frac{\sqrt{5}}{16}|c_0||c_3|^2|c_6|\right)N^2v_0+O(Nv_0). \quad (18)$$

In the above expression we have chosen the phases ϕ_m of the variational coefficients c_m in such a way as to minimize $\langle V\rangle$, and in the specific example we can arrange them so that all the off-diagonal matrix elements are negative. One of the phases can have any value, and we make the choice $\phi_0=0$. The rest of them can be expressed in terms of, say, ϕ_1. We have found that up to $m=6$ $[m\neq 0]$, the expression

$$\phi_m = m\phi_1+(m+1)\pi \quad (19)$$

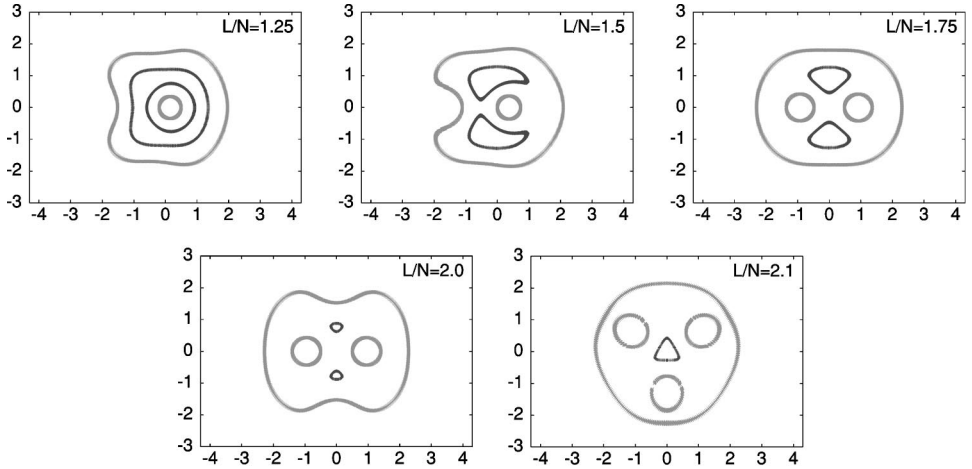

FIG. 4. Lines of constant density for $L/N=1.25$, 1.5, 1.75, 2.0, and 2.1 in a plane perpendicular to the z axis. On the darker curves $|\Psi|^2=0.3n_0$, and on the lighter curves $|\Psi|^2=0.1n_0$.

gives the lowest energy.

It is convenient to introduce the variable $X=|c_2|^2+|c_3|^2$, which is linear in l to leading order, and make use of the constraints given by Eqs. (12) and (13). One finds

$$|c_0|^2=1-X-|c_1|^2-|c_4|^2-|c_5|^2-|c_6|^2,$$
$$|c_2|^2=3X-l+|c_1|^2+4|c_4|^2+5|c_5|^2+6|c_6|^2, \quad (20)$$
$$|c_3|^2=l-2X-|c_1|^2-4|c_4|^2-5|c_5|^2-6|c_6|^2.$$

Then Eq. (18) takes the form

$$\langle V\rangle=\left(\frac{1}{2}-\frac{l}{4}-\frac{31}{16}X^2+\frac{13}{8}lX-\frac{9}{32}l^2+\frac{1}{4}|c_1|^2 - \frac{\sqrt{3}}{2}|c_1||c_2||c_3|+\frac{1}{8}|c_4|^2-\frac{\sqrt{6}}{8}|c_2|^2|c_4|+\frac{5}{16}|c_5|^2 - \frac{\sqrt{10}}{8}|c_2||c_3||c_5|+\frac{17}{32}|c_6|^2-\frac{\sqrt{5}}{16}|c_3|^2|c_6|\right)N^2v_0 + O(Nv_0). \quad (21)$$

The last four terms in the above equation can lower the energy to order l^2. For c_4, for example, the energy is minimized if [see the second line of Eq. (21)]

$$\frac{\partial}{\partial|c_4|}\frac{1}{8}|c_4|^2=\frac{\partial}{\partial|c_4|}\frac{\sqrt{6}}{8}|c_2|^2|c_4| \quad (22)$$

or

$$|c_4|=\frac{\sqrt{6}}{2}|c_2|^2\propto l. \quad (23)$$

Due to the nonzero value of c_4, the energy is lowered by an amount

$$\Delta\mathcal{E}=\left(\frac{1}{8}|c_4|^2-\frac{\sqrt{6}}{8}|c_2|^2|c_4|\right)N^2v_0=-\frac{3}{16}|c_2|^4N^2v_0 \propto l^2N^2v_0. \quad (24)$$

It is remarkable that the term $\Delta\mathcal{E}$ exactly cancels the term $3|c_2|^4/16$ in the first line of Eq. (18). In a similar way, c_1, c_5, and c_6 can be expressed in terms of c_2 and c_3 (and thus X), and Eq. (18) takes the form of the effective Hamiltonian,

$$\langle V\rangle=\left(\frac{1}{2}|c_0|^4+\frac{1}{2}|c_0|^2|c_2|^2+\frac{1}{4}|c_0|^2|c_3|^2+\frac{5}{34}|c_3|^4 - \frac{1}{4}|c_2|^2|c_3|^2\right)N^2v_0+O(Nv_0), \quad (25)$$

or equivalently

$$\langle V\rangle=\left[\frac{1}{2}-\frac{l}{4}+\frac{27}{17}\left(X-\frac{l}{2}\right)^2\right]N^2v_0+O(Nv_0). \quad (26)$$

Minimizing the above expression with respect to X, we find that $X=l/2$ and thus the angular momentum has to be carried by the $m=2$ state alone, since $|c_2|^2=l/2$ and $|c_3|^2=0$ up to terms linear in l. Also, the quadratic correction to $\langle V\rangle$ vanishes. Therefore, for $L/N\to 0$, the quadrupole ($\lambda=2$) excitations are dominant. This is one of the important conclusions of our study. We show in the Appendix that a diagrammatic perturbative expansion that assumes that only the states with $m=0$, 2, and 3 are occupied by a macroscopic number of particles, while all the other states are not (but still contribute to the energy), gives the same result. If one goes to higher order in l, the interaction energy has within the perturbative scheme a term of the form $|c_2|^3|c_3|^2$, which includes all the processes that convert three $\lambda=2$ excitations to two $\lambda=3$ excitations. This term can combine with the term $|c_3|^4$, which implies that it is possible that $|c_3|^2\propto|c_2|^3\propto l^{3/2}$, which actually turns out to be the case. Then c_1, for example, is given according to the second line of Eq. (21), by

$$|c_1|=\sqrt{3}|c_2||c_3|\propto l^{5/4}. \quad (27)$$

Using similar arguments we find that

$$|c_m|^2\propto l^{m/2} \quad \text{for} \quad m\neq 1 \quad \text{and} \quad |c_1|^2\propto l^{5/2}. \quad (28)$$

The leading terms in $|c_m|^2$ are given by

$$|c_0|^2=1-\frac{1}{2}l+\frac{1}{3}l^{3/2},$$
$$|c_1|^2=l^{5/2}+2l^3,$$
$$|c_2|^2=\frac{1}{2}l-l^{3/2},$$
$$|c_3|^2=\frac{2}{3}l^{3/2}, \quad (29)$$
$$|c_4|^2=\frac{3}{8}l^2-\frac{3}{2}l^{5/2}-\frac{1173}{816}l^3,$$
$$|c_5|^2=\frac{2}{15}l^{5/2}-\frac{4}{15}l^3,$$
$$|c_6|^2=\frac{1}{144}l^3,$$

and the corresponding interaction energy is

$$\langle V\rangle=\left[\frac{1}{2}-\frac{l}{4}+O(l^4)\right]N^2v_0+O(Nv_0). \quad (30)$$

The above equation is another basic result of our study, namely that the interaction energy drops linearly with the angular momentum up to the order we have examined, for $L/N\to 0$, in agreement with our numerical simulations and with those of Refs. [7] and [9].

C. Analytical results for $l \approx 1$

We now turn to the region $L/N \approx 1$. When the angular momentum per particle is exactly equal to 1, the lowest-energy state is the one where $|c_1|^2 = 1$, and corresponds to a vortex state. We consider the two cases $l < 1$ and $l > 1$ separately, starting with $l < 1$.

1. Analytical results for $l < 1$

The simplest way to create a state with $l < 1$ from that with $l = 1$ is to transfer particles from the $m = 1$ state to the $m = 0$ state. However, the energy can be even lower if also the $m = 2$ state is populated, because of the off-diagonal term $|c_0||c_1|^2|c_2|$. The interaction energy up to order $\overline{l} = 1 - L/N$ is found by minimizing the potential energy, retaining only the coefficients c_0, c_1, and c_2. This is

$$\langle V \rangle = \left(\frac{1}{4}|c_1|^4 + |c_0|^2|c_1|^2 + \frac{3}{4}|c_1|^2|c_2|^2 - \frac{\sqrt{2}}{2}|c_0||c_1|^2|c_2| \right) N^2 v_0 + O(N v_0), \tag{31}$$

where we have used the fact that for this case too the phases may be shown to be given by Eq. (19). Equation (19) is valid for small negative $L/N - 1$ at least up to $m = 4$. Thus in this limit

$$|c_0|^2 \propto |c_2|^2 \propto \overline{l}. \tag{32}$$

To obtain the coefficients of proportionality, it is convenient to use the following parametrization:

$$\begin{aligned} |c_0|^2 &= (1+\alpha)\overline{l}, \\ |c_1|^2 &= 1 - (1+2\alpha)\overline{l}, \\ |c_2|^2 &= \alpha \overline{l}, \end{aligned} \tag{33}$$

where α is a variational parameter. Minimizing the interaction energy in Eq. (31) with respect to α, we find that $\alpha = 1$. More generally, using similar arguments we find that to leading order

$$|c_m|^2 \propto \overline{l}^{|m-1|}, \tag{34}$$

and the explicit expressions for the coefficients are

$$\begin{aligned} |c_0|^2 &= 2\overline{l} - \frac{3}{2}\overline{l}^2, \\ |c_1|^2 &= 1 - 3\overline{l} + \frac{27}{8}\overline{l}^2, \\ |c_2|^2 &= \overline{l} - \frac{9}{4}\overline{l}^2, \\ |c_3|^2 &= \frac{3}{8}\overline{l}^2, \\ |c_4|^2 &= \frac{\overline{l}^3}{12}, \end{aligned} \tag{35}$$

and the interaction energy to order $\overline{l}^3$ is

$$\langle V \rangle = \left[\frac{1}{4} + \frac{\overline{l}}{4} + O(\overline{l}^4) \right] N^2 v_0 + O(N v_0). \tag{36}$$

The above equation implies that also in the region $l < 1$ the interaction energy varies linearly with the angular momentum to the order we have examined, which is also in agreement with the numerical simulations. The coefficient of the linear term is the same as the one we found for small values of the angular momentum.

Equations (30) and (36) as well as the numerical results (see Fig. 2) strongly suggest that the interaction energy $\langle V \rangle$ drops linearly as a function of L/N in the whole region $0 \leqslant L/N \leqslant 1$. The same result was derived by Butts and Rokhsar [7] numerically within the mean-field approximation. In Ref. [9], Bertsch and Papenbrock performed exact diagonalizations of degenerate states of a given L and found that up to machine accuracy the energy of the lowest state for a given L varies linearly with L in the range $2 \leqslant L \leqslant N$, in agreement with our analytic expansions. See also note added in proof.

2. Analytical results for $l > 1$

We turn now to the case $l > 1$. We calculate the difference in energy between the states $|1^N\rangle$ and $|1^{N-1}, (\lambda+1)^1\rangle$ by a method similar to that which for small l led to Eq. (16). The energy ϵ_λ of this 2^λ-pole excitation with $L = N + \lambda$, for $\lambda \ll N$, is given by

$$\epsilon_\lambda = \lambda \hbar \omega - \frac{1}{2}\left(1 - \frac{\lambda+2}{2^\lambda} \right) N v_0 + O(v_0). \tag{37}$$

This formula implies that for $l > 1$, the single-particle excitations with the lowest energy per unit of angular momentum are those with $\lambda = 4$ or 5, which means that the actual angular momentum carried by the particles is $m = 5$ or 6. In contrast to the low-angular-momentum case, here both $|c_5|^2$ and $|c_6|^2$ vary linearly with $\overline{l}$, $|c_5|^2 \propto |c_6|^2 \propto \overline{l}$, where $\overline{l} = L/N - 1$. In addition, in this regime we find that the energy has corrections of higher order than linear. Using similar arguments to those given before for small l, we find, to order $\overline{l}^2$,

$$\begin{aligned} |c_0|^2 &= 0.1213\overline{l}^2, \\ |c_1|^2 &= 1 - 0.2241\overline{l}, \\ |c_2|^2 &= 0.1934\overline{l}^2, \\ |c_5|^2 &= 0.1205\overline{l}, \\ |c_6|^2 &= 0.1036\overline{l}, \\ |c_9|^2 &= 1.7 \times 10^{-3}\overline{l}^2, \\ |c_{10}|^2 &= 1.3 \times 10^{-3}\overline{l}^2, \\ |c_{11}|^2 &= 8.6 \times 10^{-3}\overline{l}^2, \end{aligned} \tag{38}$$

and the interaction energy is

$$\langle V\rangle=\left[\frac{1}{4}-\frac{5\overline{l}}{64}+6.7\times10^{-3}\overline{l^2}+O(\overline{l^3})\right]N^2v_0+O(Nv_0). \tag{39}$$

If we compare the expressions (36) and (39) for the interaction energy, we see that there is a change in its slope, $\partial\langle V\rangle/\partial L$, as L passes N, from $-Nv_0/4$ for $L<N$ to $-5Nv_0/64$ for $L>N$.

D. Results for higher values of L/N

We mentioned earlier that as the angular momentum per particle increases even further, there are certain ranges of values of L/N over which the state with the lowest energy has a specific symmetry. The lowest value of L/N for which this occurs is ≈1.75 and the symmetry of the state is twofold, i.e., only $c_{2m}\neq0$. We have examined analytically as an example the case $L/N=2$. Keeping only the first three nonzero coefficients, which are the dominant ones, we find to order $\overline{l}=L/N-2$ that

$$\begin{aligned}|c_0|^2&=\beta(\overline{l})-\overline{l}/4,\\ |c_2|^2&=1-2\beta(\overline{l}),\\ |c_4|^2&=\beta(\overline{l})+\overline{l}/4,\end{aligned} \tag{40}$$

where

$$\beta(\overline{l})=\frac{3092-48\sqrt{6}}{12695}+\frac{17(64\sqrt{6}+109)}{10156}\overline{l}\approx0.2343+0.4449\overline{l}, \tag{41}$$

or

$$\begin{aligned}|c_0|^2&\approx0.2343+0.1949\overline{l},\\ |c_2|^2&\approx0.5314-0.8897\overline{l},\\ |c_4|^2&\approx0.2343+0.6949\overline{l},\end{aligned} \tag{42}$$

and the corresponding interaction energy is

$$\langle V\rangle=[A-B\overline{l}+C\overline{l^2}+O(\overline{l^3})]N^2v_0+O(Nv_0), \tag{43}$$

where

$$\begin{aligned}A&=\frac{3}{16}+\frac{\beta_0}{32}(7-4\sqrt{6})+\frac{\beta_0^2}{256}(64\sqrt{6}-109),\\ B&=\frac{1}{512}(4+85\beta_0),\end{aligned} \tag{44}$$

and $\beta_0=\beta(0)$. Numerically Eq. (43) is

$$\langle V\rangle\approx[0.1773-0.0467\overline{l}+0.0170\overline{l^2}+O(\overline{l^3})]N^2v_0+O(Nv_0). \tag{45}$$

Just beyond $L/N=2$ the lowest-energy state passes through a first-order phase transition and the slope of the interaction energy exhibits a small negative discontinuity. Figure 4 shows lines of constant density, $|\Psi|^2=\text{const}$, for $L/N=2$. The occurrence of two nodes in the density reflects the presence of two displaced vortices, and thus we see that the lowest-energy state of the system has two separated vortices and not a doubly quantized vortex. This clearly demonstrates the instability of the double-quantized vortex state to formation of two vortices plus surface waves.

IV. BEYOND THE MEAN-FIELD APPROXIMATION

Another way of approaching the problem of rotation is to diagonalize the Hamiltonian within the space of degenerate states. This approach goes beyond the mean-field approximation, since in mean-field theory the many-body wave function is a product of single-particle states, whereas more generally the true many-body state has correlations between the particles. This technique can be used by taking into account the whole set of states [9], but it is convenient and pedagogical to work in a restricted space, appropriately chosen.

As an example, we consider small negative $L/N-1$. From the analysis of Sec. III C we know that in this limit the states with $m=1$, 0, and 2 are dominant. Therefore, the eigenstates

$$|\mu,\tilde{l}\rangle=|0^{\tilde{l}+\mu},1^{N-\tilde{l}-2\mu},2^{\mu}\rangle \tag{46}$$

with N particles and $L=N-\tilde{l}$ units of angular momentum are expected to provide a good basis for describing the low-lying states for $\tilde{l}\ll N$. We restrict ourselves to this limit and demonstrate how one can derive an effective Hamiltonian which can be diagonalized exactly. In the limit we consider, $\tilde{l}$ is $\ll N$, and thus $\mu\sim\tilde{l}\ll N$. The diagonal matrix elements in the Hamiltonian are, up to terms of order N,

$$\langle\mu|V|\mu\rangle=\left(\frac{1}{4}N(N-1)+\frac{1}{2}\tilde{l}N+\frac{3}{4}\mu N\right)v_0, \tag{47}$$

and the off-diagonal matrix elements are

$$\langle\mu+1|V|\mu\rangle\approx\frac{\sqrt{2}}{4}Nv_0\sqrt{(\mu+\tilde{l}+1)(\mu+1)}. \tag{48}$$

Ignoring for the moment the (diagonal) first term of Eq. (47), which corresponds to the interaction energy of the state $|1^N\rangle$, we see from Eqs. (47) and (48) that we have to diagonalize the Hamiltonian

$$\tilde{H}=\left[\frac{1}{2}a_0^\dagger a_0+\frac{1}{4}a_2^\dagger a_2+\frac{\sqrt{2}}{4}(a_2^\dagger a_0^\dagger+a_2a_0)\right]Nv_0, \tag{49}$$

which can be done exactly by use of a Bogoliubov transformation. Here a_m is an annihilation operator that destroys a particle with angular momentum $m\hbar$. Introducing the operators c and d given by

$$c=a_0^\dagger+\sqrt{2}a_2 \quad\text{and}\quad d=\sqrt{2}a_0+a_2^\dagger, \tag{50}$$

we may write the Hamiltonian as

$$\tilde{H}=\frac{N}{4}(d^{\dagger}d-1)v_0. \tag{51}$$

Acting on states of the type (46), the operator $d^{\dagger}d-c^{\dagger}c$ is diagonal, and has an eigenvalue $N-L$. Therefore, $d^{\dagger}d$ can be eliminated and from Eq. (51) we obtain

$$\tilde{H}=\frac{N}{4}(N-L-1)v_0+\frac{Nv_0}{4}c^{\dagger}c. \tag{52}$$

The total interaction energy is thus the eigenenergy of $\tilde{H}$ plus the diagonal part $N(N-1)v_0/4$, or

$$\begin{aligned}\langle V\rangle&=\frac{N}{4}(N-1)v_0+\frac{N}{4}(N-L-1+\langle c^{\dagger}c\rangle)v_0+O(v_0)\\&=\frac{N(2N-L-2)}{4}v_0+\frac{1}{4}\langle c^{\dagger}c\rangle Nv_0+O(v_0).\end{aligned} \tag{53}$$

In the ground state $\langle c^{\dagger}c\rangle=0$, and the energy given by Eq. (53) is the same as that derived numerically in Ref. [9]. The presence of the term $\langle c^{\dagger}c\rangle$ in Eq. (53) implies that the excited states in this limit of small negative $L/N-1$ are separated from the ground state by an amount

$$\Delta E=\frac{N}{4}v_0+O(v_0). \tag{54}$$

We have also performed numerical diagonalization, and we have confirmed the above result (53), as well as Eq. (54). The average occupancy of single-particle states for the lowest-energy state and $L=N$ is

$$|c_1|^2=1-\frac{2}{N}+O\left(\frac{1}{N^2}\right),\quad |c_0|^2=|c_2|^2=\frac{1}{N}+O\left(\frac{1}{N^2}\right), \tag{55}$$

and thus in the limit $N\to\infty$ there is agreement between the mean-field approximation and the present one. The result of Eq. (55) is in agreement with Ref. [6], where the largest eigenvalue of the single-particle density matrix was found to be $1-2/N$. The two results gave identical answers because both studies considered only trial wave functions with no radial excitations, $n_r=0$, as is appropriate in the weak-interaction regime defined in Sec. II.

V. SUMMARY AND CONCLUSIONS

To summarize, we have studied the lowest-energy states of a system of rotating, weakly interacting harmonically trapped bosons. Within the mean-field approximation, for $L/N\to 0$ we find that the angular momentum is carried mainly by quadrupole ($|m|=2$) excitations. We have demonstrated that diagrammatic perturbation theory also leads to the same results as the method we have used here.

For $L/N=1$, the angular momentum is carried by particles in the $m=1$ state, while for small negative $L/N-1$ the $m=0$ and $m=2$ states are also populated. In the limits $L/N\to 0$ and $L/N\to 1$, the energy is a linear function of the angular momentum up to the order we have explored, while numerically this linearity persists in the whole region $0\leqslant L/N\leqslant 1$.

For small positive $L/N-1$, the states which carry the additional angular momentum are those with $m=5$ and $m=6$. In addition, as L passes N the derivative of the interaction energy with respect to the angular momentum changes abruptly. We have also found that for $L/N\approx 1.75$ there is a second-order phase transition and for $1.75\leqslant L/N\leqslant 2.03$ the lowest-energy state has twofold symmetry. At $L/N\approx 2.03$, there is a first-order phase transition to a state with threefold symmetry. More generally, for higher values of L/N a vortex array develops.

The Gross-Pitaevskii wave function is a power series in $\tilde{z}=x+iy$. Thus if one truncates the series at $m=m_{\max}$, the wave function will have $m_{\max}$ nodes. In the vicinity of a node at $\tilde{z}=\tilde{z}_0$, the wave function varies as $\tilde{z}-\tilde{z}_0$ and therefore each node corresponds to a singly quantized vortex having the same sense as the total angular momentum. It is instructive to study how the vortex lines move as the angular momentum is increased. For low angular momentum, the condensate wave function has only $m=0$ and $m=2$ components, and it is therefore proportional to $[1-(l^{1/2}/2)(\rho/a_{\rm osc})^2e^{2i\phi}]\exp(-\rho^2/2a_{\rm osc}^2)$ for the choice of $\phi_2=\pi$, according to Eq. (19) with $\phi_1=0$. This has vortices on the x axis at $x=\pm\sqrt{2}/l^{1/4}a_{\rm osc}$. With increasing angular momentum, components of the wave function with odd m grow, and the twofold symmetry of the cloud is broken, as may be seen in Fig. 3 for $L/N=0.1$, one of the vortices moving to larger distances and the other to smaller ones. The c_3 term leads to a third vortex at large distances from the origin. For $L/N=1$, there is only one vortex, which is at the origin. With further increase in L/N, the velocity field is at first still dominated by a vortex close to the origin, but subsequently a second vortex moves into the cloud until at $L/N\approx 1.75$ the twofold symmetry is restored. As L/N increases the distance between the two vortices does not change appreciably until $L/N\approx 2.03$ at which point the lowest-energy state changes discontinuously to a configuration of three vortices.

In this paper, we have also investigated effects not included in mean-field theory by diagonalizing a model Hamiltonian for L close to, but less than, N. We find that for $L=N$, the occupancy of the $m=1$ state is 1, with corrections of order $1/N$. We have calculated the energy up to terms of order N. Finally, we also found that the low-lying excited states are separated from the lowest state of the same angular momentum by energies of order Nv_0.

In this study, we have examined the limit of weak interactions. When the interaction energy per particle nU_0 becomes comparable to or greater than $\hbar\omega$, components of the wave function that are not members of the lowest multiplet in the absence of interaction must be included. Calculations for this regime based on the Gross-Pitaevskii equation have been carried out by Isoshima and Machida [15]. Comparison of our results with theirs is difficult because these authors calculated the lowest-energy state in a rotating frame, rather than the lowest-energy state for a given angular momentum.

One question of importance both conceptually and because of its relevance to experiment is whether or not the states are stable to small perturbations, and if they are not, what is the lifetime of the state. The answer to these questions depends on the nature of the perturbation, namely whether it is due to a deformation of the trap or to interactions with particles outside the condensate, and we shall discuss this elsewhere.

In our calculations above, we have shown for a particular example that the Gross-Pitaevskii approach gives correctly the contribution to the energy of order N^2. This result, which is alluded to in Ref. [7], is more general, and in another study [16] it has been shown how the Gross-Pitaevskii approach is recovered as the first term in an expansion in powers of $1/N$. The method may be extended to calculate contributions to the energy of order N, which are in excellent agreement with results obtained by numerical diagonalization of the Hamiltonian.

Note added in proof. In a recent paper [17] it has been demonstrated that the linear L dependence of the interaction energy for $2 \geqslant L \geqslant N$ exhibited in Fig. 2 and discussed in Secs. III and IV indeed corresponds to an eigenvalue of the Hamiltonian. In addition, two recent papers [18,19] provide proofs that this eigenvalue corresponds to the wave function proposed in [9]. It has not been possible, however, to prove that this eigenvalue is the lowest in energy.

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APPENDIX: PERTURBATION THEORY APPROACH

We show in this appendix that one can use perturbation theory to derive an effective Hamiltonian in the region $L/N \rightarrow 0$, corresponding to Eq. (25). We assume that only the states with $m=0$, 2, and 3 are macroscopically occupied. However, other states (the $m=1$, 4, 5, and 6 ones in this case) give corrections to the energy that can be treated perturbatively. Let us demonstrate how this works by considering the interaction energy up to order l^2. As long as both c_2 and c_3 vary as $l^{1/2}$, the only processes that contribute to the interaction energy up to l^2 are shown in Fig. 5.

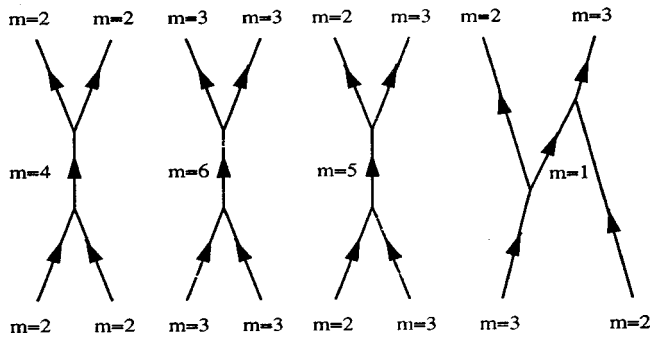

FIG. 5. The four diagrams contributing to the interaction energy to order l^2.

Let us consider the first process on the left as an example. The matrix element $\mathcal{M}$ corresponding to the vertex, where two particles with $m=2$ scatter to states with $m=0$ and $m=4$, is equal to

$$\mathcal{M} = \frac{\sqrt{6}}{16} N_2 \sqrt{N} v_0 . \tag{A1}$$

From Eq. (16) we find that the difference in the energy between the intermediate state and the initial state is

$$\delta\epsilon = -\frac{N v_0}{8} + O(v_0). \tag{A2}$$

In perturbation theory, the leading correction to the energy is given by

$$\frac{|\mathcal{M}|^2}{\delta\epsilon} = -\frac{3}{16} N_2^2 v_0 = -\frac{3}{16} |c_2|^4 N^2 v_0 , \tag{A3}$$

which is precisely the same as Eq. (24) (plus terms of order $N v_0$). Similarly, the other diagrams shown above give $-5|c_3|^4/544$, $-|c_2|^2|c_3|^3/8$, and $-3|c_2|^2|c_3|^2/4$ in units of $N^2 v_0$, respectively, and are identical to the corrections given by the terms in the last four lines of Eq. (18).

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