Low-lying excitations from the yrast line of weakly interacting trapped bosons

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Through an extensive numerical study, we find that the low-lying, quasidegenerate eigenenergies of weakly interacting trapped N bosons with total angular momentum L are given in the case of small L/N and sufficiently small L by $E = L\hbar\omega + g[N(N-L/2-1) + 1.59\,n(n-1)/2]$, where ω is the frequency of the trapping potential and g is the strength of the repulsive contact interaction. The last term arises from the pairwise repulsive interaction among n octupole excitations and describes the lowest-lying excitation spectra from the yrast line. In this case, the quadrupole modes do not interact with themselves and, together with the octupole modes, exhaust the low-lying spectra that are separated from others by energy gaps linear in N.

The yrast state, which is a subject of active research in nuclear physics [1], is the lowest-energy state of a system of particles for a given total angular momentum (AM). This state is important in that the whole of the excitation energy is used up for the rotation of the system and hence the system is at zero temperature, opening up the possibility of performing precise spectroscopic measurements of energy levels close to the yrast state. Recently, Mottelson [2] has pointed out that similar problems arise in rotating Bose-Einstein condensates (BECs) of trapped atomic vapor [3]. Two recent observations of vortices in trapped BECs [4] have lent a great impetus to theoretical studies of this subject [2,5–12].

The yrast state is obtained by distributing a given AM L over N bosons so as to minimize the total energy. When the trapping potential is harmonic, there would be a huge number of such partitions for $L \gg 1$ and hence a huge degeneracy were it not for the interactions [2]. The problem thus reduces to finding how a weak interaction lifts the degeneracy, selects the yrast state, and determines the low-lying excitations from this state. Wilkin *et al.* [6] have found that when the interaction is attractive, all the AM in the yrast state resides in the center-of-mass motion of the system. Mottelson [2] discussed that low-lying excitations are well described by collective modes whose excitation operators are given by

$$\hat{Q}_\lambda = \frac{1}{\sqrt{N\lambda!}} \sum_{p=1}^{N} (x_p + iy_p)^\lambda, \qquad (1)$$

where λ is an integer and x_p and y_p are the position operators of the pth particle. The corresponding excitation energy is given by [2]

$$\epsilon_\lambda = -2gN\left(1 - \frac{1}{2^{\lambda-1}}\right), \qquad (2)$$

where g denotes the strength of the contact interaction. Equation (2) suggests that for the case of attractive interactions (i.e., $g<0$), the AM of the yrast state is carried by the dipolar ($\lambda=1$) mode, in agreement with Ref. [6] while for the case of repulsive interactions it is carried by the quadrupole ($\lambda=2$) or octupole ($\lambda=3$) modes [2] as they have the greatest energy gain per unit of AM. A more elaborate study taking the mode-mode interaction into account has shown that the quadrupole modes have slightly larger energy gains than the octupole modes [7].

Bertsch and Papenbrock [9] have performed numerical diagonalization for small systems ($N=25$ and 50), finding that the energy of the yrast line for $L \le N$ can be given by $E = L\hbar\omega + gN(N-L/2-1)$, where ω is the frequency of the trapping potential. The corresponding eigenstate was very recently shown to exist [10] (see also Refs. [11,12]). This state partitions the AM equally among the particles [9,11,12] and smoothly crosses over to the many-body single vortex state [6] as L approaches N.

In this paper, we report on the results of our extensive numerical study of this system with up to 640 000 particles and for a total AM up to 30. Our primary finding is that of the *lowest-lying* excitation spectra from the yrast line that arise from the pairwise repulsive interaction between octupole modes; the corresponding interaction energy is given by $1.59\,gn(n-1)/2$, where n is the number of excited octupole modes [13]. These energy levels are separated from the other excitations including the one discussed in Ref. [7] by energy gaps linear in N. We have also found that for small L/N and sufficiently small L, all the many-body eigenstates have surprisingly large overlap (~ 0.99) with trial wave functions defined by

$$\prod_{\lambda=1}^{L} (\hat{Q}_\lambda)^{n_\lambda}|0\rangle \quad \text{with} \quad \sum_{\lambda=1}^{L} \lambda n_\lambda = L, \qquad (3)$$

where n_λ is a non-negative integer and $|0\rangle$ describes the exact many-body ground state of the system with $L=0$.

The model we study is the same as that of Refs. [6–9]. We consider a system of weakly interacting bosons subject

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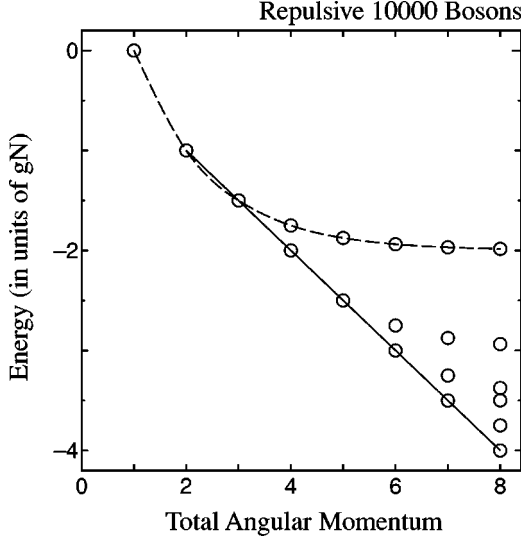
FIG. 1. The excitation spectra for $N=10\,000$ and $L \leq 8$. The energy is measured in units of gN and the yrast line is shown as a solid line. The collective excitations $\hat{Q}_\lambda |0\rangle$ ($\lambda \leq 8$) are linked by a dashed curve and their energy values are given in Table I. Except for the state $\hat{Q}_1|0\rangle$, the states that include excitations of the center-of-mass motion are omitted. Each state has a very large overlap (≥ 0.994) with the corresponding trial wave function. These states are given in the ascending order of energy as $\hat{Q}_1|0\rangle$ for $L=1$; $\hat{Q}_2|0\rangle$ for $L=2$; $\hat{Q}_3|0\rangle$ for $L=3$; $(\hat{Q}_2)^2|0\rangle$, $\hat{Q}_4|0\rangle$ for $L=4$; $\hat{Q}_2\hat{Q}_3|0\rangle$, $\hat{Q}_5|0\rangle$ for $L=5$; $(\hat{Q}_2)^3|0\rangle$, $(\hat{Q}_3)^2|0\rangle$, $\hat{Q}_2\hat{Q}_4|0\rangle$, $\hat{Q}_6|0\rangle$ for $L=6$; $(\hat{Q}_2)^2\hat{Q}_3|0\rangle$, $\hat{Q}_3\hat{Q}_4|0\rangle$, $\hat{Q}_2\hat{Q}_5|0\rangle$, $\hat{Q}_7|0\rangle$ for $L=7$; $(\hat{Q}_2)^4|0\rangle$, $\hat{Q}_2(\hat{Q}_3)^2|0\rangle$, $(\hat{Q}_2)^2\hat{Q}_4|0\rangle$, $(\hat{Q}_4)^2|0\rangle$, $\hat{Q}_3\hat{Q}_5|0\rangle$, $\hat{Q}_2\hat{Q}_6|0\rangle$, $\hat{Q}_8|0\rangle$ for $L=8$. The sets $[(\hat{Q}_2)^3|0\rangle, (\hat{Q}_3)^2|0\rangle]$ for $L=6$ and $[(\hat{Q}_2)^4|0\rangle, \hat{Q}_2(\hat{Q}_3)^2|0\rangle]$ for $L=8$ are quasidegenerate and these states are shown on or extremely near the yrast line.

to a given AM and trapped in a parabolic confining potential. The system is isotropic in the x-y plane and strongly confined in the z direction so that all the particles occupy the lowest-energy state in this direction. The problem is thus essentially two dimensional. The many-body Hamiltonian

TABLE I. Energies of the collective modes that are excited by acting on the ground state of $N=10\,000$ bosons with the excitation operator $\hat{Q}_\lambda$. The agreement with Eq. (2) is perfect (within the machine accuracy) for $\lambda \leq 3$ and excellent for $\lambda \geq 4$.

λ	1	2	3	4	5	6	7	8
ϵ_λ /gN	0	-1	$-3/2$	-1.7499	-1.8749	-1.9373	-1.9686	-1.9842

for this system can be written as $\hat{H} = \Sigma_i \hat{h}_i + \hat{V}$. Here $\hat{h}_i$ denotes the single-particle Hamiltonian for the ith particle,

$$\hat{h}_i = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2}\right) + \frac{M\omega^2}{2}(x_i^2 + y_i^2), \qquad (4)$$

where M is the mass of the boson, ω is the frequency of the trap, and $\hat{V} = (4\pi\hbar^2 \tilde{g}/M)\Sigma_{i<j}\delta^{(2)}(\mathbf{r}_i - \mathbf{r}_j)$ describes the interaction between particles ($\tilde{g}$ is the dimensionless "scattering length"). In this paper we consider the case of $\tilde{g}>0$, i.e., repulsive interactions.

The single-particle spectrum is given by $E_{n,m} = \hbar\omega(2n + |m| + 1)$, where n and m denote the radial and AM quantum numbers, respectively. When only low-lying states of the many-boson system are concerned, we may assume that all the particles are in states with $n=0$. The single-particle states are then labeled only by m and described by $\phi_m(z) = (z^m/\sqrt{\pi m!})\exp(-|z|^2/2)$, where $z \equiv x+iy$, and the lengths are measured in units of $(\hbar/M\omega)^{1/2}$. We use these single-particle states as a basis set to rewrite the many-body Hamiltonian as

$$\hat{H} = \hbar\omega\sum_{m \geq 0} m\, b_m^\dagger b_m + g\sum_{m_1 \sim m_4} V_{m_1 m_2 m_3 m_4}\, b_{m_1}^\dagger b_{m_2}^\dagger b_{m_3} b_{m_4}, \qquad (5)$$

where $g \equiv \tilde{g}\hbar\omega$, the operators b_m and $b_m^\dagger$ annihilate and create one boson in the single-particle state ϕ_m, respectively, and $V_{m_1 m_2 m_3 m_4}$ is the two-body matrix element given as [9]

TABLE II. Values of the overlap integrals between the numerically found low-lying quasidegenerate states with $N=10\,000$ for various values of L and the corresponding normalized trial wave functions (shown below each value of the overlap). These values are close to unity for small L/N and sufficiently small L.

	Lowest	First excited	Second excited	Third excited	Fourth excited	Fifth excited
$L=9$	0.9951	0.9977				
	$(\hat{Q}_2)^3\hat{Q}_3|0\rangle$	$(\hat{Q}_3)^3|0\rangle$				
12	0.9804	0.9815	0.9959			
	$(\hat{Q}_2)^6|0\rangle$	$(\hat{Q}_2)^3(\hat{Q}_3)^2|0\rangle$	$(\hat{Q}_3)^4|0\rangle$			
15	0.9820	0.9846	0.9936			
	$(\hat{Q}_2)^6\hat{Q}_3|0\rangle$	$(\hat{Q}_2)^3(\hat{Q}_3)^3|0\rangle$	$(\hat{Q}_3)^5|0\rangle$			
18	0.9374	0.9363	0.9812	0.9906		
	$(\hat{Q}_2)^9|0\rangle$	$(\hat{Q}_2)^6(\hat{Q}_3)^2|0\rangle$	$(\hat{Q}_2)^3(\hat{Q}_3)^4|0\rangle$	$(\hat{Q}_3)^6|0\rangle$		
30	0.7674	0.7447	0.9105	0.9418	0.9593	0.9735
	$(\hat{Q}_2)^{15}|0\rangle$	$(\hat{Q}_2)^{12}(\hat{Q}_3)^2|0\rangle$	$(\hat{Q}_2)^9(\hat{Q}_3)^4|0\rangle$	$(\hat{Q}_2)^6(\hat{Q}_3)^6|0\rangle$	$(\hat{Q}_2)^3(\hat{Q}_3)^8|0\rangle$	$(\hat{Q}_3)^{10}|0\rangle$

$$V_{m_1 m_2 m_3 m_4} = \frac{\delta_{m_1+m_2, m_3+m_4} (m_1+m_2)!}{2^{m_1+m_2} \sqrt{m_1! \, m_2! \, m_3! \, m_4!}}. \quad (6)$$

Given a total AM L, the state may be spanned by the Fock states $|n_0, n_1, \ldots, n_L\rangle$ with $\Sigma_{i=0,L} n_i = N$ and $\Sigma_{j=0,L} j n_j = L$, where n_i denotes the occupation number of the ith single-particle state ϕ_i, i.e., $b_i^\dagger b_i |n_0, n_1, \ldots, n_L\rangle = n_i |n_0, n_1, \ldots, n_L\rangle$. Numerical diagonalization of the two-body interaction $\hat{V}$ is performed within the Hilbert subspace subject to these constraints.

The energy eigenvalue corresponding to the ith many-body eigenstate with total AM L may be written as $L\hbar\omega + \epsilon_{L,i}$, where $\epsilon_{L,i}$ denotes the interaction energy. Because the lowest-energy eigenvalue with total AM L ($2 \leq L \leq N$) is given by $\epsilon_L = gN(N - L/2 - 1)$, the unique state with $L=0$, which is composed of N bosons in a single-particle state ϕ_0 is the ground state for $gN \ll \hbar\omega$, and it will therefore be denoted as $|0\rangle$. Our trial wave functions are constructed by acting on the ground state $|0\rangle$ with the collective operators $\{\hat{Q}_\lambda\}$ whose second quantized forms are given by $\hat{Q}_\lambda = (1/\sqrt{N}) \Sigma_m \sqrt{(m+\lambda)!/m! \lambda!} \, b_{m+\lambda}^\dagger b_m$.

Figure 1 shows the energy spectra for $N = 10\,000$ and $L \leq 8$, where the energy is measured in units of gN. Our numerical results show that all the energy eigenstates for $L \leq 8$ have remarkably large overlaps (≥ 0.994) with the corresponding trial wave functions given in Eq. (3). Among the eigenstates, only "intrinsic" ones, i.e., those that do not include dipole excitations, are shown in Fig. 1 (the only exception being the state $\hat{Q}_1|0\rangle$ for $L=1$) as the dipole mode
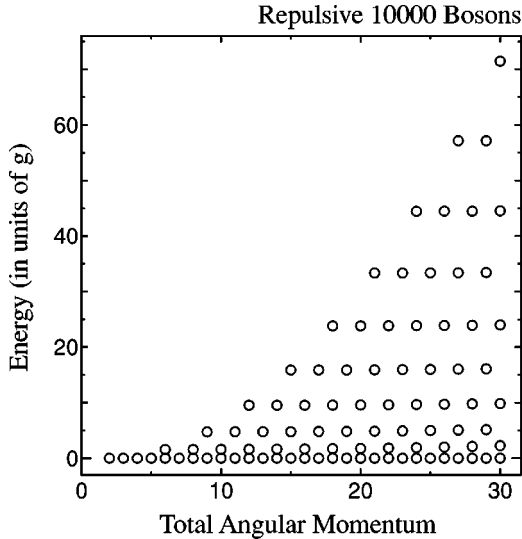
Repulsive 10000 Bosons

FIG. 2. The low-lying, quasidegenerate eigenstates for $N = 10\,000$ and $2 \leq L \leq 30$ are shown by open circles. These states are well described by the quadrupole and octupole excitation modes as seen in Table II. These energy values, which are measured from the yrast line, are well described by $1.59 \times n(n-1)/2$ in units of g. Here, n is the number of excited octupole modes. As the total AM increases, the interconversion between these two modes becomes apparent (see Table V), which is also suggested by the level repulsion between the lowest and first-excited states for larger L.

TABLE III. The deviations of overlap integrals from unity are shown for $N = 5000, 10\,000, 20\,000$ and $L = 6, 8, 10, 12, 14, 16, 18$ where each overlap integral is the one between a normalized trial wave function with n quadrupole excitations [i.e., $\propto (\hat{Q}_2)^n |0\rangle$] and a numerically obtained lowest-energy state for $L = 2n$ (n an integer). These values seem to include not only a factor of L/N but also another factor like L^s ($s \sim 2$) for small L.

	$L=6$	8	10	12	14	16	18
$N=5000$	0.0049	0.0117	0.0227	0.0385	0.0596	0.0861	0.1179
10 000	0.0025	0.0059	0.0115	0.0196	0.0307	0.0450	0.0626
20 000	0.0012	0.0030	0.0058	0.0099	0.0156	0.0230	0.0323

corresponds to the center-of-mass motion that does not affect the interaction in a harmonic trap. For example, for $L=6$ only the intrinsic eigenstates $(\hat{Q}_2)^3|0\rangle$, $(\hat{Q}_3)^2|0\rangle$, $\hat{Q}_2\hat{Q}_4|0\rangle$, and $\hat{Q}_6|0\rangle$ are shown among all the eigenstates for $L=6$ and they are identified in the ascending order of energy as $(\hat{Q}_2)^3|0\rangle$, $(\hat{Q}_3)^2|0\rangle$, $\hat{Q}_2\hat{Q}_4|0\rangle$, $\hat{Q}_1\hat{Q}_2\hat{Q}_3|0\rangle$, $(\hat{Q}_1)^2(\hat{Q}_2)^2|0\rangle$, $\hat{Q}_6|0\rangle$, $\hat{Q}_1\hat{Q}_5|0\rangle$, $(\hat{Q}_1)^2\hat{Q}_4|0\rangle$, $(\hat{Q}_1)^3\hat{Q}_3|0\rangle$, $(\hat{Q}_1)^4\hat{Q}_2|0\rangle$, and $(\hat{Q}_1)^6|0\rangle$. We should note here that two states $(\hat{Q}_2)^3|0\rangle$ and $(\hat{Q}_3)^2|0\rangle$ are seen as "a single circle" in Fig. 1 due to their *quasidegeneracy*. The energy difference between them is caused by mode-mode interactions and is on the order of g [2,7,12]. Two states $(\hat{Q}_2)^4|0\rangle$ and $\hat{Q}_2(\hat{Q}_3)^2|0\rangle$ for $L=8$ are also quasidegenerate. The yrast line is shown by a solid line in Fig. 1 and the other states are separated from this line by energy gaps roughly equal to or greater than $gN/4$. The energy difference $gN/4$ corresponds to the replacement of the factor $(\hat{Q}_2)^2$ included in the yrast states with $\hat{Q}_4$.

In Fig. 1, the collective excitations discussed by Mottelson, $\hat{Q}_\lambda|0\rangle$ ($\lambda = 1, 2, \ldots, 8$), are linked by a dashed curve. The energies of these states are given in Table I. These values are very well described by Eq. (2); in particular, for $\lambda \leq 3$ the agreement is perfect within the machine accuracy [9].

For higher (but not very large) AM, the low-lying states are again well described by the collective excitations. In particular, the quadrupole ($\lambda = 2$) and octupole ($\lambda = 3$) modes describe well the low-lying, quasidegenerate states as shown in Table II. These quasidegenerate states for $2 \leq L \leq 30$ are shown in Fig. 2 where the energies are measured from the yrast line and are of the order of g. We note that the other

TABLE IV. Energies (in units of g) of the low-lying quasidegenerate states with $L=18$ for various values of N. They are measured from the yrast line. As the ratio L/N becomes small, the convergence of these energies can be seen.

	$N=10\,000$	40 000	160 000	640 000
First excited	1.721	1.622	1.597	1.590
Second excited	9.564	9.538	9.532	9.530
Third excited	23.82	23.82	23.82	23.82

TABLE V. Values of the overlap integrals between the lowest/first-excited states and some trial wave functions for $N = 10\,000$ and $L = 30$. The interconversion between the quadrupole and octupole modes makes a much larger contribution to the yrast state than other modes such as $\hat{Q}_4$.

	$(\hat{Q}_2)^{15}|0\rangle$	$(\hat{Q}_2)^{12}(\hat{Q}_3)^2|0\rangle$	$(\hat{Q}_2)^9(\hat{Q}_3)^4|0\rangle$	$(\hat{Q}_2)^{13}\hat{Q}_4|0\rangle$	$(\hat{Q}_2)^{10}(\hat{Q}_3)^2\hat{Q}_4|0\rangle$
Lowest	0.7674	0.5307	0.1045	0.1338	0.0737
First excited	0.5400	0.7447	0.1928	0.0937	0.1035

excitations are separated from these in Fig. 2 by energy gaps linear in N ($\gtrsim gN/4$).

However, the overlap integrals between the collective trial wave functions and the numerically obtained low-lying eigenstates become small even for small L/N as L increases. In fact, in Table III, the deviations of these overlaps from unity seem to include not only a factor of L/N but also another factor like L^s ($s \sim 2$) for small L. Thus these trial wave functions describe the low-lying states well for small L/N and sufficiently small L.

Moreover, for small L/N and sufficiently small L, the energies of these quasidegenerate states are found to be described by $1.59gn(n-1)/2$, where n is the number of excited octupole modes in each state [13,14]. This energy ''quantization'' can also be seen in the data for $N = 640\,000$ and $L = 18$ in Table IV as $1.590 \approx 1.59 \times 2(2-1)/2$, $9.530 \approx 1.59 \times 4(4-1)/2$, and $23.82 \approx 1.59 \times 6(6-1)/2$. Here, 2, 4, and 6 are the number of excited octupole modes in the first, second, and third excited states for $L = 18$, as seen in Table II.

These results show that the quadrupole modes do not interact with themselves or with the octupole mode in the limit of $L/N \to 0$ while the octupole modes undergo a pairwise repulsive interaction. Although the mode-mode interactions were discussed in Refs. [2,7,12], such concrete quasiparticle features of these modes were not pointed out previously. Because of such quasiparticle features, the yrast states are well described by $(\hat{Q}_2)^n|0\rangle$ for even L and by $(\hat{Q}_2)^{n'}\hat{Q}_3|0\rangle$

for odd L in that limit (n, n' are integers). The lowest energy for sufficiently small AM L is therefore simply given by the sum of the excitation energies of the quadrupole modes (and the energy of an octupole mode for odd L).

As the total AM increases, however, the interconversion between these two modes becomes significant. This is seen in Table V and is also suggested by the level repulsion between the lowest and first-excited states for larger L in Fig. 2. Although contributions by the modes $\hat{Q}_4$, $\hat{Q}_5$, and $\hat{Q}_6$ to the yrast states have been claimed [7], the interconversion between modes $\hat{Q}_2$ and $\hat{Q}_3$ makes a greater contribution than these three modes, as seen in Table V.

Whereas the yrast state is analytically given for $L \lesssim N$ [11,12], its relations to collective excitations for small L/N and sufficiently small L (especially the interconversion effects between the quadrupole and octupole modes) remain unclear. An understanding of these relations may help us clarify the integrability in a two-dimensional Bose system with a harmonic potential that includes weak repulsive δ-function interactions or a hidden symmetry of the Hamiltonian [15].

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