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, quasi-degenerate eigenenergies of weakly-interacting trapped $N$ bosons with total angular momentum $L$ are given in case of small $L/N$ and sufficiently small $L$ by $E = L\hbar\omega + g[N(N - L/2 - 1) + 1.59n(n - 1)/2]$, where $\omega$ 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 $N$-linear energy gaps.

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 $^2$ $^5$ $^6$ $^7$.

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 large number of such partitions for $L \gg 1$ and hence a huge degeneracy, were it not for the interactions $^8$ $^9$. 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

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

where $\lambda$ is an integer, and $x_p$ and $y_p$ are the position operators of the $p$-th particle. The corresponding excitation energy is given by $^2$

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

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 $^2$.

Bertsch and Papenbrock $^9$ have performed numerical diagonalization for small systems ($N = 25$ and $50$), finding that the energy of the Yrast line for $L \leq N$ can be given by $E = L\hbar\omega + gN(N - L/2 - 1)$, where $\omega$ is the frequency of the trapping potential. The corresponding eigenstate was very recently shown to exist $^9$ (see also Refs. $6$ $7$ $8$). This state partitions the AM equally among the particles $6$ $7$ $8$ 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 640000 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 energy gain is given by $1.59gn(n - 1)/2$, 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. $6$, by $N$-linear energy gaps. We have also found that for small $L/N$ and sufficiently small $L$ all the many-body eigenstates have surprisingly large overlap ($\sim 0.99$) with trial wavefunctions defined by

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

where $n_\lambda$ 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. $6$ $7$ $8$. We consider a system of weakly-interacting bosons subject to a given AM and trapped in a parabolic confining...
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create one boson in the single-particle state described by \(\phi\).

We may assume that all the particles are in states with \(|\bar{z}\rangle\) of the trap, and \(\hat{m}\) describes the interaction between particles \((\bar{g}\) is the dimensionless ‘scattering length’). In this paper we consider the case of \(\bar{g} > 0\), 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 \(\phi_m(z) = \left(z^m/\sqrt{\pi m!}\right)\exp(-|z|^2/2)\), 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

\[
\hat{H} = \hbar\omega \sum_{m \geq 0} m b_m^\dagger b_m + g \sum_{m_1 \sim m_4} V_{m_1m_2m_3m_4} b_{m_1}^\dagger b_{m_2} b_{m_3} b_{m_4},
\]

where \(g \equiv \bar{g}\hbar\omega\), the operators \(b_m\) and \(b_m^\dagger\) annihilate and create one boson in the single-particle state \(\phi_m\), respectively, and \(V_{m_1m_2m_3m_4}\) is the two-body matrix element given as

\[
V_{m_1m_2m_3m_4} = \frac{\delta_{m_1+m_2,m_3+m_4}(m_1 + m_2)!}{2m_1!m_2!m_3!m_4!} \sqrt{m_1!m_2!m_3!m_4!}.
\]

Given a total AM \(L\), the state may be spanned by the Fock states \(|n_0, n_1, \ldots, n_L\rangle\) with \(\sum_{i=0}^{L} n_i = N\) and \(\sum_{j=0}^{L} j n_j = L\), where \(n_i\) denotes the occupation number of the \(i\)-th single particle state \(\phi_i\), i.e., \(b_i^\dagger b_i|n_0, n_1, \ldots, n_L\rangle = |n_0, n_1, \ldots, n_L\rangle\). 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 \(i\)-th 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 \(\phi_0\), is the ground state for \(gN \ll \hbar\omega\), and it will therefore be denoted as \(|0\rangle\). Our trial wavefunctions are constructed by acting on the ground state \(|0\rangle\) with the collective operators, \(|Q_\lambda\rangle\), whose second quantized forms are given by \(Q_\lambda = (1/\sqrt{N}) \sum_m \sqrt{(m + \lambda)!/m!\lambda!} b_{m+\lambda}^\dagger b_m\).

Figure 1 shows the excitation spectra for \(N = 10000\) and \(L \leq 8\), where the energy is measured in units of \(gN\). The Yrast line is shown as a solid line. The collective excitations, \(Q_\lambda|0\rangle\) \((\lambda \leq 8)\), are linked by a dashed curve, and their energy values are given in Table I. Except for the state \(|Q_1\rangle\), the states that include excitations of the center-of-mass motion are omitted. Each state has a very large overlap \((\geq 0.994)\) with the corresponding trial wavefunction. These states are given in the ascending order of energy as \(|Q_1\rangle\) for \(L = 1\); \(|Q_2\rangle\) for \(L = 2\); \(|Q_3\rangle\) for \(L = 3\); \(|Q_4\rangle\) for \(L = 4\); \(|Q_5\rangle\) for \(L = 5\); \(|Q_6\rangle\) for \(L = 6\); \(|Q_7\rangle\) for \(L = 7\); \(|Q_8\rangle\) for \(L = 8\). The sets, \(|Q_1\rangle, |Q_2\rangle, |Q_3\rangle\) for \(L = 6\) and \(|Q_1\rangle, |Q_2\rangle, |Q_3\rangle\) for \(L = 8\), are quasi-degenerate, and these states are shown on or extremely near the Yrast line.

![FIG. 1. The excitation spectra for N = 10000, L ≤ 8. The energy is measured in units of gN, and the Yrast line is shown as a solid line. The collective excitations, Q_λ|0\rangle (λ ≤ 8), are linked by a dashed curve, and their energy values are given in Table I. Except for the state 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 wavefunction. These states are given in the ascending order of energy as Q_1|0\rangle for L = 1; Q_2|0\rangle for L = 2; Q_3|0\rangle for L = 3; Q_4|0\rangle for L = 4; Q_5|0\rangle for L = 5; Q_6|0\rangle for L = 6; Q_7|0\rangle for L = 7; Q_8|0\rangle for L = 8. The sets, [Q_1|0\rangle, Q_2|0\rangle, Q_3|0\rangle] for L = 6 and [Q_1|0\rangle, Q_2|0\rangle, Q_3|0\rangle] for L = 8, are quasi-degenerate, and these states are shown on or extremely near the Yrast line.](image-url)
for \( L = 8 \) are also quasi-degenerate. 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 \( Q_4 \).

In Fig. 1, the collective excitations discussed by Mottelson, \( Q_\lambda|0\) \((\lambda = 1, 2, \ldots, 8)\), 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.

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 well describe the low-lying, quasi-degenerate states as shown in Table I. These quasi-degenerate states for \( 2 \leq L \leq 30 \) are shown in Fig. 2, where the energies are measured from the Yrast line and are on the order of \( g \). We note that the other excitations are separated from these in Fig. 2 by \( N \)-linear energy gaps (\( \geq gN/4 \)).

However, the overlap integrals between the collective trial wavefunctions and the numerically-obtained low-lying eigenstates become small even for small \( L/N \) as \( L \) increases. In fact, in Table I, 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 wavefunctions 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 quasi-degenerate states are found to be described by \( 1.59 \times n(n-1)/2 \), where \( n \) is the number of excited octupole modes in each state \( |\lambda\rangle \). This energy ‘quantization’ can also be seen in the data for \( N = 640000 \), \( L = 18 \) in Table I as \( 1.590 \simeq 1.59 \times 2(2-1)/2 \), \( 9.530 \simeq 1.59 \times 4(4-1)/2 \) and \( 23.82 \simeq 1.59 \times 6(6-1)/2 \). 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 I.

These results show that the quadrupole modes do not interact with themselves or with the octupole mode in the limit of \( L/N \rightarrow 0 \), while the octupole modes undergo a pairwise repulsive interaction. Although the mode-mode interactions were discussed in Refs. 2, 3, 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 \((n, n': \) 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 \( L \). Whereas the Yrast state is analytically given for \( L \leq N \), 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 delta-function interactions or a hidden symmetry of the Hamiltonian.
TABLE I. Energies of the collective modes that are excited by acting on the ground state of \(N = 10000\) bosons with the excitation operator \(Q_\lambda\). The agreement with eq. (2) is perfect (within the machine accuracy) for \(\lambda \leq 3\) and excellent for \(\lambda \geq 4\).

| \(\lambda\) | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|---|---|---|---|---|---|---|---|---|
| \(\epsilon_\lambda/gN\) | 0  | -1 | -3/2 | -1.7499 | -1.8749 | -1.9373 | -1.9686 | -1.9842 |

TABLE II. Values of the overlap integrals between the numerically found low-lying quasi-degenerate states with \(N = 10000\) for various values of \(L\) and the corresponding normalized trial wavefunctions (shown on the second line in each cell). These values are close to unity for small \(L/N\) and sufficiently small \(L\).
TABLE III. The deviations of overlap integrals from unity are shown for $N = 5000, 10000, 20000$ and $L = 6, 8, 10, 12, 14, 16, 18$, where each overlap integral is the one between a normalized trial wavefunction with $n$ quadrupole excitations (i.e., $\propto (\hat{Q}_2)^n|0\rangle$) and a numerically-obtained lowest-energy state for $L = 2n$ ($n$: 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 $L$.

| $N$   | $L = 6$ | $8$ | $10$ | $12$ | $14$ | $16$ | $18$ |
|-------|---------|-----|-----|-----|-----|-----|-----|
| $5000$| 0.0049  | 0.0117| 0.0227| 0.0385| 0.0596| 0.0861| 0.1179|
| $10000$| 0.0025  | 0.0059| 0.0115| 0.0196| 0.0307| 0.0450| 0.0626|
| $20000$| 0.0012  | 0.0030| 0.0058| 0.0099| 0.0156| 0.0230| 0.0323|

TABLE IV. Energies (in units of $g$) of the low-lying quasi-degenerate 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.

| $N$   | $10000$ | $40000$ | $160000$ | $640000$ |
|-------|---------|---------|----------|----------|
| 1st-excited | 1.721  | 1.622  | 1.597    | 1.590    |
| 2nd-excited | 9.564  | 9.538  | 9.532    | 9.530    |
| 3rd-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 wavefunctions for $N = 10000$ 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                                   |
| 1st-excited | 0.5400                        | 0.7447                                   | 0.1928                                   | 0.0937                                   | 0.1035                                   |