Perturbative Spectrum of Trapped Weakly Interacting Bosons in Two Dimensions

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Abstract

We study a trapped Bose-Einstein condensate under rotation in the limit of weak, translational and rotational invariant two-particle interactions. We use the perturbation-theory approach (the large-$N$ expansion) to calculate the ground-state energy and the excitation spectrum in the asymptotic limit where the total number of particles $N$ goes to infinity while keeping the total angular momentum $L$ finite. Calculating the probabilities of different configurations of angular momentum in the exact eigenstates gives us a clear view of the physical content of excitations. We briefly discuss the case of repulsive contact interaction.

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The study of low-lying excitations of the weakly interacting, trapped Bose-Einstein condensed gas under rotation is of considerable experimental [1,2] and theoretical interest [3]. Theoretical studies have focused on the Thomas-Fermi limit of strong interactions [3], as well as on the limit of weak interactions [4–7], which we consider in this paper. Wilkin et al. [4] studied the case of attractive interaction, and Mottelson and Kavoulakis et al. [5] developed a theory for repulsive interactions. They compared the mean-field approach and exact numerical results obtained by diagonalization in a subspace of degenerate states [6]. Bertsch and Papenbrock [7] performed numerical diagonalization for small systems and showed that the interaction energy of the lowest-energy states decreases linearly with angular momentum $L$. Nakajima and Ueda [8] found through an extensive numerical study, in the limit where the angular momentum per particle is much smaller than one, that low-lying excitation energies, measured from the energy of the lowest state are given by $0.795 n(n - 1)$, where $n$ is the number of octupole excitations. Recently, Kavoulakis et al. [9] rederived these results analytically with use of the diagrammatic perturbation-theory approach in the asymptotic limit $N \to \infty$. In this paper we present a systematic method for calculating the excitation spectrum for the weak, translationally and rotationally symmetric interaction in the asymptotic limit, where the total number of particles $N$ goes to infinity, while keeping the total angular momentum $L$ finite. We also discuss the probabilities of different configurations of the angular momentum in the exact eigenstates.

Our starting point is the two-dimensional Hamiltonian $H = H_0 + V$, where

$$H_0 = \sum_{i=1}^{N} \left( -\frac{1}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right)$$

is the one-particle part, including the kinetic energy of the particles, and the potential energy due to the trapping potential. The trapping potential is approximated by a two-dimensional, isotropic harmonic oscillator with the frequency set to one. The system is in the ground state for the motion in the direction of the axis of rotation. The two-body interaction between the particles is given by

$$V = \sum_{i<j} v(|r_i - r_j|),$$

where an arbitrary potential $v$ possesses translational and rotational symmetries. We also assume that the interaction $v$ is weak. This allows us to work within the subspace of single-particle states with no radial excitations

$$\psi_n(z) = (\pi n!)^{-1/2} z^n \exp\left(-\frac{1}{2} |z|^2 \right),$$

where $z = x + iy$ and $n$ is the angular momentum quantum number. The energy levels and the corresponding wave functions are found by diagonalizing the interaction $V$ in this Hilbert space. Basis functions for the many-body problem are $\psi(z_1, z_2, \ldots, z_N) = \varphi(z_1, z_2, \ldots, z_N) \prod_{i=1}^{N} \exp\left(-\frac{1}{2} |z_i|^2 \right)$, where $\varphi$ is a homogeneous polynomial of degree $L$. For simplicity, we omit the exponentials from the wave functions. Suitable basis functions for such polynomials are given by

\[2\]
where the set \( \{ \lambda_1, \lambda_2, \ldots, \lambda_q \} \) denotes any partition of \( L \) such that \( \sum_{i=1}^q \lambda_i = L \) and \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_q > 0 \) for \( q \leq N \). The prime denotes the sum over mutually different indices \( i_1, i_2, \ldots, i_q \), while the numbers \( \nu_1, \nu_2, \ldots, \nu_p \) denote the frequencies of appearance of equal \( \lambda_i \)'s. Note that the number of distinct monomial terms \( z_1^{\lambda_1} z_2^{\lambda_2} \cdots z_q^{\lambda_q} \) in \( B_\lambda \) is given by \( d_\alpha = N(N-1)\cdots(N-q+1)/(\nu_1!\nu_2!\cdots\nu_p!) \), where \( \nu_1 + \nu_2 + \cdots + \nu_p = q \). Owing to the translational and rotational symmetries of the two-particle interaction \( v(|\mathbf{r}_i - \mathbf{r}_j|) \), for non-negative integers \( n \) and \( m \) we have

\[
v(|z_1 - z_2|) (z_1 + z_2)^n (z_1 - z_2)^2 m P(z_3, z_4, \ldots, z_N) = c_{2m} (z_1 + z_2)^n (z_1 - z_2)^2 m P(z_3, z_4, \ldots, z_N),
\]

(5)

where \( P \) denotes an arbitrary polynomial. The coefficient \( c_n \) is given by

\[
c_n = \frac{\int_0^\infty dr r^{2n+1} v(r) \exp(-r^2/2)}{\int_0^\infty dr r^{2n+1} \exp(-r^2/2)}.
\]

(6)

and represents the interaction energy \( v(r) \) of the relative motion of two bosons in the single-particle state \( r^n \exp(-r^2/2) \) with the angular momentum \( n \). To proceed, let us now define symmetric functions of two variables

\[
b_{ij}(z_1, z_2) = \frac{1}{2} (z_i^j z_2^j + z_1^j z_2^j), \quad i \geq j.
\]

(7)

The action of the potential \( v(|\mathbf{r}_i - \mathbf{r}_j|) \) on \( b_{ij} \) is given by

\[
v(|z_1 - z_2|) b_{ij}(z_1, z_2) = \sum_{l=0}^{[q]} \alpha_{ij}^{kl} b_{kl}(z_1, z_2),
\]

(8)

where \( i + j = k + l = n \). This restriction is a consequence of the conservation of total angular momentum for a rotationally symmetric potential. Also, the coefficients \( \alpha_{ij}^{kl} \)

\[
\alpha_{ij}^{kl} = \frac{2 - \delta_{kl}}{2} \sum_{p=0}^{[q]} c_{2p} S_{i,j}^{2p} S_{n-2p,2p},
\]

(9)

where

\[
S_{i,j}^q = \sum_{r+s=q} (-)^s \binom{i}{r} \binom{j}{s},
\]

(10)

satisfy the summation rule \( \sum_{l=0}^{[q]} \alpha_{ij}^{kl} = c_0 \), as a consequence of translational symmetry. The coefficients \( \alpha_{ij}^{kl} \) in fact represent the two-body matrix element \( V_{ijkl} \) (see Ref. [11]) of the interaction potential \( V \). Next, by using Eqs. (11) and (12) we obtain

\[
V B_1^n(z_1, z_2, \ldots, z_N) = c_0 \binom{N}{2} B_1^n(z_1, z_2, \ldots, z_N) \text{ for } B_1 = \sum_{i=1}^N z_i.
\]

(11)
As a result, $B^n_i(z_1, z_2, \ldots, z_N)$ is an exact eigenstate and the corresponding eigenvalue is $c_0 \binom{N}{2}$. Furthermore, owing to translational invariance the action of the potential $V$ on the product $B^n_i B_\lambda$ reduces to

$$V B^n_i B_\lambda = B^n_i V B_\lambda$$

for any $n$ and partition $\lambda$. Specially, if $A$ is an eigenstate with energy $E$, then $B^n_i A$ is also an eigenstate with the same energy.

Generally, for any partition $\lambda$ we find

$$V B_\lambda = \sum_\mu a^\mu_\lambda B_\mu,$$  \hspace{1cm} (13)

where $\mu$ is the partition obtained by substituting a pair of numbers $\{k, l\}$ for a $\{i, j\}$ in partition $\lambda$, such that $i \geq j$, $k \geq l$, and $i+j = k+l$, for all distinct pairs $\{i, j\}$ and all allowed $\{k, l\}$. Note that any partition $\lambda = \{\lambda_1, \ldots, \lambda_q\}$ can be written as $\lambda = 0^{n_0} 1^{n_1} 2^{n_2} \ldots l^{n_l} \ldots$, with $\sum_i n_i(\lambda) = N$ and $\sum_i \lambda_i n_i(\lambda) = L$. In the second quantized approach, the number $n_i(\lambda)$ can be interpreted as the number of particles with the angular momentum $i$ in the partition $\lambda$. The diagonal coefficient is

$$a^\lambda_\lambda = \sum_{\{i,j\}} a_{ij}^{ij} \frac{2 - \delta_{i,j}}{2} n_i(\lambda)[n_j(\lambda) - \delta_{i,j}],$$  \hspace{1cm} (14)

where the sum goes over all distinct pairs $\{i, j\}$, $i \geq j \geq 0$ contained in partition $\lambda$. The sum contains $\binom{K_1}{2} + K_2$ terms, where $K_1$ is the number of $n_i$'s greater than zero, and $K_2$ is the number of $n_i$'s greater than one, in partition $\lambda$ ($i \geq 0$). The nondiagonal coefficient can be expressed as

$$a^\mu_\lambda = \alpha_{ij}^{kl} \frac{2 - \delta_{i,j}}{2} n_k(\mu)[n_l(\mu) - \delta_{k,l}],$$  \hspace{1cm} (15)

where $\{i, j\}$ ($\{k, l\}$) are contained in partition $\lambda$ ($\mu$), respectively. The general matrix element has the form $a^\mu_\lambda = \alpha_{ij}^{kl} \delta_{\lambda_\mu} N^2 + \beta_{\lambda_\mu} N + \gamma_{\lambda_\mu}$. Note that this matrix is not Hermitian since our initial basis $\{B_\lambda\}$ is orthogonal but not orthonormal, i.e., $\langle B_\lambda | B_\mu \rangle = d_\lambda \prod_i \lambda_i!$. Since the interaction is Hermitian, changing the basis to orthonormal would render the matrix $\{a^\mu_\lambda\}$ Hermitian. The matrix $\{a^\mu_\lambda\}$ has dimension $\mathcal{P}(L)$, which is the number of partitions of $L$. It had been shown \[12,14\] that the eigenvalue problem can be reduced to $\mathcal{P}(L) - \mathcal{P}(L-1) - 1$ dimensions and recursively solved for the general interaction up to $L = 5$. For $L = 6$, the problem reduces to the diagonalization of the $3 \times 3$ matrix, which can be accomplished using the $1/N$ expansion. Motivated by this approach, in this paper we propose a similar strategy. In the limit where the angular momentum $L$ is much smaller than the number of particles $N$ we use perturbation theory in the large-$N$ expansion to calculate the interaction energies and derive analytical results. In the zeroth order, the standard perturbation-theory approach gives $A_\lambda = B_\lambda$ for eigenstates and $E^{(0)}_\lambda = a^\lambda_\lambda$ for the corresponding energy. The eigenenergy with the first-order corrections is

$$E^{(1)}_\lambda = a^\lambda_\lambda + \sum_{\mu \neq \lambda} \frac{a^\mu_\lambda a^\lambda_\mu}{a^\lambda_\lambda - a^\mu_\mu},$$  \hspace{1cm} (16)
The above expression is applicable if the condition $a_0^0 a_0^0 \ll (a_0^0 - a_0^0)^2$ is satisfied for all partitions $\mu \neq \lambda$. It can be easily checked using relations (14) and (17) that $a_0^0 a_0^0 \leq N$ and $(a_0^0 - a_0^0)^2 \sim N^2$. One finds that the dominant contributions are those with $j$ or $l$ equal to zero, in Eq.(13), and they produce corrections to the energy of order $N^0$.

We can label the exact interaction energies and eigenstates as $E_\lambda$ and $A_\lambda$, respectively, such that in the limit $N \to \infty$ and finite $L$, the energy $E_\lambda$ goes to $E_\lambda^{(0)}$ and $A_\lambda$ goes to $B_\lambda$. For an exact eigenstate $A_\lambda(N, L)$, the state $B_\lambda' A_\lambda(N, L)$ is an exact eigenstate $A_\lambda(N, L + n)$, where $\lambda' = 0^{(n_0 - n)}1^{(n_1 + n)}2^{n_2} \ldots$. According to translational invariance, we obtain the exact identity for eigenenergies

$$E_{0^{(n_0 - n)}1^{(n_1 + n)}2^{n_2}} = E_{0^{n_0}1^{n_1}2^{n_2}}^{(0)}.$$  

Hence, $A_{0^{n_0}1^{n_1}2^{n_2}} = B_1^{n_1} A_{0^{(n_0 + n_1)}2^{n_2}}$ and $E_{0^{n_0}1^{n_1}2^{n_2}}^{(0)} = E_{0^{(n_0 + n_1)}2^{n_2}}$. The part $1^{n_1}$ in the partition $\lambda$ denotes $n_1$ unit angular momenta which can be realized only as the angular momenta due to the center-of-mass motion. Therefore we consider only the eigenstates with partition $\lambda = 0^{n_0}2^{n_2}3^{n_3} \ldots l^{n_l} \ldots$, i.e., the states involving quadrupoles, octupoles, and higher $l$ poles. In this case, we have

$$E_\lambda^{(0)} = c_0 \left( \frac{n_0(\lambda)}{2} \right) + \sum_{i \geq 2} c_i^{-} n_i(\lambda) n_0(\lambda) + \sum_{i \geq j \geq 2} \frac{2 - \delta_{ij}}{2} n_i(\lambda)[n_j(\lambda) - \delta_{ij}].$$  

For special partition $\lambda = 0^{(N-1)}1$, we obtain the excitation energy for a general weak interaction $E_\lambda^{(0)} - E_0^{(0)} = N(\alpha_{00}^0 - \alpha_{00}^0)$. In the case of contact interaction it reduces to the $\epsilon_l = -c_0 N(1 - 2^{-(l-1)})$. Now, we include corrections

$$E_\lambda^{(1)} = E_\lambda^{(0)} + \sum_{i \geq j \geq 2} c_{ij} n_i(\lambda)[n_j(\lambda) - \delta_{ij}][n_i(\lambda) + 1] - \sum_{i \geq j \geq 2} c_{ij} n_i(\lambda)[n_i(\lambda) + 1 + \delta_{i,j}][n_j(\lambda) + 1],$$  

where

$$c_{ij} = \frac{\alpha_{ij}^{1+j,0} \alpha_{ij}^{2-j,0} - \delta_{i,j}}{\alpha_{00}^0 + \alpha_{ij}^{0} - \alpha_{ij}^{1+j,0} - \alpha_{ij}^{0} + \alpha_{ij}^{2-j,0} - \alpha_{ij}^{0}}. $$  

In the case of repulsive delta interaction, Eqs. (18) and (19) simplify significantly, because all coefficients $c_n$ are zero for $n \neq 0$, so $\alpha_{ij}^{kl} = 2^{(-n)}(2-\delta_{k,l}){n \choose k} c_0$, $n = i + j = k + l$. From Eq.(18) we easily find the lowest-order energy $E_\lambda^{(0)}$

$$E_\lambda^{(0)} = c_0 \left\{ \frac{N^2}{2} - N \left[ \frac{L + 2}{4} - \sum_{i \geq 4} \left( \frac{i}{2^i - 1} - 1 \right) n_i \right] \right\}. $$  

One can calculate the first-order correction for arbitrary partition, so, for example, the eigenenergy for the partition $\lambda = 0^{n_0}2^{n_2}3^{n_3}4^{n_4}$ is

$$E_\lambda^{(1)} = c_0 \left\{ \frac{N^2}{2} - \frac{N}{8} (2L + 4 - n_4) + \frac{27}{68} n_3(n_3 - 1) + n_4 \left( \frac{81}{52} n_2 + \frac{27}{41} n_3 + \frac{99}{194} n_4 + \frac{93}{388} \right) \right\} + O(1/N).$$  

(22)
This result is in complete agreement with the results obtained in Refs. [11,12]. We see that in the special case of \( n_l = 0 \) for \( l \geq 4 \), the zeroth-order energy

\[
E^{(0)}_\lambda = c_0 \left[ \frac{N^2}{2} - \frac{N(L + 2)}{4} \right]
\]

is degenerated, but the corrections \( \frac{27}{68} n_3 (n_3 - 1) \) remove this degeneracy if \( n_2 \geq 2 \). Hence, for the repulsive delta interaction the ground state is unique and defined by \( N = n_0 + n_2, L = 2n_2 \) or \( N = n_0 + n_2 + 1, L = 2n_2 + 3 \), depending on \( L \) being even or odd. Therefore, our analysis confirms the conjecture of Smith and Wilkin [11], in the limit of large \( L \). The exact eigenstates for \( L \leq 5 \) do not depend on details of interaction, and can be expanded in the standard basis \( B_\lambda \). For example, in the \( L = 2 \) case we have \( B_1^2 = B_2 + 2B_{11} \) and \( A_2 = \frac{1}{N} B_{11} - \frac{N-1}{2N} B_2 \) and in the \( L = 3 \) case we have

\[
\begin{align*}
B_1^3 &= B_3 + 3B_{21} + 6B_{111}, \\
B_1 A_2 &= -\frac{N - 1}{2N} B_3 - \frac{N - 3}{2N} B_{21} + \frac{3}{N} B_{111}, \\
A_3 &= \frac{(N - 1)(N - 2)}{3N^2} \left[ B_3 - \frac{3}{N - 1} B_{21} + \frac{12}{(N - 1)(N - 2)} B_{111} \right].
\end{align*}
\]

It is interesting to consider the probability of the configuration \( B_\mu \) in the exact eigenstate \( A_\lambda \), since it gives us a physical picture of the excitations. One can easily calculate the probability using the formula

\[
w_\mu(A_\lambda) = \frac{\langle B_\mu | A_\lambda \rangle^2}{\langle B_\mu | B_\mu \rangle \langle A_\lambda | A_\lambda \rangle}. \tag{23}
\]

For the \( L = 3 \) case, the probabilities are given in Table 1. We see that the probability of the configuration \( B_1L \) in any exact state other than \( A_1L \) tends to zero, in the limit when \( N \to \infty \) and \( L \) finite. Of course, this is not a surprise, as we labeled the exact states to obey the condition \( w_\mu(A_\lambda) \to \delta_{\mu, \lambda} \) in the large-\( N \) limit.

The eigenstates \( \tilde{\epsilon}_L = \sum (z_{i_1} - B_1/N) \cdots (z_{i_L} - B_1/N) \), with \( L \leq N \) are common to all interactions and these are the ground states for the repulsive delta interaction [13,14]. There is a simple relation between these states and the exact eigenstates \( A_\lambda \) we have discussed up to now. Generally, \( \tilde{\epsilon}_L = A_{2L/2} \) for even \( L \) and \( \tilde{\epsilon}_L = A_{3(\lambda-3)/2} \) for odd \( L \). For \( L \ll N \) \( \tilde{\epsilon}_L \) is dominated by \( \{2^{L/2}\} \) or \( \{32^{(L-3)/2}\} \) configurations, depending on \( L \) being even or odd.

Of special interest are "vortex" states \( \tilde{\epsilon}_{L=N} \). The probability that every particle carries a unit of angular momentum is easily calculated for low \( N \) and is given by \( w_{11} (\tilde{\epsilon}_2) = 1/2, w_{13} (\tilde{\epsilon}_3) = 4/9, w_{15} (\tilde{\epsilon}_4) = 15/32, w_{15} (\tilde{\epsilon}_5) = 296/625 \). It seems that \( w_{1N} (\tilde{\epsilon}_N) \approx 1/2 \), and this is in contrast with the naive expectation that all particles contribute with a unit of angular momentum in the vortex state \( \tilde{\epsilon}_N \) [11]. Note that in this case our perturbative approach is not valid, hence the probabilities of configurations \( \{2^{L/2}\} \) and \( \{32^{(L-3)/2}\} \) are small.

In conclusion, we studied a trapped Bose-Einstein condensate under rotation in the limit of weak, translational and rotational invariant two-particle interactions. We have used the perturbation-theory approach to calculate the ground-state energy and the excitation spectrum in the asymptotic limit where the total number of particles \( N \) goes to infinity while
keeping the total angular momentum $L$ finite. Calculating the probabilities of configurations $B_\mu$ in the exact eigenstates $A_\lambda$ gives us a clear view on the physical content of excitations $A_\lambda$. In addition, we have briefly discussed the case of repulsive delta interaction.

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TABLE I. The probabilities of configurations $B_\mu$ in exact states $A_\lambda$ for the $L = 3$ case.

|      | $B_{111}$                      | $B_{21}$                | $B_3$               |
|------|--------------------------------|-------------------------|---------------------|
| $B_1^3$ | $(1 - \frac{1}{N})(1 - \frac{2}{N})$ | $\frac{3}{N}(1 - \frac{1}{N})$ | $\frac{1}{N^2}$     |
| $B_1A_2$ | $\frac{3}{N}(1 - \frac{2}{N})$ | $(1 - \frac{3}{N})$ | $\frac{3}{N}(1 - \frac{1}{N})$ |
| $A_3$ | $\frac{4}{N^2}$ | $\frac{3}{N}(1 - \frac{2}{N})$ | $(1 - \frac{1}{N})(1 - \frac{2}{N})$ |