Weakly Interacting Bose-Einstein Condensates Under Rotation: Mean-field versus Exact Solutions

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(March 21, 2022)

We consider a weakly-interacting, harmonically-trapped Bose-Einstein condensed gas under rotation and investigate the connection between the energies obtained from mean-field calculations and from exact diagonalizations in a subspace of degenerate states. From the latter we derive an approximation scheme valid in the thermodynamic limit of many particles. Mean-field results are shown to emerge as the correct leading-order approximation to exact calculations in the same subspace.

PACS numbers: 03.75.Fi, 05.30.Jp, 67.40.Db, 67.40.Vs

Following the observation of Bose-Einstein condensation\textsuperscript{[1]} in vapours of alkali atoms\textsuperscript{[2]}, considerable attention has been devoted to the behaviour of these systems under rotation. Matthews et al.\textsuperscript{[3]} reported the observation of vortex states in a two-component system, and Madison et al.\textsuperscript{[4]} demonstrated the existence of vortex states in a stirred one-component Bose-Einstein condensate. Numerous authors have considered the problem of rotation in these systems theoretically\textsuperscript{[5–11]}. Many of them focused on the Thomas-Fermi regime of strong interactions between the atoms\textsuperscript{[5–7]}, where the coherence length is much smaller than the spatial extent of the system and where the cloud is expected to exhibit properties like those of a bulk superfluid such as \textsuperscript{4}He. The other interesting limit, to be considered here, is that of weak interactions between the atoms, where the coherence length is much larger than the size of the cloud of atoms and where one expects to see properties similar to those of superfluid nuclei\textsuperscript{[12]}.

The problem of rotation in the limit of weak interactions has also been considered previously. Wilkin et al.\textsuperscript{[8]} studied the case of effective attraction between the atoms and showed that, in the ground state of the system, angular momentum is carried by the center of mass. Butts and Rokhsar\textsuperscript{[9]} examined the problem of effective repulsion between the atoms. They included the kinetic energy of the particles and the potential energy due to the trapping potential and where

\[ \hat{V} = \frac{1}{2} U_0 \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j) \]

is the two-body interaction between particles, which is assumed to be of zero range. Here \( M \) is the atomic mass, \( \omega \) is the frequency of an isotropic trapping potential, and \( U_0 = 4\pi \hbar^2 a/M \) is the strength of the effective two-body interaction, with \( a \) being the scattering length for atom-atom collisions. We assume that \( a > 0 \), i.e., we treat only the case of repulsive effective interactions between the atoms. We further restrict our attention to the limit of weak interactions,

\[ nU_0 \ll \hbar \omega, \]

where \( n \) is the density of the condensed atoms. If the system has angular momentum \( L \), this condition allows us to work in subspaces of states which are degenerate in the absence of interactions. All other states differ by an energy of order \( \hbar \omega \), which is much larger than \( nU_0 \) by assumption. Finally, we assume that the cloud of atoms rotates about some axis, and that the system is in its ground state with respect to this axis, which implies that our problem is essentially two-dimensional. In the absence of interactions for the harmonic oscillator potential in two dimensions the single particle energies are

\[ e = (2n_r + |m| + 1) \hbar \omega, \]
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 system all the atoms are in states with \( n_r = 0 \), and with \( m \) being zero or having the same sign as the total angular momentum.

Let us describe briefly the two methods which have been used to attack the problem of rotation, starting with the mean-field approach \[7, 14\]. Within this approximation the many-body wavefunction with \( N \) particles and \( L \) units of angular momentum \( \Psi_{L,N}(r_1, r_2, \ldots, r_N) \) is a Fock state simply expressed as a product of single particle states:

\[
\Psi_{L,N}(r_1, r_2, \ldots, r_N) = \Psi(r_1) \times \Psi(r_2) \ldots \Psi(r_N).
\]  

(5)

It is natural to expand the single-particle states \( \Psi(r_i) \) in the basis of the harmonic-oscillator eigenstates \( \Phi_m(r_i) \) with angular momentum \( m \hbar \) along the axis of rotation:

\[
\Psi(r_i) = \sum_{m=0}^{\infty} c_m \Phi_m(r_i),
\]  

(6)

where \( c_m \) are variational parameters. The quantity \( |c_m|^2 \) gives the probability for the occupancy of state \( \Phi_m \). One imposes two constraints on the parameters \( c_m \). The wavefunction must be normalized,

\[
\sum_{m} |c_m|^2 = 1,
\]  

(7)

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

\[
\sum_{m} m|c_m|^2 = L/N.
\]  

(8)

The expectation value of the interaction energy \( \hat{V} \) in the state given by Eq. (6) is

\[
\langle \hat{V} \rangle = \frac{1}{2} (N - 1) U_0 \int |\Psi|^4 \, dr.
\]  

(9)

Minimizing this energy with respect to the \( c_m \) subject to the constraints of Eqs. (6) and (8), one obtains the mean field energy and corresponding wavefunction.

Turning to the “exact” approach to this problem, it is convenient to work in the basis \( |N_0, N_1, N_2, \ldots \rangle \) where \( N_m \) is the number of particles with angular momentum \( m \hbar \). The constraints on particle number and angular momentum now take the form:

\[
\sum_{m} N_m = N; \sum_{m} mN_m = L.
\]  

(10)

It is convenient to write the interaction energy as

\[
\hat{V} = \frac{1}{2} U_0 \sum_{i,j,k,l} I_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l,
\]  

(11)

where \( a_k \) and \( a_k^\dagger \) are annihilation and creation operators respectively, and

\[
I_{i,j,k,l} = \int \Phi_i^*(r) \Phi_j^*(r) \Phi_k(r) \Phi_l(r) \, dr
\]  

\[
= \frac{(i+j)!}{2^{(i+j)}} \sqrt{i!j!k!l!} \int |\Phi_0(r)|^4 \, dr
\]  

(12)

when \( i + j = k + l \) and zero otherwise. The final step is to diagonalize the matrix \( \hat{V} \) in the space of the states \( |N_0, N_1, N_2, \ldots \rangle \) which satisfy the constraints of Eq. (10).

Before turning to a comparison of these methods, it is useful to consider their advantages and disadvantages. On the one hand, the mean-field approximation gives the energy in the asymptotic limit \( L \) and \( N \to \infty \) with \( L/N \) fixed. This limit is not directly accessible to the exact method since the dimensionality of the space increases dramatically with increasing \( L \) and \( N \). On the other hand, the exact method provides the entire spectrum of excited states and a lower ground state energy than the mean-field result. The mean-field assumption of a simple product wavefunction ignores correlations between the particles which are contained in the exact diagonalization. The mean-field energy offers only an upper bound for the true ground state energy. To be more specific, the leading term in the ground state energy of the system must grow like \( N^2 \) for the interaction considered. As we show below, the energy obtained by the exact method in the asymptotic limit is bounded from below by an expression which has the same \( N^2 \) coefficient as the mean-field result. Thus, the exact energy differs from the mean-field value by terms of order \( N \) or less. In addition, we will suggest simple methods for computation of the order \( N \) correction to the ground state energy in the asymptotic limit.

The spirit of the mean field approximation is that the wavefunction is composed of a large number of states with occupation numbers in the vicinity of \( N|c_m|^2 \) but that these states are of measure zero in the full Hilbert space considered. Up to a staggering related to the phases of the \( c_m \), the wavefunction should then be a smooth and differentiable function of occupation number for single particle states containing a finite fraction of the particles. Such states are amenable to simple treatment. States with \( c_m = 0 \) in a mean field description will require special treatment. Consider the particular case \( L = 2N \) using a Hilbert space \( 0 \leq m \leq 4 \). In mean field theory it is found that the only non-zero coefficients are \( c_0 \), \( c_2 \), and \( c_4 \). Initially retaining only these states, we will consider the basis of states

\[
|k\rangle = |k, 0, N - 2k, 0, 0\rangle.
\]  

(13)

Write the wavefunction as

\[
|L = 2N, N\rangle = \sum_k (-1)^k \psi_k |k\rangle,
\]  

(14)

where the \( k \)-dependent phase has been chosen to minimize the resulting energy. The eigenvalue equation has the form

\[
\hat{V}_{k,k} \psi_k - \hat{V}_{k,k-1} \psi_{k-1} - \hat{V}_{k,k+1} \psi_{k+1} = \mathcal{E}_{2N,N} \psi_k,
\]  

(15)
where $\hat{V}_{k,k'} = \langle k|\hat{V}|k' \rangle$ is the matrix element of the interaction between the states $|k\rangle$ and $|k'\rangle$ given by Eq. (13). The two-body interaction $\hat{V}$ connects only states for which $k - k' = \pm 1$, or 0.

Assuming that $\psi_k$ is smooth and differentiable over a suitable range, we expand the wavefunction as

$$\psi_{k\pm1} = \psi_k \pm \partial_k \psi_k + \frac{1}{2} \partial_k^2 \psi_k$$

(16)

to obtain the eigenvalue equation

$$-\frac{1}{2}(\hat{V}_{k,k-1} + \hat{V}_{k,k+1}) \partial_k^2 \psi_k + V_{\text{eff}} \psi_k = \mathcal{E}_{2N,N} \psi_k,$$

(17)

where the effective potential is

$$V_{\text{eff}}(k) = \hat{V}_{k,k} - \hat{V}_{k,k-1} - \hat{V}_{k,k+1}.$$  

(18)

The leading term in the energy is of order $N^2$ and is simply the minimum value of $V_{\text{eff}}(k)$. This minimum occurs at

$$k_0 = N \frac{16\sqrt{5} - 28}{64\sqrt{6} - 109}.$$  

(19)

The occupancy of the $m = 0$ and $m = 4$ states is $k_0/N$ in the asymptotic limit; the occupancy of $m = 2$ is $1 - 2k_0/N$. This is precisely the result found in Ref. [4] within the mean-field approximation. Numerical exploration for $N > 10^9$ indicates that the energy of the minimum of the effective potential, $V_{\text{eff}}(k_0)$, can be described by the approximate form

$$\tilde{\mathcal{E}}_{2N,N} \approx \left(0.177256895N^2 - 0.366043N + O(N^0)\right) v_0,$$

(20)

where $v_0 = U_0 \int |\Phi_0|^4 \, d\mathbf{r}$, with $\Phi_0(\mathbf{r})$ being the ground state of the harmonic oscillator. As expected, the $N^2$ coefficient in this expression is identical to the corresponding term in the mean field [4]. In general, the properties of the minimum of $V_{\text{eff}}(k)$ reproduce the leading $N^2$ term of mean field theory.

Expanding $V_{\text{eff}}(k)$ around $k_0$, we find that the effective potential has the form

$$V_{\text{eff}}(k) = \tilde{\mathcal{E}}_{2N,N} + \frac{1}{2} d (k - k_0)^2 v_0,$$

(21)

where $\tilde{\mathcal{E}}_{2N,N}$ is given by Eq. (20) and where the constant $d \approx 0.3732$ is necessarily positive and of $O(N^0)$. The leading, “kinetic energy” term in Eq. (17) is positive with $\hat{V}_{k,k-1} + \hat{V}_{k,k+1} \approx 0.0381N^2$. That this term is of $O(N^2)$ is a consequence of the fact that $\hat{V}$ is a two-body operator. The ground-state energy for this harmonic oscillator problem is readily found to be

$$\mathcal{E}_{2N,N} = \tilde{\mathcal{E}}_{2N,N} + \frac{1}{2} \hbar \Omega$$

(22)

with

$$\hbar \Omega = \sqrt{d (\hat{V}_{k,k-1} + \hat{V}_{k,k+1})} \approx 0.1192N v_0.$$  

(23)

The effective oscillator length corresponding to Eq. (17) is proportional to $(|\langle k_0 | \hat{V} | k_0 \rangle| / d)^{1/4}$ and is of order $N^{1/2}$. This demonstrates the consistency of our assumptions: The ground state wavefunction $\psi_k$ is a Gaussian centered at $k_0$ with a width of order $N^{1/2}$. It contains significant contributions from a large number of states, which, however, is only a vanishingly small fraction of all the states in our Hilbert space. Combining Eqs. (20), (21), and (23) we obtain a ground state energy of

$$\mathcal{E}_{2N,N} = \left(0.177256895N^2 - 0.366046N + O(N^0)\right) v_0.$$  

(24)

The general conclusion from this analysis is that the correct $O(N^2)$ contribution to the energy can be obtained by determining the classical minimum of the effective potential energy, $V_{\text{eff}}(k)$. Quantum fluctuations lead to corrections of order $N$. Since the kinetic energy term is positive, these corrections are necessarily positive and this leading term thus provides a lower bound on the ground state energy. By contrast, the mean-field approach leads to minimizing the same classical potential but provides an upper bound on the energy as a consequence of its variational character. Thus, the ground state energy is trapped between upper and lower bounds with the same leading term. Thus, we conclude that the $O(N^2)$ contribution to the ground state energy obtained by mean field theory is exact in the large $N$ limit.

While the space considered in the above example was severely limited, this method can be generalized to include as many states as necessary. Our analysis holds provided that the states included are occupied by a finite fraction of the total number of particles. If this is true, roughly $N^{1/2}$ states for each of the variables in the multi-dimensional space will make significant contributions to the wave function and the approximation of differentiability is valid. One can then derive an eigenvalue equation of the form of Eq. (17), of multi-dimensional coupled harmonic oscillators. A crucial assumption in establishing the asymptotic validity of the mean field result is the positivity of the “inertial” parameters such as the coefficient of $\partial_k^2 \psi_k$ in the case of Eq. (17). We have verified that this is true in a number of specific cases, and we believe that it is true in general.

Let us now return to the states $m = 1$ and $m = 3$ in our example. These states are not macroscopically occupied, i.e., the corresponding $c_1$ and $c_3$ are zero in a mean field calculation. The expansion of Eq. (14) cannot be used for their description, and their incorporation requires some care. To include their effects, we approximate $|L = 2N, N\rangle_0$ by the single state $|k = k_0\rangle$ of Eq. (13). Starting with this state, we build a basis of states containing $n_1$ particles with $m = 1$ state and $n_3$ particles with $m = 3$, being careful to conserve particle number and angular momentum. The effect of these
states with odd $m$ values can then be obtained by diagonalizing $\hat{V}$ in this basis. If $0 \leq (n_1 + n_3) \leq 2Q$, there will be $(Q+1)^2$ states in this basis. Convergence of this calculation to arbitrary accuracy can be obtained by choosing $Q$ to be large but none the less of order $N^0$. This confirms the fact that the states $m = 1$ and $m = 3$ are not macroscopically occupied. In the present case, the lowest eigenvalue of this matrix converges rapidly to an asymptotic value of $-0.1812N\nu_0$. The linear contribution to the energy from such states is general. An improved description of $\{L = 2N, N\}_0$ would lead to changes in this energy of order $N^0$.

We are now able to obtain the asymptotic ground state energy for the case $L = 2N$ correct to order $N$ by combining this correction for the odd $m$ states with the result of Eq. (24). We find

$$\mathcal{E}_{2N,N} \approx (0.177256895N^2 - 0.487576N + O(N^0)) \nu_0.$$  \hfill (25)

This result is in remarkable agreement with the expression

$$\mathcal{E}_{2N,N} \approx (0.177256752N^2 - 0.487848N + O(N^0)) \nu_0$$ \hfill (26)

obtained by direct numerical diagonalization in the same truncated space $0 \leq m \leq 4$ for values of $100 \leq N \leq 220$. Note that the case $N = 220$ requires diagonalization of a matrix of dimension $305990$. The small discrepancies obtained are a consequence of the limited range of $N$ for which exact diagonalization is possible and the largest values of $Q$ considered in our approximate calculation. These restrictions are absent in calculations within the same Hilbert space $0 \leq m \leq 4$ for $L = N/2$. It is then possible to consider $N$ as large as 600. All states have an occupation number of order $N$, and the final matrix diagonalization in our approximate treatment is not required. In this case, the quadratic terms in the ground state energy agree to 10 significant figures, and the linear terms differ by 1 part in $10^6$.

Additional evidence comes from exact diagonalizations (with no truncation in $m$) for the case $L = 2N$ for $4 \leq N \leq 24$. The resulting energies are well described by

$$\mathcal{E}_{2N,N} \approx (0.1749N^2 - 0.5206N + 0.0028)\nu_0.$$ \hfill (27)

As argued above, mean field theory suggests that only states with even $m$ are macroscopically occupied in the ground state for $L = 2N$. This is supported by exact diagonalizations for the same range of $N$ from which we have excluded single-particle states with odd $m$. The energy is then found to be

$$\mathcal{E}_{2N,N} \approx (0.1755N^2 - 0.2980N - 0.0905)\nu_0.$$ \hfill (28)

Comparing the coefficients of $N^2$ and $N$ in Eqs. (27) and (28), we see that only the latter is materially affected by this truncation. This is consistent with our assertion that states which are not occupied macroscopically contribute to the energy at order $N$.

In summary we have adopted a “correspondence principle approach” to describe repulsive two-body interactions between the particles in a Bose-Einstein condensate by assuming that the wavefunction in the $N \to \infty$ limit is a smooth and differentiable function of the occupation number. This approach leads us to the result that mean field theory provides an exact determination of the $N^2$ term in the ground state energy and permits determination of the contribution to this energy of order $N$. Butts and Rokhsar have arrived at a similar conclusion.\footnote{D. A. Butts, and D. S. Rokhsar, Nature 397, 327 (1999).} Evidently, the same arguments can be used to describe the spectrum of excited states. The present methods would appear to be a useful and practical supplement to mean field methods whenever these are of value.

G.M.K. was supported by the European Commission, TMR program, under contract No. ERBFMBICT 983142, and S.M.R. under contract No. ERB4001G 970292. We would like to thank C. J. Pethick for helpful discussions and M. Koskinen for advice regarding numerical questions. G.M.K. would like to thank the Foundation of Research and Technology, Hellas (FORTH) for its hospitality, and S.M.R. would like to acknowledge financial support from the “Bayerische Staatsministerium für Wissenschaft, Forschung und Kunst”.

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