

Rotational spectra of weakly interacting Bose-Einstein condensates

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We study the spectrum of rotating Bose-Einstein condensates in the limit of weak repulsive interactions and present analytical and numerical results for energies and wave functions. While the low-lying states are of collective nature, the high-lying states are dominated by single-particle excitations and can be accurately approximated by simple polynomial expressions. In the limit that the number of particles is large compared to the number of excited quanta, the single-particle states become excellent approximations to the eigenstates, and a rather simple ordering scheme is obtained.

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The experimental realization of Bose-Einstein condensation in atomic vapors [1–3] has received much interest in recent years [4]. Very recently, experiments have started to investigate Bose-Einstein condensates under rotation. Matthews *et al.* created vortices in a two-component condensate [5], and Madison *et al.* studied rotations of a one-component gas [6]. Theoretical studies have focused on the Thomas-Fermi regime of strong interactions [7,8] or on the limit of weak interactions between the atoms [9–17]. While the former case is more closely related to the experiment, the latter case allows for exact (numerical or analytical) solutions and is of particular theoretical interest. Wilkin *et al.* studied the case of attractive interactions [10] and employed a composite boson/fermion picture [12,14] to describe configurations beyond the one-vortex state in few-body boson systems. Mottelson [11] and the Copenhagen group [15,16] analyzed the mean-field theory in the weak-interaction limit. In Ref. [13], the authors studied the ground states using exact diagonalization techniques. So far, research has been restricted to the low-lying states in rotating Bose-Einstein condensates. It is the purpose of this paper to study higher excited states in the rotational spectrum.

The paper is organized as follows. We will first introduce the Hamiltonian and the Hilbert space. This will be done using second quantization and by an approach in configuration space. After the presentation of some exact results concerning the ground state, we study the most energetic non-spurious states. We finally investigate the regime where the number of bosons is large compared to the number of excited quanta and classify the complete spectrum.

The Hamiltonian is

$$H = \sum_{j=1}^N \left\{ -\frac{1}{2} \nabla_j^2 + \frac{1}{2} \mathbf{r}_j^2 \right\} + g \sum_{i < j} 2\pi \delta(\mathbf{r}_i - \mathbf{r}_j),$$

where the trap frequency is set to $\hbar\omega = 1$ and g is a dimensionless coupling. In the limit of weak repulsive interactions $0 < g \ll 1$ and maximal alignment of angular momentum with the z axis, the Hamiltonian becomes essentially two-dimensional [11,15]. In what follows, we restrict ourselves to this limit and fix the total angular momentum to L .

The problem then consists in diagonalizing the contact interaction in the Hilbert space of degenerate oscillator states at total energy L (setting the ground-state energy to zero) [20]. We will analyze the problem in second quantization and in configuration space. While analytical results will be derived in both representations, numerical work is most easily done using second quantization [18,19]. Let us start with the second quantized two-body interaction

$$\hat{V} = \sum_{i < j} 2\pi \delta(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2} \sum_{i,j,k,l} \frac{(k+l)!}{2^{k+l} \sqrt{i!j!k!l!}} \delta_{k+l}^{i+j} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \quad (1)$$

The operators \hat{a}_m and \hat{a}_m^\dagger annihilate and create one boson in the single-particle oscillator state $|m\rangle$ with energy $m\hbar\omega$ and angular momentum $m\hbar$, respectively, and fulfill bosonic commutation rules. For total angular momentum L , the Fock space is spanned by states $|\alpha\rangle \equiv |n_0, n_1, \dots, n_k\rangle$ with $\sum_{i=0,k} n_i = N$, $\hat{a}_j^\dagger \hat{a}_j |n_0, n_1, \dots, n_k\rangle = n_j |n_0, n_1, \dots, n_k\rangle$ and $\sum_{j=0,k} j n_j = L$. Here n_j denotes the occupation of the j th single-particle state $|j\rangle$.

Turning to configuration space, we use complex single-particle coordinates $z = x + iy$ such that $\langle z | j \rangle = \phi_j(z) = (\pi j!)^{-1/2} z^j \exp(-\frac{1}{2}|z|^2)$. Basis functions for the many-body problem are $\psi(z_1, \dots, z_N) \prod_{j=1}^N \exp(-\frac{1}{2}|z_j|^2)$, where $\psi(z_1, \dots, z_N)$ is a homogeneous polynomial of degree L that is totally symmetric in its coordinates. For representations of such polynomials, see, e.g., Ref. [21]. In what follows, we will omit the exponentials when working in configuration space and identify wave functions directly by their polynomial part. Let $\psi(z_1, \dots, z_N)$ be such a polynomial.

Consider the two-body operator

$$\hat{W}_{ij} = \sum_{m,n,k,l} \frac{(k+l)!}{2^{k+l} n! m! k! l!} \delta_{m+n}^{k+l} z_i^n z_j^m \{ \partial_{z_j}^k \partial_{z_i}^l |_{z_i=z_j=0} \}. \quad (2)$$

Here it is understood that the derivatives act only on the polynomial part of the wave function and that they are evaluated at $z_i = z_j = 0$. A direct computation (e.g., in second quantization) shows that the operator (2) has the same matrix elements as the contact interaction $2\pi \delta(\mathbf{r}_i - \mathbf{r}_j)$. Performing the sums in Eq. (2) and introducing coordinates $R_{ij} = (z_i + z_j)/\sqrt{2}$ and $r_{ij} = (z_i - z_j)/\sqrt{2}$ leads to the following:

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$$\begin{aligned}
 & 2\pi\delta(\mathbf{r}_i - \mathbf{r}_j)\psi(z_1, \dots, z_i, \dots, z_j, \dots, z_N) \\
 &= \hat{W}_{ij}\psi(z_1, \dots, z_i, \dots, z_j, \dots, z_N) \\
 &= \psi\left(z_1, \dots, \frac{z_i + z_j}{2}, \dots, \frac{z_j + z_i}{2}, \dots, z_N\right). \quad (3)
 \end{aligned}$$

Thus, the contact interaction $2\pi\delta(\mathbf{r}_i - \mathbf{r}_j)$ acts on a wave function by replacing the i th and j th argument by its mean value. Note that the center of mass

$$z_c = \frac{1}{N} \sum_{j=1}^N z_j$$

is left invariant under the action of the contact interaction.

Let us now consider the spectrum of states at angular momentum L . States may be classified by their angular momentum quantum numbers L and L_{cm} , and by their energies $E_n = L + g\epsilon_n$. The angular momentum of the center of mass is denoted as L_{cm} and is given by

$$\hat{L}_{\text{cm}} = z_c \sum_{j=1}^N \partial_{z_j} = \frac{1}{N} \sum_k \sqrt{k+1} \hat{a}_{k+1}^\dagger \hat{a}_k \sum_l \sqrt{l+1} \hat{a}_l^\dagger \hat{a}_{l+1}, \quad (4)$$

where the differential operator is understood to act only on the polynomial part of the wave function. The functions z_c and

$$q_k(z_1, \dots, z_N) = \sum_{j=1}^N (z_j - z_c)^k, \quad k \geq 2 \quad (5)$$

are eigenfunctions of \hat{L}_{cm} with eigenvalues one and zero, respectively. Products $z_c^{\lambda_1} q_{\lambda_2} \dots q_{\lambda_N}$ with λ being a partition of L are eigenstates of \hat{L}_{cm} with eigenvalue $L_{\text{cm}} = \lambda_1$ and span the Hilbert space [20] at angular momentum $2 \leq L \leq N$. Note that they do not form an orthogonal basis. Let $|L, L_{\text{cm}}, \epsilon_n\rangle$ denote an eigenstate of the Hamiltonian (1). Due to an $\text{SO}(2,1)$ symmetry, one has $z_c |L, L_{\text{cm}}, \epsilon_n\rangle \propto |L+1, L_{\text{cm}}+1, \epsilon_n\rangle$ [22,23]. It is therefore of particular interest to find the “nonspurious” eigenstates (i.e., those with no excitations of the center-of-mass coordinate) since all other states can simply be obtained by multiplication with powers of z_c [22,10,17]. Note, however, that the spurious states are particularly important in the case of attractive contact interactions since the center of mass carries all angular momentum in the ground state [10].

Figure 1 shows the spectrum of nonspurious states for $N=50$ bosons and angular momenta $2 \leq L \leq 18$. Note that there are several high-lying levels that approach constant values as L increases. This is particularly the case for the two most energetic levels, and these are well separated from their neighbors for all values of L . As has been observed earlier in exact diagonalizations [13] and mean-field calculations [7,15], the ground states depend linearly on total angular momentum.

Based on numerical results, we suggested in Ref. [13] that the ground-state wave function is

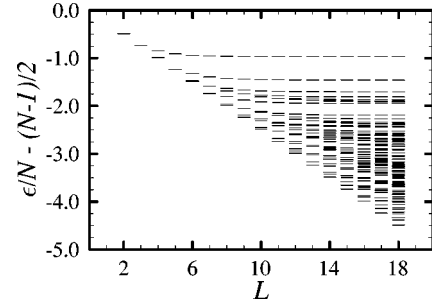


FIG. 1. Spectrum of nonspurious states for a system of $N=50$ particles as a function of angular momentum.

$$\begin{aligned}
 \psi_0(z_1, \dots, z_N) &= \sum_{1 \leq p_1 < p_2 < \dots < p_L \leq N} (z_{p_1} - z_c) \\
 &\quad \times (z_{p_2} - z_c) \dots (z_{p_L} - z_c) \quad (6)
 \end{aligned}$$

and the ground-state energy is

$$\epsilon_0 = \frac{1}{2} \left(N(N-1) - \frac{NL}{2} \right). \quad (7)$$

Very recently, Jackson and Kavoulakis [17] showed the existence of an eigenstate with energy (7) while Smith and Wilkin [24] proved that the wave function (6) indeed has eigenvalue (7). This proof was given using the second quantized form of the interaction. As an application of Eq. (3), we now present a shorter proof in configuration space. We expand

$$\psi_0 = \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \sum_{1 \leq p_1 < \dots < p_k \leq N} z_{p_1} \dots z_{p_k}.$$

Applying operator (2) to this expansion and using the prescription (3) yields

$$\begin{aligned}
 \hat{W}_{ij}\psi_0 &= \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \left\{ \sum_{1 \leq p_1 < \dots < p_k \leq N}^{\neq i,j} z_{p_1} \dots z_{p_k} \right. \\
 &\quad + (z_i + z_j) \sum_{1 \leq p_1 < \dots < p_{k-1} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-1}} \\
 &\quad \left. + \frac{1}{4} (z_i + z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-2}} \right\}.
 \end{aligned}$$

Using $(z_i + z_j)^2 = (z_i - z_j)^2 + 4z_i z_j$ in the third term enclosed in brackets, one obtains

$$\begin{aligned}
 \hat{W}_{ij}\psi_0 &= \psi_0 + \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \\
 &\quad \times \left\{ \frac{1}{4} (z_i - z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-2}} \right\}.
 \end{aligned}$$

Summing over $\Sigma_{i < j}$ and using the identity

TABLE I. Numerical data for the states ψ_1 and ψ_2 as a function of angular momentum L for $N=50$. The energy expectation values $\langle \psi_j | \hat{V} | \psi_j \rangle$ approach energies $\epsilon_1 = (N-1)(N-2)/2 = 1176$ and $\epsilon_2 = [(N-2)^2 - 1]/2 = 1151.5$, respectively. The widths $\Gamma_j^2 = \langle \psi_j | \hat{V}^2 | \psi_j \rangle - \langle \psi_j | \hat{V} | \psi_j \rangle^2$ are small compared to the level spacing [which is of order $O(N)$], and the overlap with the exact eigenstates is close to 1.

L	8	12	16	20
$\langle \psi_1 \hat{V} \psi_1 \rangle$	1176.325	1176.019	1176.001	1176.000
Γ_1	0.6	0.2	0.03	0.01
$1 - \langle \psi_1 \psi_{\text{exact}} \rangle ^2$	2×10^{-4}	6×10^{-6}	2×10^{-7}	$< 10^{-7}$
$\langle \psi_2 \hat{V} \psi_2 \rangle$	1153.031	1151.604	1151.508	1151.501
Γ_2	1.4	0.3	0.09	0.03
$1 - \langle \psi_2 \psi_{\text{exact}} \rangle ^2$	3×10^{-3}	9×10^{-5}	5×10^{-6}	4×10^{-7}

$$\begin{aligned}
 & \sum_{i < j} \left\{ (z_i - z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i, j} z_{p_1} \dots z_{p_{k-2}} \right\} \\
 &= -kN \sum_{1 \leq p_1 < \dots < p_k \leq N} z_{p_1} \dots z_{p_k} \\
 &+ N(N-k+1)z_c \sum_{1 \leq p_1 < \dots < p_{k-1} \leq N} z_{p_1} \dots z_{p_{k-1}}
 \end{aligned}$$

one arrives directly at the desired result $\hat{V}\psi_0 = \epsilon_0\psi_0$.

Another exact result is readily obtained for $L=4$ and arbitrary N . Employing Eq. (3), one may show that

$$\hat{V} \sum_{1 \leq i < j \leq N} (z_i - z_j)^4 = \frac{1}{2} \left(N^2 - \frac{11}{4}N + \frac{3}{2} \right) \sum_{1 \leq i < j \leq N} (z_i - z_j)^4. \quad (8)$$

Unfortunately, we are not able to generalize this result to higher values of angular momentum. Note, however, that wave functions (6) and (8) comprise the set of nonspurious states for $L=4$.

Let us consider the most energetic nonspurious states. Since the ground state has mainly collective character [11,13,15], one may expect that single-particle excitations are considerably higher in energy. The simplest single-particle excitation is certainly the state where $N-1$ bosons are in the harmonic-oscillator ground state and one excited boson carries all the angular momentum. The corresponding nonspurious state is given by [compare with Eq. (5)]

$$\psi_1(z_1, \dots, z_N) = q_L(z_1, \dots, z_N). \quad (9)$$

Numerical computations show that this ansatz has almost unit overlap with the most energetic nonspurious eigenstate. Its energy approaches the asymptotic eigenvalue $\epsilon_1 = \frac{1}{2}(N-1)(N-2)$ exponentially fast with increasing values of angular momentum L . This is the energy of $N-1$ interacting bosons in the single-particle ground state. The energy contribution of the highly excited particle is exponentially suppressed for sufficiently large angular momenta. Table I pre-

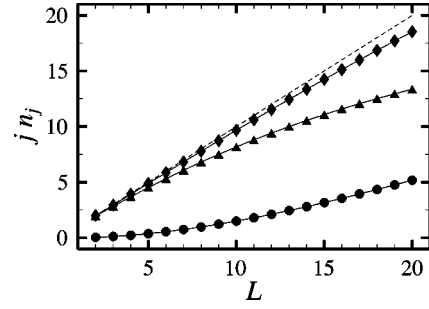


FIG. 2. Structure of state ψ_1 : Single-particle angular momenta $n_j = j \langle \psi_1 | \hat{n}_j | \psi_1 \rangle$ as a function of angular momentum L for different single-particle orbitals j in a system of $N=50$ bosons ($j=L-1$: circles; $j=L$: triangles; sum of both: diamonds; total angular momentum: dashed line).

sents numerical values obtained for the overlaps with the exact numerical eigenfunction, energies $\langle \psi_1 | \hat{V} | \psi_1 \rangle$, and widths $\Gamma_1^2 = \langle \psi_1 | \hat{V}^2 | \psi_1 \rangle - \langle \psi_1 | \hat{V} | \psi_1 \rangle^2$. The presented results show that Eq. (9) is a highly accurate approximation to the exact eigenstate. This can be understood in more detail by applying the operator (1) to ψ_1 ,

$$\hat{V}\psi_1 = \frac{1}{2}(N-1)(N-2)\psi_1 + 2^{1-L} \sum_{i < j} (z_i + z_j - 2z_c)^L. \quad (10)$$

For sufficiently large L , the “remainder” $\sum_{i < j} (z_i + z_j - 2z_c)^L$ is numerically found to have significant overlap only with a small number of eigenstates in the bulk. This explains the quality of our ansatz. Note that $\psi_0 \propto \psi_1$ for $L=2$ and $L=3$. Note also that $\hat{V}\psi_1 = [1 + (-1)^L 2^{1-L}] \psi_1$ for $N=3$. The ansatz (9) describes ψ_1 as an excitation of one particle relative to the center of mass. This picture is confirmed by the computation of selected single-particle occupation numbers $n_j = \langle \psi_1 | \hat{n}_j | \psi_1 \rangle$ shown in Fig. 2. The main contribution to the total angular momentum stems from the single-particle orbital $\phi_L(z)$ and a smaller part is carried by the orbital $\phi_{L-1}(z)$.

Let us now consider the second highest nonspurious state. Naively, one would expect that this state is mainly given by a configuration where $N-2$ particles are in the harmonic-oscillator ground state while the remaining two particles carry $L-2$ and two units of angular momentum. This picture would correspond to the state $q_2 q_{L-2}$. However, our numerical computations show that this state has significant overlap with the highest nonspurious state (9) as well. (We recall that products of functions q_λ are not orthogonal.) We therefore use the ansatz

$$\begin{aligned}
 \psi_2(z_1, \dots, z_N) &= \frac{N-1}{N} q_2(z_1, \dots, z_N) q_{L-2}(z_1, \dots, z_N) \\
 &- \psi_1(z_1, \dots, z_N)
 \end{aligned} \quad (11)$$

and find almost unit overlap with the numerically obtained exact eigenstate for sufficiently large values of total angular momentum. It approaches the numerically determined en-

ergy $\epsilon_2 = \frac{1}{2}[(N-2)^2 - 1]$ exponentially fast with increasing L . Details concerning overlaps and width are presented in Table I. The dominant contributions to the total angular momentum of ψ_2 stem from the orbitals $\phi_2(z)$, $\phi_{L-3}(z)$, and $\phi_{L-2}(z)$. As expected, the ansatz (11) describes mainly a few-boson excitation. The single-particle character of the two most energetic states differs strongly from the collective behavior found for the ground state ψ_0 . This observation is similar to the case of bosons in the Thomas-Fermi regime [25] and to the case of many-fermion systems such as atomic nuclei [26].

We checked that the numerical results agree with ansatz (9) and (11) for various numbers of bosons. The convergence is determined by L only and depends weakly on N . The spectrum depicted in Fig. 1 seems to suggest that there are more states that may be approximated by simple polynomial expressions; however, we do not see an obvious generalization of the expressions (9) and (11) to account for further states.

Let us consider the regime $N \gg L \sim O(N^0)$, where the ground state is occupied by a macroscopic number of bosons, i.e., $n_0 \sim O(N)$. While low-lying states have been computed in Refs. [11,15], we aim at a general understanding of the full spectrum within this regime. Equation (1) shows that the diagonal matrix elements of \hat{V} are of order $O(N^2)$. In leading order, off-diagonal elements involve change of the ground state occupation by one unit. They are therefore of order $O(N^{1/2})$ and small compared to the diagonal elements. In a first approximation, one may then neglect any off-diagonal elements and take the single-particle states as eigenstates. One obtains from Eq. (1)

$$\hat{V}|n_0, n_1, n_2, \dots, n_k\rangle = \epsilon_{\{n_j\}}|n_0, n_1, n_2, \dots, n_k\rangle + O(N^{1/2}), \quad (12)$$

$$\epsilon_{\{n_j\}} = \frac{1}{2}n_0(n_0 - 1) + 2n_0 \sum_{k \geq 0} 2^{-k}n_k.$$

Note that typical energies are of the order $O(N^2)$ while energy differences for two different states are of order $O(N)$. Small energy differences may occur for two configurations $\{n_j\}$ and $\{n'_j\}$ that differ only in the occupation of the orbitals $j=0,2,3$. Both configurations should have an identical number of bosons and angular momentum, i.e., $n_0 + n_2 + n_3 = n'_0 + n'_2 + n'_3$ and $2n_2 + 3n_3 = 2n'_2 + 3n'_3$. The energy difference of such configurations is only of order $\sim O(N^0)$, which is much smaller than a typical spacing. Thus there are quasidegenerate levels in the spectrum, and the ground state becomes quasidegenerate for $L=6$ and $L \geq 9$. These observations have also been made by Mottelson [11].

Note that the single-particle states have almost good quantum number L_{cm} . One finds $\hat{L}_{\text{cm}}|n_0, n_1, n_2, \dots, n_k\rangle \approx n_1|n_0, n_1, n_2, \dots, n_k\rangle$, and corrections are of order $O(L/N)$. This can be seen by applying the operator (4) to a state with $n_0 \sim O(N)$. Thus, the nonspurious states are comprised of configurations with $n_1=0$. We may now discuss the order of the spectrum of nonspurious states. According to Eq. (12), this ordering is led by two observations. (i) The lower the number of bosons in the ground state, the lower the total energy of this state. (ii) For two configurations with

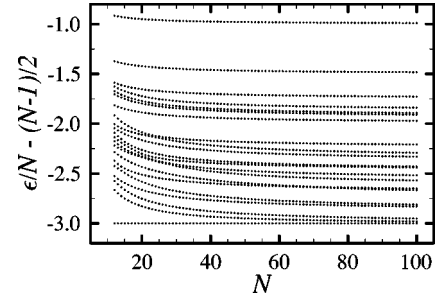


FIG. 3. Spectrum of nonspurious states for $L=12$ as a function on the number of bosons N .

equal numbers of excited bosons, the higher energetic one has the highest single-particle orbital occupied. This ordering scheme favors collective motion above single-particle excitations. Deviations from this scheme are caused by the quasidegeneracy of configurations discussed above. The validity of our arguments and of Eq. (12) is confirmed by numerically computing and analyzing the spectrum for $N=46000$ in the regime $2 \leq L \leq 18$. The numerical energies agree well with the analytical result (12). This is different for the wave functions at quasidegeneracies. Numerical eigenstates are superpositions of the quasidegenerate single-particle basis states. This is expected since the neglect of off-diagonal matrix elements becomes invalid for degenerate levels.

Let us finally examine the N dependence of the spectra at fixed L as shown in Fig. 3. The spectrum evolves rather smoothly with increasing N and levels tend to be clustered at high N . For instance, there is a triplet of states at lowest energies. This is due to the quasidegeneracy discussed above, and the triplet is comprised of configurations with

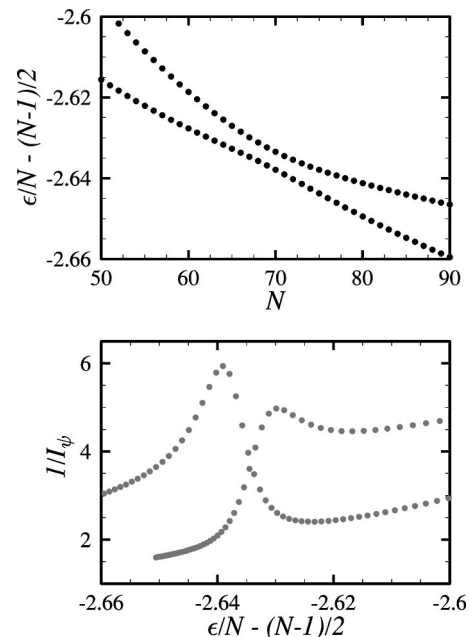


FIG. 4. Avoided crossing. Top: Two energies as a function of N . Bottom: Number of participating basis states as a function of energy. Results are taken from one avoided crossing at $L=12$.

$\{n_2=6\}$, $\{n_3=4\}$, and $\{n_2=3, n_3=2\}$. Such quasidegeneracies indicate a high degree of integrability and regularity. However, there are also a few quasidegeneracies at midvalues of N . Closer inspection reveals that these are avoided crossings. As an example, we present in Fig. 4 (top) the avoided crossing at $N \approx 70$. The enlargement of the energy clearly indicates an avoided crossing. Further evidence comes from analyzing the wave-function structure, i.e., we follow the inverse participation [27]

$$I_\psi = \sum_{\alpha} |\langle \alpha | \psi \rangle|^4 \quad (13)$$

of an eigenstate $|\psi\rangle$ in the basis of single-particle basis states $|\alpha\rangle$. The inverse $1/I_\psi$ measures the number of basis states that have significant overlap with the eigenstate $|\psi\rangle$; it is a one-number quantity that describes the wave-function structure. Figure 4 (bottom) shows that the wave-function structure changes at the avoided crossing. The simple ordering obtained for the spectrum at large values of N is thus lost when decreasing N . We also recall that avoided crossings indicate some degree of level repulsion and chaoticity [28]. Therefore, we do not expect that all states may be described by simple polynomial expressions. Note, however, that the high-lying nonspurious states and the ground state do not interact with their neighboring levels, a further confirmation of their regularity.

In summary, we have studied the rotational spectrum of Bose-Einstein condensates in the limit of weak repulsive interactions. The most energetic nonspurious states are well separated from neighboring levels and their energies approach constant values with increasing angular momentum. These states can accurately be approximated by simple polynomial expressions. They exhibit single-particle behavior and differ thereby from the collective behavior of the ground state. In the limit of a macroscopic occupation of the ground state and small total angular momentum, the single-particle states become approximate eigenstates. We obtain a simple ordering scheme for the entire excitation spectrum that energetically favors collective behavior over single-particle behavior. This ordering scheme is expected to break down when leaving the limit of $L/N \ll 1$ since some states undergo avoided crossings. While this introduces chaotic behavior in the involved states, the ground state and the highest excited nonspurious states appear to remain simple and regular. Parts of the analytical results presented in this work, including a proof concerning the ground-state wave function, are based on a particularly useful and novel representation of the contact interaction in configuration space.

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