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Condensates of \( p \)-Wave Pairs Are Exact Solutions for Rotating Two-Component Bose Gases

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We derive exact analytical results for the wave functions and energies of harmonically trapped two-component Bose-Einstein condensates with weakly repulsive interactions under rotation. The isospin symmetric wave functions are universal and do not depend on the matrix elements of the two-body interaction. The comparison with the results from numerical diagonalization shows that the ground state and low-lying excitations consist of condensates of \( p \)-wave pairs for repulsive contact interactions, Coulomb interactions, and the repulsive interactions between aligned dipoles.

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Exact analytical solutions for interacting quantum many-body systems are very rare [1,2]. However, they are of tremendous interest, since they may provide us with further insight into the correlations of quantum-mechanical many-body systems. Even rarer are cases where the exactly solvable quantum many-body system can also potentially be realized experimentally. A famous example is the celebrated Laughlin state [3] and its generalizations [4] that describe the two-dimensional electron gas in the quantum Hall regime. In recent years, the advances with ultracold atomic quantum gases have significantly broadened the range of experimentally accessible many-body systems that are also solvable exactly. An example is the interacting Bose gas in one dimension. Here, the Bethe ansatz offers an analytic solution to the Lieb-Liniger model [5], and the fermionization of bosons in the Tonks-Girardeau [6] limit has been observed [7,8].

Exact analytical solutions exist also for single-component dilute and weakly interacting Bose-Einstein condensates under rotation [9–17]. For a large class of repulsive two-body interactions, the exact ground state of \( N \) bosons at angular momentum \( L \) results from projecting the unique state, where \( L \) particles carry one unit of angular momentum onto the subspace with zero angular momentum for the center of mass [14–16]. In this Letter, we generalize this exact solution to the interesting case of a two-component Bose gas [18–20] and arrive at a very appealing result: As in the single-component case, the exact solutions at angular momentum \( L \) are states where \( L \) bosons carry one unit of angular momentum each, and as before one has to project out excitations of the center of mass. In the two-component case, however, isospin enters as a good quantum number, and eigenstates can be labeled by the number of isospin-singlet \( p \)-wave pairs that enter the wave function. Isospin was introduced in nuclear physics by Heisenberg [21] and—like ordinary spin—is based on the SU(2) symmetry of two-component systems. The comparison with numerical results shows that, for repulsive contact interactions, Coulomb forces, and repulsive forces between aligned dipoles [22], the ground state contains a maximum number of isospin-singlet \( p \)-wave pairs. This Letter also explains the recent study by Bargi et al. [19], who found by numerical diagonalization that the yrast energy of two-component Bose gases is a simple function of angular momentum.

We consider a harmonically trapped two-component dilute gas of \( N \) bosons of a first species \( \uparrow \) and \( M \) bosons of a second species \( \downarrow \). We assume that the interactions are perturbatively weak and of equal strength between those that are intraspecies and interspecies. This special case of equal scattering lengths is approximately realized in gases of \( ^{87}\text{Rb} \) and gases of \( ^{23}\text{Na} \) [23]. Let us list the conserved quantities involved in this problem. Besides the isospin \( T \), the total angular momentum \( L \), the angular momentum of the center of mass \( L_c \), the total number of bosons \( A = M + N \), and the isospin projection \( T_z = (M - N)/2 \) are conserved. There is no simple basis that reflects these symmetries simultaneously. In second quantization, the conservation of \( L, A, T_z \), and \( T \) is straightforward, while the conservation of \( L, M, N, \) and \( L_c \) is most easily expressed in the configuration space within first quantization.

We will employ both pictures in what follows. Single-particle states \( \phi_{nlm} \) of the spherical harmonic oscillator have energies \( E_{nl} = \hbar \omega (2n + l + 3/2) \). We are interested in low-energetic states at high angular momentum. For weakly perturbative interactions, only single-particle states with no radial excitation \( (n = 0) \) can contribute, and we can limit ourselves to maximally aligned states with \( m = l \). Thus, single-particle states with single-particle angular momentum \( l \) are
\[ \phi_{00}(z) = z^l \exp(-|z|^2/2) \] and \[ \phi_{0i}(w) = (w^l \exp(-|w|^2/2) \]
for the bosons of the species \( l \) and \( i \), respectively. We denote the coordinates of bosons belonging to the \( l \) species by \( z_j = x_j + iy_j \) (\( j = 1, \ldots, N \)) and by \( w_j = u_j + iv_j \) (\( j = 1, \ldots, M \)) for the \( i \) species. Here, \( x \) and \( y \) \((u \) and \( v)\) are the two Cartesian coordinates perpendicular to the axis of rotation for the \( l \) \((i)\) species. In what follows, we omit the ubiquitous Gaussians from the single-particle wave functions. Let \( \hat{b}_{l}^{\dagger} \) and \( \hat{b}_{l}^{\dagger} \) create a boson in the states corresponding to \( z^l \) and \( w^i \), respectively. The corresponding annihilation operators are \( \hat{b}_{l} \) and \( \hat{b}_{l} \), and the creation and annihilation operators fulfill the canonical commutation relations for bosons.

In the case of a single species of boson under rotation, the ground state at angular momentum \( L \) consists essentially of \( L \) bosons carrying one unit of angular momentum each, while the remaining \( N - L \) bosons carry no angular momentum [12]. Small modifications of this picture are due to the preservation of the angular momentum of the center of mass. Remarkably, the two-component case is somewhat similar, and Bargi et al. [19] numerically found that the ground state consists entirely of single-particle states with angular momenta \( l = 0 \) and \( l = 1 \). For \( L \leq N \leq M \), there are \( L + 1 \) such states (labeled by the number of bosons of the species \( l \) that are in the single-particle state with \( l = 1 \)). What is the ground state for repulsive interactions in the space spanned by these states? To address this question for a two-component system, we recall the essence of Hund’s rule: For repulsive interactions, the interaction energy is minimized for wave functions that are antisymmetric in position space. In fermionic electron systems such as atoms and quantum dots, this leads to a symmetric spin wave function. The same reasoning applied to the present case of a two-species Bose gas would require the isospin wave function to be antisymmetric, too, thus making the total wave function symmetric under particle exchange. The operator

\[ \hat{B}^{\dagger} = \frac{1}{\sqrt{2}} (\hat{b}_{1}^{\dagger} \hat{b}_{0}^{\dagger} - \hat{b}_{0}^{\dagger} \hat{b}_{1}^{\dagger}) \]  

creates an isospin-singlet \( p \)-wave pair (i.e., \( L = 1 \) and \( T = T_{z} = 0 \)). This pair is antisymmetric in position space and antisymmetric in isospin space, and thus totally symmetric under exchange. Thus, the interaction energy is minimized for condensates of isospin-singlet pairs. In general, we have \( N \neq M \), and the ground-state wave function will also consist of unpaired bosons. The states

\[ |\lambda_{T} \rangle = (\hat{T}_{-})^{N_{T}} (\hat{b}_{0}^{\dagger})^{A_{T} - \tau} (\hat{b}_{1}^{\dagger})^{\tau} (\hat{B}^{\dagger})^{\tau} |0 \rangle \]  

have angular momentum \( L \), isospin \( T = A/2 - \tau \), isospin projection \( T_{z} = (M - N)/2 \), and consist entirely of single-particle states with angular momenta \( l = 0 \) and \( l = 1 \). Here, \(|0 \rangle\) denotes the vacuum, and \( \tau = 0, 1, \ldots, \min(L, N) \) is the number of isospin-singlet pairs. The isospin operators are \( \hat{T}_{z} = \sum_{l=0}^{\infty} \hat{b}_{l}^{\dagger} \hat{b}_{l} / 2 \) and \( \hat{T}^{2} = \hat{T}^{-}_{z} + T(T + 1) \). The eigenvalues of \( \hat{T}_{z} \) and \( \hat{T}^{2} \) are denoted as \( T_{z} \) and \( T(T + 1) \), respectively. Let us understand the state (2) in detail, starting from the right. The application of the pair operators \( \hat{B}^{\dagger} \) to the vacuum yields a state of \( 2\tau \) bosons with quantum numbers \( L = \tau, T = 0, \) and \( T_{z} = 0 \). The operators \( \hat{b}_{l}^{\dagger} \) yield the angular momentum \( L \) we seek and increase the number of bosons to \( L + \tau \), while keeping isospin \( T = T_{z} = (L - \tau)/2 \) a good quantum number. The application of the operators \( \hat{b}_{0}^{\dagger} \) increases the number of bosons to \( A \) and keeps isospin a good quantum number. Finally, \( \hat{T}^{2} \) yields the angular momentum \( T_{z} \) and \( \hat{T}^{2} \) yields \( T(T + 1) \). Thus, the observation by Bargi et al., together with an adaptation of Hund’s rule for bosons and isospin symmetry, leads to eigenstates (2) consisting of condensates of isospin-singlet \( p \)-wave pairs. Note that these arguments are independent of the details of the repulsive interaction. These are the main result of the present Letter. As in the single-component case, minor modifications of this picture are due to the conserved angular momentum of the center of mass. Let us contrast our results to BCS pairing in Fermi systems. In BCS theory, a weakly attractive interaction leads to the formation of Cooper pairs (i.e., pairs of fermions in time-reversed orbits). The resulting BCS ground state is a condensate of spin-singlet \( s \)-wave pairs, where the symmetric configuration-space wave function optimizes the interaction energy. In our case, we deal with bosons and with repulsive interactions, and this modifies the picture accordingly.

Let us compute the energies of the states (2). We generalize and extend the results of Ref. [14] to the case of two-component Bose gases and sketch the main steps. The Hilbert space \( \mathcal{H}^{(N)}_{L} \) of \( N \) identical bosons \( l \) at total angular momentum \( L \) is spanned by products \( e_{A_{l}}(z_{1})e_{A_{l}}(z_{2}) \ldots e_{A_{l}}(z_{N}) \)

(3)

with \( A_{l} + A_{l} + \ldots + A_{l} = L \) of elementary symmetric polynomials

and keeps isospin a good quantum number. The operators \( \hat{b}_{l}^{\dagger} \) increase the number of bosons to \( A \) and keeps isospin a good quantum number. Finally, \( \hat{T}^{2} \) yields the angular momentum \( T_{z} \) and \( \hat{T}^{2} \) yields \( T(T + 1) \). Thus, the observation by Bargi et al., together with an adaptation of Hund’s rule for bosons and isospin symmetry, leads to eigenstates (2) consisting of condensates of isospin-singlet \( p \)-wave pairs. Note that these arguments are independent of the details of the repulsive interaction. These are the main result of the present Letter. As in the single-component case, minor modifications of this picture are due to the conserved angular momentum of the center of mass. Let us contrast our results to BCS pairing in Fermi systems. In BCS theory, a weakly attractive interaction leads to the formation of Cooper pairs (i.e., pairs of fermions in time-reversed orbits). The resulting BCS ground state is a condensate of spin-singlet \( s \)-wave pairs, where the symmetric configuration-space wave function optimizes the interaction energy. In our case, we deal with bosons and with repulsive interactions, and this modifies the picture accordingly.

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(3)

of direct products of the Hilbert spaces of each component. Products of elementary symmetric polynomials are linearly independent and form a basis. In the absence of interactions, all states in the Hilbert space are degenerate. Perturbatively weak interactions will lift this degeneracy.
The two-body interaction for a two-component mixture of Bose gases can be written as

\[ V = \sum_{m \geq 0} v_m \hat{V}_m = \sum_{m \geq 0} v_m (\hat{A}_m + \hat{B}_m + \hat{C}_m). \]  

(5)

Here, \( v_m \) is a matrix element and

\[ \hat{A}_m = \sum_{1 \leq i < j \leq M} (z_i - z_j)^m (\partial_{z_i} - \partial_{z_j})^m, \]

(6)

\[ \hat{B}_m = \sum_{1 \leq i < j \leq M} (w_i - w_j)^m (\partial_{w_i} - \partial_{w_j})^m, \]

(7)

\[ \hat{C}_m = \sum_{1 \leq i, j \leq M} (z_i - w_j)^m (\partial_{z_i} - \partial_{w_j})^m \]

(8)

are the interactions between bosons of species \( \uparrow \), between bosons of species \( \downarrow \), and the interspecies interaction, respectively. By construction, the interaction preserves angular momentum \( L \) (i.e., the degree of the monomial wave function it is acting on), is of two-body nature, and—due to its translationally invariant form (only differences of coordinates and derivatives appear)—preserves the angular momentum \( L_c \) of the center of mass. Furthermore, the interaction (5) is invariant under the exchange of \( z_i \leftrightarrow w_k \) and therefore preserves isospin. For the zero-ranged contact interaction, we have \( v_m = (-1/2)^m/m! \) [14].

The action of the operators (6) on elementary symmetric polynomials is particularly simple [14]:

\[ \hat{A}_m e_\lambda(z) = \hat{B}_m e_\mu(w) = 0 \quad \text{for} \quad m \geq 3, \]

\[ \hat{C}_m e_\lambda(z) e_\mu(w) = 0 \quad \text{for} \quad m \geq 3, \]

(9)

\[ \hat{A}_m e_1(z) = \hat{B}_m e_1(w) = \hat{C}_m R = 0 \quad \text{for} \quad m \geq 1. \]

Here, \( R = \frac{1}{4} [e_1(z) + e_1(w)] \) denotes the center of mass. Equations (9) show that only the terms \( 0 \leq m \leq 2 \) of the Hamiltonian (5) are of interest when acting on products \( e_\lambda(z) e_\mu(w) \). For the operators \( \hat{V}_0 \) and \( \hat{V}_1 \), we find

\[ \hat{V}_0 = A(A - 1)/2, \quad \hat{V}_1 = A(\hat{L} - \hat{L}_c), \]

\[ \hat{L} = \sum_{i=1}^{N} z_i \partial_{z_i} + \sum_{j=1}^{M} w_j \partial_{w_j}, \]

(10)

\[ \hat{L}_c = \frac{1}{A} \left( \sum_{i=1}^{N} \sum_{k=1}^{M} z_i w_k \partial_{z_i} \partial_{w_k} \right). \]

Only \( \hat{V}_2 \) is truly nontrivial, and

\[ \hat{V}_2 e_\lambda(z) e_\mu(w) = 2(\lambda \mu + \mu M + 2\lambda \mu) e_\lambda(z) e_\mu(w) \]

\[ + 2(N - \lambda + 1)(\mu + 1) e_{\lambda-1}(z) e_{\mu+1}(w) \]

\[ + 2(M - \mu + 1)(\lambda + 1) e_{\lambda+1}(z) e_{\mu-1}(w), \]

\[ - 2A(N - \lambda + 1) e_{\lambda-1}(z) e_{\mu+1}(w)R \]

\[ - 2A(M - \mu + 1) e_{\lambda+1}(z) e_{\mu-1}(w)R. \]

(11)

Equation (11) shows that the set

\[ \mathcal{M} \equiv \{ R^n e_\lambda(z) e_{L-\lambda-n}(w) \} \quad \text{with} \quad 0 \leq \lambda \leq \min(L, N), \]

\[ 0 \leq n \leq L - \lambda \]

(12)

spans a subspace in Hilbert space at angular momentum \( L \) that is left invariant by \( \hat{V}_2 \). This subspace contains the states \( e_\lambda(z) e_{L-\lambda}(w) \) which are linear combinations of the eigenstates (2). The states \( e_\lambda(z) e_{L-\lambda}(w) \) are, however, not eigenstates of the center-of-mass momentum. Let \( \hat{P}_0 \) be the projector onto wave functions with zero angular momentum of the center of mass, i.e., \( \hat{P}_0 \psi(z, w) = \psi(z - R, w - R) \) for any wave function \( \psi(z, w) \). The wave functions \( P_0 e_\lambda(z) e_{L-\lambda}(w) \) are in the subspace spanned by \( \mathcal{M} \) [14].

Thus, the states \( \hat{P}_0 [\chi_{\lambda}] \) from Eq. (2) are eigenstates of the Hamiltonian (5). Note that these states do not depend on the matrix elements \( v_m \) of the interaction.

To compute the corresponding eigenvalues, we make the ansatz \( P_0 \psi_{L,n} \) for the eigenfunction with

\[ \psi_{L,n} = \sum_{\lambda = 0}^{\min(L, N)} c^{(n)}_\lambda e_\lambda(z) e_{L-\lambda}(w). \]

(13)

Here, \( n \) is an additional label that distinguishes between \( \min(L, N) + 1 \) different wave functions. Our results below suggest that \( n \) is the number of isospin-singlet pairs. The eigenvalue equation \( \hat{P}_0 \psi_{L,n} = E_n P_0 \psi_{L,n} \) requires the coefficients \( c^{(n)}_\lambda \) to fulfill

\[ 0 = [LM + (2L + N - M - 2\lambda) - e_n] c^{(n)}_\lambda \]

\[ + (N - \lambda)(L - \lambda) c^{(n)}_{\lambda+1} + \lambda(M - L + \lambda) c^{(n)}_{\lambda-1}. \]

(14)

Here, \( e \) enters the energy eigenvalue

\[ E_n = A(A - 1) \frac{V_0}{2} + AL v_1 + 2v_2 e_n. \]

(15)

Note that the eigenvalue problem (14) does not depend on the matrix elements of the two-body interaction. For the solution of the eigenvalue problem, we make the ansatz

\[ c^{(n)}_\lambda = \sum_{k=0}^{n} \beta_k \lambda^k. \]

(16)

Here, we concealed the fact that the coefficients \( \beta_k \) also depend on \( n \). We insert the ansatz (16) into Eq. (14) and compare the coefficients of \( \lambda^n \), \( m = 0, \ldots, n + 2 \). This yields

\[ e_n = AL - n(A + 1 - n), \]

(17)

which enters the energy (15). The coefficients \( \beta_k, \ k < n \) are recursively defined in terms of \( \beta_n \) (which sets the normalization). The quantum number \( n \) acquires the values \( n = 0, 1, 2, \ldots, \min(L, N) \), and the lowest energy is obtained for \( n = \min(L, N) \).

Figure 1 shows the energy spectrum of a two-component Bose-Einstein condensate with \( N = 4 \) and \( M = 8 \) particles per species, respectively, as a function of the angular momentum \( L \). The broken lines connect states with energies \( E_n \) from Eq. (15) for fixed \( n = 0, 1, 2, \ldots \) (from top to
The ground state has \( n = \min(L, N) \). Note that \( c^{(0)}_\lambda = 1 \) solves the eigenvalue problem (14) and yields the state \( \psi_{L,0} = c_L(z_1, \ldots, z_N, w_1, \ldots, w_M) \). This state is totally symmetric under the exchange of any particles, has maximum isospin \( T = A/2 \), and contains no isospin-singlet \( p \)-wave pairs. For \( L \leq N \), the ground state (13) with \( n = L \) has coefficients \( c^{(L)}_\lambda / c^{(L)}_0 = (-1)^{\lambda}(M - L + \lambda)!(N - \lambda)!/[\lambda!(M - L)!N!] \) and can be rewritten as \( \hat{S} \prod_{k=1}^n (z_k - w_k) \). Here, the symmetrization operator \( \hat{S} \) ensures the symmetry under exchange of bosons of each species, and the antisymmetry between the two species in position space is evident. We thus believe that the label \( n \) of the energies (15) has to be identified with the number \( \tau \) of isospin-singlet \( p \)-wave pairs of the eigenstates \( \hat{P}_{0,\tau}\chi_\tau \) with \( |\chi_\tau\rangle \) from Eq. (2).

The reasoning that led to the isospin-singlet \( p \)-wave condensates (2) was based on general arguments regarding repulsive interactions in SU(2)-symmetric two-component systems. To check our arguments, we performed numerical computations for Coulomb interactions and repulsive interactions between aligned dipoles. For the Coulomb interaction, the relevant matrix elements are \( v_0 = \sqrt{\pi}/2 \), \( v_1 = -v_0/4 \), and \( v_2 = 3v_0/64 \), respectively, and we refer the reader to Ref. [16] for the analytical derivation. The comparison with numerical results shows that the exact results (15) again describe the ground states and low-lying excitations. Finally, we consider repulsive interactions between dipoles aligned perpendicular to the trap plane. The comparison of the numerical spectra and the analytical results (15) yields \( v_0 = 6.868 \), \( v_1 = -3.188 \), and \( v_2 = 0.755 \), respectively. Again, the ground state and low-lying excitations are described by the analytical results.

In summary, we showed that low-lying states of rotating two-component Bose gases with weak repulsive interactions are condensates of isospin-singlet \( p \)-wave pairs and we derived analytical expressions for the energies and the corresponding wave functions. The wave functions are universal, as they do not depend on the details of the two-body interaction. Numerical computations demonstrate that these eigenstates are the ground states and some of the low-lying excitations for the contact interaction, the Coulomb interaction, and repulsive interactions between aligned dipoles.

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