Bosonic molecules in rotating traps

Igor Romanovsky, Constantine Yannouleas, Leslie O. Baksmaty, and Uzi Landman
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430
(Dated: To appear in Phys. Rev. Lett.)

We present a variational many-body wave function for repelling bosons in rotating traps, focusing on rotational frequencies that do not lead to restriction to the lowest Landau level. This wave function incorporates correlations beyond the Gross-Pitaevskii (GP) mean field approximation, and it describes rotating boson molecules (RBMs) made of localized bosons that form polygonal-ring-like crystalline patterns in their intrinsic frame of reference. The RBMs exhibit characteristic periodic dependencies of the ground-state angular momenta on the number of bosons in the polygonal rings. For small numbers of neutral bosons, the RBM ground-state energies are found to be always lower than those of the corresponding GP solutions, in particular in the regime of GP vortex formation.

PACS numbers: 05.30.Jp, 03.75.Hh

Recent experimental advances in the field of trapped ultracold neutral bosonic gases have enabled control of the strength of interatomic interactions over wide ranges, from the very weak to the very strong. This control is essential for experimental realizations of novel states of matter beyond the well-known Bose-Einstein condensate. In this context, the linear 1D Tonks-Girardeau regime of impenetrable trapped bosons has generated intensive theoretical activity and several experimental realizations of it have been reported most recently.

Here we address the properties of strongly-repelling impenetrable bosons in rotating ring-shaped or 2D harmonic traps. To this end, we recall that impenetrable bosons are “localized” relative to each other, and exhibit nontrivial intrinsic crystalline correlations. For a small number of bosons, \( N \), these crystalline arrangements are reminiscent of the structures exhibited by the well-studied rotating electron molecules (REMs) in quantum dots under high magnetic fields. Consequently, we use in the following the term rotating boson molecules (RBMs). A central result of our study is that the point-group symmetries of the intrinsic crystalline structures give rise to characteristic regular patterns (see below) in the ground-state spectra and associated angular momenta of the RBMs as a function of the rotational frequency for neutral bosons (or the magnetic field for charged bosons).

An unexpected result of our studies is that the rotation of repelling bosons (even those interacting weakly) does not necessarily lead to formation of vortices, as is familiar from the case of rotating Bose-Einstein condensates (BECs). In particular, for small \( N \), we will show that the Gross-Pitaevskii energies (including those corresponding to formation of vortices) remain always higher compared to the ground-state energies of the RBMs. Of course, we expect that the rotating BEC will become the preferred ground state for sufficiently large \( N \) in the case of weakly repelling neutral bosons. We anticipate, however, that it will be feasible to test our unexpected results for small \( N \) by using rotating optical lattices, where it is established that a small finite number of atoms can be trapped per given site.

In a non-rotating trap, it is natural to describe a localized boson (at a position \( \textbf{R}_j \)) by a simple displaced gaussian. When the rotation of the trap is considered, the gaussian needs to be modified by a phase factor, determined through the analogy between the one-boson Hamiltonian in the rotating frame of reference and the planar motion of a charged particle under the influence of a perpendicular magnetic field \( B \) (described in the symmetric gauge). That is, the single-particle wave function of a localized boson is

\[
\varphi_j(\textbf{r}) \equiv \varphi(\textbf{r}, \textbf{R}_j) = \frac{1}{\sqrt{\pi} \lambda} \exp \left[ \frac{\left( \textbf{r} - \textbf{R}_j \right)^2}{2 \lambda^2} - i \textbf{r} \cdot (\textbf{Q} \times \textbf{R}_j) \right],
\]

with \( \textbf{Q} \equiv \hat{z}/(2\lambda^2) \) and the width of the Gaussian \( \lambda \) is a variational parameter; \( \lambda \equiv l_B = \sqrt{\hbar e/(\epsilon B)} \) for the case of a perpendicular magnetic field \( \textbf{B} \), and \( \lambda = l_0 = \sqrt{\hbar/(2mB)} \) in the case of a rotating trap with rotational frequency \( \Omega \). Note that we consider a 2D trap, so that \( \textbf{r} \equiv (x, y) \) and \( \textbf{R} \equiv (X, Y) \). The hamiltonian corresponding to the single-particle kinetic energy is given by \( H_K(\textbf{r}) = (\textbf{P} - \hbar \textbf{Q} \times \textbf{r})^2/(2m) \), for the case of a magnetic field, and by \( H_K(\textbf{r}) = (\textbf{P} - \hbar \textbf{Q} \times \textbf{r})^2/(2m) - m\Omega^2 r^2/2 \), for the case of a rotating frame of reference.

A toroidal trap with radius \( r_0 \) can be specified by the confining potential

\[
V(\textbf{r}) = \frac{\hbar \omega_0}{2} \left( r - r_0 \right)^n / r_0^n,
\]

with \( l_0 = \sqrt{\hbar/(m\omega_0)} \) being the characteristic length of the 2D trap. For \( n \gg 2 \) and \( l_0/r_0 \to 0 \) this potential approaches the limit of a toroidal trap with zero width, which has been considered often in previous theoretical studies (see, e.g., Ref. [11]). In the following, we consider the case with \( n = 2 \), which is more realistic from the experimental point of view. In this case, in the limit \( r_0 = 0 \), one recovers a harmonic trapping potential.
The many-body Hamiltonian is given by $\mathcal{H} = \sum_{i=1}^{N} [H_{K}(r_{i}) + V_{i,j}(r_{i},r_{j})] + \sum_{i<j}^{N} V(r_{i},r_{j})$, with the interparticle interaction being given by a contact potential $V_{i,j} = g\delta(r_{i} - r_{j})$ for neutral bosons and a Coulomb potential $V_{C} = Z^{2}e^{2}/|r_{i} - r_{j}|$ for charged bosons. The parameter that controls the strength of the interparticle repulsion relative to the zero-point kinetic energy is given by $R_{s} = gm/(2\pi^{2}\hbar^{2})$ (for a contact potential and $R_{r} = Z^{2}e^{2}/(\hbar\omega_{0})$) for a Coulomb repulsion.

For a given value of the dimensionless rotational frequency, $\Omega/\omega_{0}$, the projection yields wave functions and energies for a whole rotational band comprising many angular momenta. In the following, we focus on the ground-state wave function (and corresponding angular momentum and energy) associated with the lowest energy in the band.

Fig. 1(a) displays the ground-state energy $E_{P}^{PRJ}$ of $N = 8$ bosons in a toroidal trap as a function of the dimensionless rotational frequency $\Omega/\omega_{0}$, with $\omega_{0}$ being the trap frequency. The prominent features in Fig. 1(a) are: (i) the energy diminishes as $\Omega/\omega_{0}$ increases; this is an effect of the centrifugal force, and (ii) the $E_{P}^{PRJ}$ curve consists of linear segments, each one associated with a given angular momentum $L$. Most remarkable is the regular variation of the values of $L$ with a constant step of $N$ units (here $N = 8$) [see inset in Fig. 1(a) and Fig. 1(c)]. These preferred angular momenta $L = kN$ with integer $k$, are reminiscent of the so-called “magic angular momenta” familiar from studies of electrons under high-magnetic fields in 2D semiconductor quantum dots. The preferred angular momenta reflect the intrinsic molecular structure of the localized impenetrable bosons. We note, that the $(0,8)$ polygonal-ring arrangement is obvious in the single-particle density associated with the UBHF permanent [see Fig. 2(b)]; $(0,8)$ denotes no particles in the inner ring and 8 particles in the outer one. After restoration of symmetry, however, the single-particle (sp) density is circularly symmetric [see the PRJ sp-density in Fig. 2(c)] and the intrinsic crystallinity becomes “hidden”; it can, however, be revealed via the conditional probability distribution [CPD, see Fig. 2(d)]. We note the Gross-Pitaevskii sp-density in Fig. 2(a), which is clearly different from the PRJ density in Fig. 2(c).

The internal structure for charged bosons in a toroidal trap (not shown) is similar to that of neutral bosons (Fig. 2), i.e., a $(0,8)$ ring arrangement, portrayed also in the stepwise variation (in steps of 8 units) of the total angular momenta associated with (i) the RBM ground states [thick solid line (showing steps and marked as PRJ); online black] and (ii) the UBHF solutions (thin solid line; online red).

To construct an RBM variational many-body wave function describing $N$ impenetrable bosons in the toroidal trap, we use $N$ displaced orbitals $\varphi(r,R_{i})$, $i = 1,2,...,N$ [see Eq. (1)] centered at the vertices of a regular polygon. Then, we first construct an unrestricted Bose Hartree-Fock (UBHF) permanent $\Phi^{UBHF}$ of $\Phi^{UBHF} \propto \sum_{P_{(i<m)}} \varphi_{1}(r_{1})\varphi_{2}(r_{2})...\varphi_{N}(r_{N})$. The UBHF permanent breaks the circular symmetry of the many-body hamiltonian. The “symmetry dilemma” is resolved through a subsequent “symmetry-restoration” step accomplished via projection techniques [12, 13, 14], i.e., we construct a many-body wave function with good total angular momentum by applying the projection operator $P_{L} = (1/2\pi) \int_{0}^{2\pi} d\theta \exp[i\theta(L - L')]$, so that the final RBM wave function is given by

$$
|\Psi^{PRJ}_{N,L}\rangle = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta |\Phi^{UBHF}_{N}(\theta)\rangle e^{i\delta L}.
$$

$|\Phi^{UBHF}_{N}(\theta)\rangle$ is the original UBHF permanent rotated by an azimuthal angle $\theta$. We note that, in addition to having good angular momenta, the projected (PRJ) wave function $|\Psi^{PRJ}_{N,L}\rangle$ has also a lower energy than that of $|\Phi^{UBHF}_{N}\rangle$ [see, e.g., $E_{L}^{PRJ} - E^{UBHF}$ in Fig. 1(b)].

The projected ground-state energy is given by

$$
E_{L}^{PRJ} = \int_{0}^{2\pi} h(\theta)e^{i\delta L} d\theta / \int_{0}^{2\pi} n(\theta)e^{i\delta L} d\theta,
$$

where $h(\theta) = \langle \Phi^{UBHF}_{N}(\theta = 0) | H | \Phi^{UBHF}_{N}(\theta) \rangle$ and $n(\theta) = \langle \Phi^{UBHF}_{N}(\theta = 0) | \Phi^{UBHF}_{N}(\theta) \rangle$; the latter term ensures proper normalization.

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For anticipates the emergence of concentric ring structures. rally in a toroidal trap. Indeed, in harmonic traps, one than the simple \((0, 1, 2, 3, 4, \ldots)\) arrangement that appears naturally in a toroidal trap. Indeed, in harmonic traps, one anticipates the emergence of concentric ring structures. For \(N = 6\) neutral bosons in a harmonic trap, we observe that, as in the case of a toroidal trap, the ground-state energy as a function of the reduced rotational frequency, \(\Omega/\omega_0\), [Fig. 3(a)] is composed of linear segments, but now the corresponding magic angular momenta [Fig. 3(b)] vary in steps of \(N - 1 = 5\) units. This indicates an RBM consisting of two polygonal rings; denoted as a \((1, 5)\) structure, with the inner ring having a single boson and the outer ring five.

In Fig. 4(a), we display the RBM and mean-field GP ground-state energies of \(N = 6\) strongly repelling (i.e., \(R_3 = 50\)) neutral bosons in a harmonic trap as a function of the reduced angular frequency of the trap. The GP curve (thin solid line; online red) remains well above the RBM curve (thick solid line; online green) in the whole range \(0 \leq \Omega/\omega_0 \leq 1\). The RBM ground-state angular momenta exhibit again the periodicity in steps of five units [Fig. 4(b)]. As expected, the GP total angular momenta are quantized \([L_z = 0 \text{ (no-vortex)} \text{ or } L_z = 6 \text{ (one central vortex)}]\) only for an initial range \(0 \leq \Omega/\omega_0 \leq 0.42\). For \(\Omega/\omega_0 \geq 0.42\), the GP total angular momentum takes non-integer values and ceases to be a good quantum number, reflecting the broken-symmetry character of the associated mean field, with each kink signaling the appearance of a different vortex pattern of \(p\)-fold symmetry (\(p = 1, 2, 3, 4, \ldots\)) \(\mathbb{E}\); see an example in Fig. 4(c).

The energetic superiority of the RBM wave function over the GP solution demonstrated in Fig. 4(a) was to be expected, since we considered the case of strongly repelling bosons. Unexpectedly, however, for a small number of neutral bosons the energetic advantage of the RBM persists even for weakly repelling bosons, as illustrated in Fig. 5(a). Indeed, Fig. 5(a) displays the RBM (thick solid line; online green) and GP (thin solid line; online red) ground-state energies for \(N = 6\) neutral bosons in a trap rotating with \(\Omega/\omega_0 = 0.85\) as a function of the interaction parameter \(R_3\). The surprising result in Fig. 5(a) is that the GP energy remains above the RBM curve even for \(R_3 \to 0\). Of course the RBM wave function is very close to that of a BEC without vortices when \(R_3 \to 0\) (BECs without vortices are approximately feasible for small \(N\)). However, for small \(N\), our results show that BECs with vortices (i.e., for \(L_z \geq N\)) are not the preferred many-body ground states; instead, formation of RBMs is favored. Note that the energy difference \(E_{\text{GP}} - E_{\text{PRJ}}\) increases rapidly with increasing \(R_3\), reflecting the fact that the RBM energies saturate (as is to be expected from general arguments), while the GP ener-

![FIG. 2: Single-particle densities and CPDs for \(N = 8\) bosons in a rotating toroidal trap with \(\Omega/\omega_0 = 0.2\) and \(R_3 = 50\). The remaining trap parameters are as in Fig. 1. (a) GP sp-density. (b) UBHF sp-density exhibiting breaking of the circular symmetry. (c) RBM sp-density exhibiting circular symmetry. (d) CPD for the RBM wave function [PRJ wave function, see Eq. 4] revealing the hidden point-group symmetry in the intrinsic frame of reference. The observation point is denoted by a white dot. The RBM ground-state angular momentum is \(L_z = 16\). Lengths in units of \(l_0\). The vertical scale is the same for (b), (c), and (d), but different for (a).

![FIG. 3: Properties of \(N = 6\) neutral bosons in a rotating harmonic trap as a function of the reduced rotational frequency \(\Omega/\omega_0\). The confining potential is given by Eq. 2 with \(n = 2\) and \(r_0 = 0\), and the interaction-strength parameter was chosen as \(R_3 = 50\). The intrinsic molecular structure is \((1, 5)\). (a) RBM ground-state energies, \(E_{\text{PRJ}}\). The inset shows a smaller range. The numbers denote ground-state angular momenta. (b) Total angular momenta associated with (i) the RBM ground states (thick solid line showing steps; online black) and (ii) the UBHF solutions (thin solid line; online red).]
FIG. 4: Properties of GP solutions (thin solid line; online red) versus those of RBM wave functions (thick solid line; online green) for \( N = 6 \) neutral bosons as a function of the reduced rotational frequency \( \Omega/\omega_0 \). A harmonic trap is considered, and the interaction strength equals \( R_\delta = 50 \). (a) Ground-state energies. (b) Associated ground-state angular momenta. (c) GP (BEC) sp-density at \( \Omega/\omega_0 = 0.65 \) having 7 vortices with a 6-fold symmetry (thus exhibiting breaking of the circular symmetry). (d) RBM sp-density at \( \Omega/\omega_0 = 0.65 \) which does not break the circular symmetry. (e) CPD of the RBM at \( \Omega/\omega_0 = 0.65 \) revealing the intrinsic (1,5) crystalline pattern. The white dot denotes the observation point \( r_0 \). Note the dramatic difference in spatial extent between the GP and RBM wave functions [compare (c) with (d) and (e)]. Lengths in units of \( l_0 \). The vertical scale is the same for (d) and (e), but different for (c).

 FIG. 5: Properties of GP solutions (thin solid line; online red) versus those of RBM wave functions (thick solid line; online green) for \( N = 6 \) bosons as a function of the interaction strength \( R_\delta \), and the recently demonstrated ability to experimentally control \( R_\delta \) \[1, 2, 3, 4\], we anticipate that our results could be tested in experiments involving rotating optical lattices. Detection of RBMs could be based on a variety of approaches \[5\], such as the measurement of the spatial extent [contrast the RBM and BEC spatial extents in Figs. 4(c)-4(e)], or the use of Hanbury Brown-Twiss-type experiments \[6\] to directly detect the intrinsic crystalline structure of the RBM.

This work is supported by the US D.O.E. (Grant No. FG05-86ER45234) and the NSF (Grant No. DMR-0205328).

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(LLL) only in the limit when $\lambda = \sqrt{2}l_B$ in the case of a magnetic field, or $\lambda = \sqrt{2}l_\Omega$ and $\Omega/\omega_0 = 1$ in the case of a rotating trap. LLL investigations of neutral bosons using exact diagonalization (EXD) techniques have attempted to introduce analogies with the liquid-like bosonic Laughlin and composite-fermion wave functions [see e.g., Th. Jolicoeur and N. Regnault, Phys. Rev. B 70, 241307 (2004)]. Recently, however, the possibility of localization of neutral bosons in the LLL is also attracting attention. In particular, the EXD study in Ref. [11] shows that, for small $N$, formation of vortices in the LLL is not a prevalent phenomenon, and their appearance “is restricted to the vicinity of some critical values of the rotational frequency ...”

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