Effects of finite-range Gaussian repulsion on trapped many-boson system

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We investigate a rotating system of $N$ spinless bosons confined in quasi-two-dimensional harmonic trap with repulsive finite-range Gaussian interaction potential of large $s$-wave scattering length. Exact diagonalization of the Hamiltonian matrix in subspaces of quantized total angular momenta $L_z$ is carried out to obtain the $N$-body ground states in slow rotating regime of $0 \leq L_z \leq 2N$. We study the finite-range effects of the Gaussian repulsion potential on the many-body ground state properties in different subspaces of quantized $L_z$. The study ranges from the few-body ($N = 2$) system to the many-body ($N = 16$) system, where quantum (Bose) statistics becomes perceptible. In particular, we analyze the effect of interaction range of the Gaussian potential on the ground state energy of different $L_z$ states as well on the critical angular velocity $\Omega_{1}$ of first vortex ($L_z = N$) state. For an optimal value of the range of the Gaussian interaction potential, the nucleation of the first centered vortex may begin at a lower value of the rotational angular velocity as compared to the zero-range interaction potential. Moreover, we explore the role of interaction potential range on the quantum correlation (measured in terms of the degree of condensation and the von Neumann entropy), for small systems ($N = 2$ to $8$) where an understanding of few-body effects provide valuable insight into large systems ($N = 8$ to $16$) which admit the possibility of many-body correlation. The results obtained indicate that the finite-range Gaussian interaction potential enhances the degree of condensation compared to the zero-range interaction potential.

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I. INTRODUCTION

Ever since the experimental realization of Bose-Einstein condensate (BEC) with ultracold alkali atomic vapors \cite{1,2,3}, attempts have been made to examine the role of various energy scales in the physics of quantum systems of interacting particles rotating in a trap \cite{4,5}. The decisive control over parameters such as density, effective dimensionality and the particle-particle interactions \cite{6,7} enables one to examine their effects on the quantum many-body states. With recent advances in BEC on optical lattices \cite{2} and microchip traps \cite{11,12}, the few-body systems (seem to be possible to reach) have attracted particular attention of theorists \cite{12}. An understanding of the physics of few-body systems provide an insight into the beyond mean-field physics of macroscopic ensembles \cite{13}. For dilute gas systems at low-enough temperatures, the interparticle interaction being short-ranged is usually described by zero-range ($\delta$-function) potential \cite{4}. This approach is useful in case of one dimensional system as the $\delta$-function interaction is well understood and easy to handle. Unfortunately, such an interaction potential in 2D is not self-adjoint \cite{14} and cannot be used in a manner analogous to its one dimensional counterpart. Using configuration interaction, it is shown in Ref. \cite{15} that a $\delta$-function is not suitable as a replacement for the two-body interaction in exact theories. Indeed a regularized 2D contact potential is analytically tractable \cite{16} but harder to handle it numerically. Further as the number of particles is increased beyond two, the complexity of the quantum states increases quickly and the analytical treatment becomes intractable, leaving one only with a numerical recourse. It has been demonstrated that in order to tackle the limit of zero-range interaction numerically \cite{17}, a prohibitively large Hilbert space is required to obtain the many-body ground state of the system. For numerical many-body simulation, one usually prefers a smooth, finite-range, model interaction potential. This leads us to use the finite-range Gaussian potential as a model inter-particle interaction \cite{17,18}, in the trapped interacting few-boson system. More control over the inter-particle interaction with the variation of interaction range and being expandable within finite number of basis functions of the Hilbert space, are few of the advantages of the Gaussian potential over the usual $\delta$-function potential. Besides, most of the mean field as well as the many-body calculations on harmonically confined interacting Bose gas use only the lowest-Landau-levels (LLL), in which bosons occupy single-particle states with radial quantum number $n_r = 0$ and angular momentum quantum number $m$ taking positive sign. There are studies \cite{19,20} wherein it has been argued that for slow rotating \cite{21} and moderately to strongly interacting \cite{22} bosons, it becomes necessary to consider the single-particle states beyond LLL approximation with $n_r = 0, 1, \ldots$, while $m$ is allowed to take positive as well as negative values in constructing the many-body basis states. Thus, we are motivated to study the many-body dynamics beyond the LLL approximation in moderately interacting system with finite-range Gaussian potential as an urgent issue.

In our last work \cite{23} for a non-rotating system of fixed number of bosons, we examine the ground state and the first breathing mode with a Gaussian repulsion. Our aim in the present work is to investigate in detail the problem.
(various quantum mechanical ground state properties) of rotating system of $N$ ($2 \leq N \leq 16$) spinless bosons repulsively interacting via finite-range Gaussian potential (of large $s$-wave scattering length) in a quasi-two-dimensional (quasi-2D) harmonic trap. The exact diagonalization of the many-body Hamiltonian matrix is carried out in given subspaces of quantized total angular momentum $L_z$ using Davidson iterative algorithm [24] to obtain the lowest-energy eigenstates of the system in the co-rotating frame. The whole study of the many-body ground state properties of the rotating Bose-condensed gas is carried out beyond the usual LLL approximation [19]. We focus on quite small angular momentum regime $0 \leq L_z \leq 2N$ and are mainly interested in exploring the vicinity of first central vortex ($L_z = N$) state. To study the effect of the interaction potential range on the Bose-condensed system, we used finite-range Gaussian potential to avoid the mathematical difficulties of the contact ($\delta$-function) interaction in connection to the diagonalization of the many-body Hamiltonian [23, 24]. We examine in detail the role of interaction potential range on the various quantities of interest which are experimentally accessible such as the ground state energy, degree of condensation, von Neumann entanglement entropy and critical angular frequencies of interest which are experimentally accessible such as the ground state energy, degree of condensation, von Neumann entanglement entropy and critical angular velocity $\Omega_{\perp 1}$ of first vortex state $L_z = N$. The results obtained demonstrate that the use of (repulsive) particle-particle Gaussian interaction has a dramatic effect on the many-body ground state properties.

This paper is organized as follows. In Sec. II we describe the model Hamiltonian of a rotating Bose system with finite-range Gaussian interaction in quasi-2D harmonic trap. We then introduce the single-particle reduced density matrix to delineate the criterion for the existence of BEC as well as its degree of condensation and von Neumann entanglement entropy. In our exact diagonalization calculation, we provide a justification for the adoption of Gaussian interaction potential, instead of the usual contact ($\delta$-function) potential. In Sec. III we present the exact results for a system of $N$ bosons, to explore the finite-range effects with strong $s$-wave scattering length, on the many-body ground state properties of the system. First, we examine the non-rotating system with $L_z = 0$ followed by the rotating system in different $L_z > 0$ subspaces with emphasis on the first vortex state with $L_z = N$. Finally in Sec. IV we summarize the main results of the present study.

**II. THEORETICAL MODEL**

**A. The System and The Hamiltonian**

We consider a system of $N$ interacting spinless bosons each of mass $M$, trapped in a harmonic potential $V(\mathbf{r}) = \frac{1}{2} M (\omega_z^2 r_z^2 + \omega_{\perp}^2 z^2)$. The trap with $x$-$y$ rotational symmetry is rotating around the $z$-axis with angular velocity $\Omega \equiv \Omega \hat{z}$. Here $r_{\perp} = \sqrt{x^2 + y^2}$ is the radial distance of the particle from the trap center; $\omega_{\perp}$ and $\omega_z$ are the radial and the axial frequencies respectively, of the harmonic confinement. The axially symmetric trapping potential $V(\mathbf{r})$ is assumed to be highly anisotropic with $\lambda_z = \omega_z / \omega_{\perp} \gg 1$, so that the many-body dynamics along $z$-axis is frozen. The confined system is thus effectively quasi-two-dimensional (quasi-2D) with $x$-$y$ rotational symmetry. We chose $\hbar \omega_{\perp}$ as the unit of energy and $a_{\perp} = \sqrt{\hbar / M \omega_{\perp}}$ as the corresponding unit length. Introducing $\Omega \equiv \Omega / \omega_{\perp} (\leq 1)$ as the dimensionless angular velocity and $L_z$ (scaled by $\hbar$) being the $z$ projection of the total angular momentum operator, the many-body Hamiltonian in the co-rotating frame is given as $H^{\text{rot}} = H^{\text{lab}} - \Omega L_z$ where

$$H^{\text{lab}} = \sum_{j=1}^{N} \left[ -\frac{1}{2} \nabla_j^2 \right] + \frac{1}{2} N \sum_{i \neq j} U(\mathbf{r}_i, \mathbf{r}_j) \quad (1)$$

The first two terms in the Hamiltonian correspond to the kinetic and potential energies respectively, and the third term $U(\mathbf{r}_i, \mathbf{r}_j)$, arises from the particle-particle interaction, is described by the Gaussian potential

$$U(\mathbf{r}_i, \mathbf{r}_j) = \frac{g_2}{2\pi \sigma^2} \exp \left[ -\frac{(\mathbf{r}_i - \mathbf{r}_j)^2}{2\sigma^2} \right] \quad (2)$$

with parameter $\sigma$ (scaled by $a_{\perp}$) being the effective range. The dimensionless parameter $g_2 = 4\pi a_{\perp} a_s / a_{\perp}$ is a measure of the strength of interaction where $a_s$ is the $s$-wave scattering length taken to be positive ($a_s > 0$) so that the effective interaction is repulsive. In the limit $\sigma \to 0$, the normalized Gaussian potential in Eq. (2) reduces to the zero-range contact potential $g_2 \delta(\mathbf{r} - \mathbf{r}')$, which has been used in earlier studies [4]. The values of interaction range $\sigma$ considered, may depend on the size of the system and vary from zero to the system size, $a_{\perp}$. For a fixed value of range $\sigma$, the parameter $g_2$ is adjusted such that $U(\mathbf{r}, \sigma, g_2)$ has a large $s$-wave scattering length $a_s$. In addition to being physically more realistic, the finite-range Gaussian interaction potential is expandable within a finite number of single-particle basis functions and hence computationally more feasible compared to the zero-range $\delta$-function potential [20].

Since the system being studied here is rotationally invariant in the $x$-$y$ plane, the $z$-component of the total angular momentum is a good quantum number leading to block diagonalization of the Hamiltonian matrix in each of the subspaces of $L_z$ separately [19]. To obtain the many-body eigenstates, we employ exact diagonalization of the Hamiltonian matrix in different subspaces of $L_z$ with inclusion of lowest as well as higher Landau levels in constructing the $N$-body basis states [19, 20]. The respective many-body Hilbert space may be restricted to the space spanned by the single-particle basis functions $u_{n}(\mathbf{r})$ within the 2D plane, where $n \equiv (n, m)$ is set of single-particle quantum numbers with $n = 2n_r + |m|$ where the radial quantum number $n_r = 0, 1, \ldots$ and angular momentum quantum number $|m| = 0, 1, 2, \ldots$, as discussed earlier for beyond LLL approximation. Therefore, the $N$-body variational wavefunction $\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ for a given $L_z$, is constructed...
as linear combination of the symmetrized products of a finite number of single-particle basis functions \( u_\mu (r) \) chosen to be the eigenfunctions of the non-interacting (one-body) Hamiltonian. Details of the diagonalization scheme and beyond LLL approximation employed here, has been presented in Ref. [10].

For a system of \( N \) bosons confined in a trap rotating with angular velocity \( \Omega \), the ground state is obtained by minimizing the free energy \( F(T,V,N) = E(S,V,N) - TS \) given by \( e^{-\beta F} = \text{Tr} \left[ e^{-\beta (H_{\text{lab}} - \Omega L_z)} \right] \).

At zero temperature, it reduces to \( E(S = 0, V, N) = \langle \Psi_0 \left| (H_{\text{lab}} - \Omega L_z) \right| \Psi_0 \rangle \), where \( \Psi_0 \) is the variationally obtained ground state with \( L_z \), in the non-rotating (laboratory) frame. Therefore, the many-body Hamiltonian \( H_{\text{lab}} \) in Eq. (1) is diagonalized in given subspaces of \( L_z \) to obtain the free energy \( E^{\text{rot}} (L_z, \Omega) = E^{\text{lab}} (L_z) - \Omega L_z \) in the co-rotating frame. This is equivalent to minimizing \( E^{\text{lab}} (L_z) \) subject to the constraint that the system has angular momentum expectation value \( L_z \) with angular velocity \( \Omega \) identified as the corresponding Lagrange multiplier. Fixing \( L_z \), therefore, fixes \( \Omega \) and accordingly we will mention \( L_z \) (instead of \( \Omega \)), throughout this work.

**B. Physical Quantities of Interest**

*Single-particle reduced density matrix.* The \( N \)-body ground state wavefunction \( \Psi_0 (r_1, r_2, \ldots, r_N) \) obtained variationally through exact diagonalization, is assumed to be normalized. One can then derive the zero-temperature single-particle reduced density matrix \( \rho_1 (r, r') \), by integrating out the degrees of freedom of \((N - 1)\) particles. Thus

\[
\rho (r, r') = \int \cdots \int dr_2 \, dr_3 \cdots dr_N \times \Psi_0^* (r, r_2, r_3, \ldots, r_N) \Psi_0 (r', r_2, r_3, \ldots, r_N) = \sum_{n,n'} \rho_{nn'} \, u_n^* (r) \, u_{n'} (r').
\]

The above expression is written in terms of single-particle basis functions \( u_n (r) \) with quantum number \( n \equiv (n, m) \). Being hermitian, this can be diagonalized to give

\[
\rho_1 (r, r') = \sum_{\mu} \lambda_\mu \, \chi_\mu^* (r) \chi_\mu (r') = \sum_{\mu} \lambda_\mu \, \chi_\mu (r) \chi_\mu (r'),
\]

where \( \chi_\mu (r) \equiv \sum_n c_\mu^* \, u_n (r) \) and \( \sum_{\mu} \lambda_\mu = 1 \) with \( 1 \geq \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N = 0 \). The \( \{ \lambda_\mu \} \) are the eigenvalues, ordered as above, and \( \{ \chi_\mu (r) \} \) are the corresponding eigenvectors of the single-particle reduced density matrix \( \rho_1 (r, r') \); each \( \mu \) defines a fraction of the BEC.

**Degree of condensation.** It is to be noted that the usual definition of condensation for a macroscopic system, given by the largest eigenvalue \( \lambda_1 \) of the single-particle reduced density matrix, is not appropriate for systems with small number of particles being studied here. For example, in the absence of condensation, there is no macroscopic occupation of a single quantum state and all levels are equally occupied, such a definition would imply a condensate though with small magnitude. To circumvent this situation, one introduces a quantity which is sensitive to the loss of macroscopic occupation called the degree of condensation defined as

\[
C_d = \lambda_1 - \bar{\lambda}
\]

where \( \bar{\lambda} = \frac{1}{p} \sum_{\mu=2}^{p} \lambda_\mu \) is the mean of the rest of eigenvalues. It can be seen that the degree of condensation, defined as in Eq. (5), approaches zero for equal eigenvalues, as one would expect.

**von Neumann entanglement entropy.** In order to measure the quantum correlation of a many-body ground state, we calculate von Neumann entropy \([27–29]\) defined as

\[
S_1 = - \text{Tr} (\rho_1 \ln \rho_1)
\]

with \( \rho_1 \) being the single-particle reduced density operator obtained from the many-body ground state wavefunction. In terms of eigenvalues \( \{ \lambda_\mu \} \) and eigenfunctions \( \{ \chi_\mu (r) \} \), then, the von Neumann entropy is evaluated explicitly as

\[
S_1 = - \sum_{\mu} \lambda_\mu \ln \lambda_\mu
\]

in subspaces of total angular momentum \( L_z \). The entropy \( S_1 \) also provides information about the degree of condensation \( C_d \). For instance, for a perfect BEC, the value of \( C_d \) approaches to unity correspondingly the value of \( S_1 \) is zero, from Eq. (5) and (7) respectively, since all bosons assume to occupy one and the same mode that is macroscopic eigenvalue \( \lambda_1 \sim 1 \) and \( \lambda_\mu \sim 0 \) for \( \mu > 2 \). As the condensate depletes (due to rotation or interaction), with more than one eigenvalue \( \{ \lambda_\mu \} \) becoming non-zero, \( S_1 \) increases and correspondingly \( C_d \) decreases.

**III. NUMERICAL RESULTS AND DISCUSSION**

We consider an interacting system of few to many (\( 2 \leq N \leq 16 \)) Bose atoms of \(^{87}\text{Rb}\) confined in an axially symmetric harmonic trap. The radial trapping frequency is taken to be \( \omega_\parallel = 2\pi \times 220 \text{Hz} \) corresponding to the trap length \( a_\perp = \sqrt{\hbar / M \omega_\perp} = 0.727 \mu \text{m} \) and the aspect ratio of the trap \( \lambda_z = \omega_z / \omega_\perp = \frac{\sqrt{5}}{2} \), so that the system has negligible extension \( a_z = \sqrt{\hbar / M \omega_z} = a_\perp \lambda_z^{-1/2} \) in the \( z \)-direction and its dynamics along this axis can be assumed to be completely frozen resulting in a quasi-2D system. Recent advancements in atomic physics have made it possible to tune the scattering length (from infinitely weak to strong) in ultracold atomic vapors using Feshbach resonance \([5,8]\). In the results presented here, the parameters of Gaussian interaction potential in Eq. (4) have been chosen as the interaction range \( 0 \leq \sigma \leq 0.9 \) (in units of \( a_\perp \)) and the \( s \)-wave scattering length \( a_s = 10000 \, a_0 \) where \( a_0 = 0.05292 \text{nm} \) is the
Bohr radius. The corresponding value of the dimensionless interaction parameter \( g_2 = 4\pi a_s / a \) turns out to be 9.151. It is to be noted that for a many-body system being studied here, the characteristic energy scale for the interaction is determined by the dimensionless parameter \( (N a_s / a \) \). Owing to increasing dimensionality of the Hilbert space with \( N \) making computation impractical, we vary \( a_s \), in our calculation here, to achieve suitable value of \( (N a_s / a \) \) relevant to experimental situation [4]. The scattering length \( a_s \) has been consciously chosen to be large so that the parameter \( (N a_s / a \) \) \( \sim 1 \) corresponding to moderate interaction [19, 20]. From now on we fix the parameter \( g_2 = 9.151 \) and vary the value of Gaussian range \( \sigma \) from zero (corresponding to \( \delta \)-function potential) to a value determined by the system size \( \sim a \). The \( N \)-body variational ground state wavefunction in lowest Landau-level (LLL) approximation [19, 20] is obtained through exact diagonalization of the Hamiltonian matrix for each of the subspaces of quantized total angular momentum \( 0 \leq L_z \leq 2N \) using Davidson iterative algorithm [24]. The results obtained with repulsive Gaussian interaction potential [2] allow us to study the effect of the range \( \sigma \) of interparticle interaction on the various quantum mechanically interesting properties of the Bose-condensed gas are discussed in the following.

### A. Non-rotating System

Initially, when the system is subjected to rotation with \( 0 \leq \Omega \leq \Omega_{c1} \) (where \( \Omega_{c1} \) is the critical angular velocity of the first vortex state), the angular momentum state \( L_z = 0 \) corresponds to the many-body ground state (with the lowest energy in the co-rotating frame). Here, we examine the non-rotating \( N \)-boson (\( 2 \leq N \leq 16 \)) ground state in \( L_z = 0 \) subspace as the range of interaction is varied over \( 0 \leq \sigma \leq 0.9 \) for the repulsive finite-range Gaussian interaction potential [2].

**Many-body ground state energy.** We first explore the dependence of ground state energy on the parameter \( \sigma \). In Fig. 1, we present the variation of ground state energy per particle \( E/N \) with the range of interaction \( \sigma \) for \( N = 2, 4, 8, 12 \) and 16 bosons in \( L_z = 0 \) subspace. For the smallest system with \( N = 2 \) bosons, we observe in Fig. 1(a) that the ground state energy increases initially for small values of \( \sigma \) attaining a peak at \( \sigma = 0.55 \) and then decreases monotonically as \( \sigma \) is increased further. For large values of \( \sigma \gg 1 \), when the range of interaction potential is much greater than the system size \( a \) (not shown in the figure), the ground state energy is found to approach the non-interacting value \( E/N = 0 \). The interaction energy becomes negligible. Our results on \( \sigma \)-dependence of the ground state energy of \( N = 2 \) particle in small \( \sigma \) limit is in good agreement with a recent work [17].

To examine the effect of quantum statistics, we study more than two bosons with Gaussian repulsion potential [2] and find that there is a change in \( \sigma \)-dependence of the ground state energy as the number of bosons is increased. For few boson systems with \( N \leq 4 \), the effect of quantum statistics is insignificant and the results are qualitatively similar to those presented for two bosons. It is seen from Figs. 1(a) and 1(b) that the peak of the ground state energy per particle versus \( \sigma \) plot, shifts to larger values of \( \sigma \) as the number of particles is increased from \( N = 2 \) to \( N = 4 \). For \( N = 8 \), the effect of quantum statistics begins to show up and the peak of the \( E/N \) versus \( \sigma \) plot, shifts to smaller values of \( \sigma \). This reversal in trend, of the peak position of \( E/N \) versus \( \sigma \) plot as \( N \) is increased from 2 to 8, is due to quantum statistics. For \( N > 8 \), the effect of quantum statistics becomes fully developed and the \( E/N \) versus \( \sigma \) plot exhibits a monotonic trend. Accordingly, we observe from Fig. 1(d) for \( N = 12 \) and Fig. 1(c) for \( N = 16 \) that the ground state energy changes very little for small values of \( \sigma \) but as \( \sigma \) is increased further over the range \( 0.1 \leq \sigma \leq 0.9 \), the \( E/N \) versus \( \sigma \) plot exhibits a monotonic decrease showing no peaks. The dependence of energy on the interaction range \( \sigma \) is quite identical (always decreasing) for relatively large values of \( \sigma \leq 1 \), regardless of the number of particles \( N \). It, however, shows departure for small values of \( \sigma \), namely, the ground energy increases for small number of particles \( 2 \leq N \leq 8 \) but remains constant for \( N > 8 \) as the range \( \sigma \) is increased.

**Quantum correlation.** To further analyze the effect of interaction range \( \sigma \) of the Gaussian interaction potential [2] on the quantum mechanical correlation or phase coherence of the Bose-condensed gas, we calculate the single-particle reduced density matrix defined in Eq. (1). The many-body quantum correlation is measured, here, in terms of the degree of condensation \( C_d \) and the von
Neumann entanglement entropy $S_1$ defined in Eq. (5) and (7), respectively.

![Diagram](image_url)

**FIG. 2.** (Color online) For the non-rotating system corresponding to $L_z = 0$ subspace, the $N$-body ground state of $N = 2$ (black squares), 4 (red circles), 8 (blue triangles), 12 (green rhombus) and 16 (pink stars) bosons interacting via Gaussian potential (2) with $g_\perp = 9.151$: (a) von Neumann entropy $S_1$ and (b) degree of condensation $C_d$ as a function of the interaction range $\sigma$ (in units of $a_\perp$).

We first examine quantum correlation through the dependence of von Neumann entropy $S_1$ on the interaction range $\sigma$ of the Gaussian potential (2). The results are presented in Fig. 2(a) where the values of entropy $S_1$ are plotted as a function of $\sigma$ for a system of $N = 2, 4, 8, 12$ and 16 bosons in the angular momentum subspace $L_z = 0$. We observe that for a fixed value of $\sigma$, the entropy $S_1$ gains a large value with increase in number of particles $N$. However, for a given number of bosons $N$, the value of $S_1$ decreases with $\sigma$ and the decrease in $S_1$ becomes linear at large values of $\sigma < 1$. The dependence of $S_1$ on $\sigma$ is qualitatively similar for all $N$-boson system studied here. It is interesting to note that for relatively large number of particles $N \geq 8$, the entropy $S_1$ decreases sharply with increasing $\sigma$ as the correlation per particle increases with increasing $N$. Accordingly, $S_1$ versus $\sigma$ plot for $N = 16$ bosons, the largest system considered in our case, is the steepest.

The above observation of many-body quantum correlation is further supported by the corresponding degree of condensation. In Fig. 2(b) we present the variation of degree of condensation $C_d$ versus $\sigma$ for a system of $N = 2, 4, 8, 12$ and 16 bosons. For a fixed value of $\sigma$, the degree of condensation $C_d$ decreases for increasing number of particles $N$, as is expected in order to reduce the interparticle repulsion. It is further seen from the figure that the value of $C_d$ increases with increase in $\sigma$ and the variation becomes linear for larger values of $\sigma < 1$. Consequently, with increasing $\sigma$, the degree of condensation $C_d$ increases and the correspondingly von Neumann entropy $S_1$ decreases as shown in Fig. 2(a) leading to increase in phase coherence.

The explanation for such a behavior is that as the range $\sigma$ of the Gaussian interaction potential is increased, the broadened interparticle pair-potentials begin to overlap leading to increase in many-body effects. This increased many-body effect compared to the zero-range ($\delta$-function) potential leads to an enhanced phase coherence, reflected in Figs. 2(a) and 2(b). Thus the use of finite-range Gaussian interaction potential leads to Bose-Einstein condensate with relatively lesser value of entropy and higher degree of condensation than the use of zero-range ($\delta$-function) interaction potential [30].

**B. Rotating System**

The results presented so far have been for the $L_z = 0$ (non-rotating) states. As the system is subjected to an external rotation, higher angular momentum states ($L_z > 0$) which minimize the free energy, become the ground state of the system [31]. We now examine the variation of ground state properties of the rotating system as a function of the interaction range $\sigma$ of the Gaussian repulsion (2), for a fixed number of bosons $N$ in different subspaces of quantized total angular momentum $L_z$. For the sake of comparison, the results are also provided for the non-rotating state $L_z = 0$ in their respective plots.

**Many-body state energy.** Figures 3(a) and 3(b) for a system of $N = 4$ and $N = 8$ bosons, respectively, present the variation of the lowest state energy per particle ($E/N$) in the co-rotating frame with the interaction range $\sigma$, in different subspaces of $L_z$. First, we consider a few-body system with $N = 4$ bosons and observe from Fig. 3(a) that the $\sigma$-dependence of the ground state energy per particle $E/N$ in the angular momentum subspace $L_z = 2$ is similar to the non-rotating ground state with $L_z = 0$. As the angular momentum is increased beyond $L_z = 2$, the energy per particle $E/N$ increases, in general, almost linearly with $\sigma$. For small values of $\sigma$ ($< 0.1$), the value of $E/N$ does not change significantly with $\sigma$. However, for large values of $\sigma$ ($> 0.1$), the effect of increasing rotation on $E/N$ dominates over the effect
of $\sigma$. When the particle number is increased to $N = 8$, the ground state energy $E/N$ decreases with increasing $\sigma$ for a given angular momentum ($L_z \neq 0$) and becomes almost linear for higher angular momentum states, as seen in Fig. 3(b). The trend is thus opposite to the one seen for $N = 4$ system and can be attributed to quantum (Bose-Einstein) statistics.

Quantum correlation. In order to measure the many-body quantum correlation of the rotating system with a fixed number of bosons $N$, we calculate von Neumann entanglement entropy $S_1$ and degree of condensation $C_d$ in different subspaces of total angular momentum $L_z$. In Fig. 3 we plot $S_1$ and $C_d$ as a function of interaction range $\sigma$, for a few-boson system with $N = 4$ in subspaces of $L_z = 0, 2, 4, 6, 8$. It is observed from Fig. 4(a) that for a given $\sigma$, the von Neumann entropy $S_1$ increases with increase in $L_z$. Further, it is found that $S_1$ decreases for increasing $\sigma$ in different subspaces of $L_z$, specifically at large values of $\sigma$. The decreasing behavior of $S_1$ with $\sigma$ is relatively steeper for $L_z = 0, 2, 4, 8$ and moderate for the fragmented state $L_z = 6$, thereby indicating the effect of rotation on $S_1$ similar to energy as discussed above in Fig. 3(a) for $N = 4$ bosons. It is evident from Fig. 4(b) that the degree of condensation $C_d$ increases gradually with $\sigma$ for a given $L_z$, except in the subspace $L_z = 6$, for which it is decreasing with $\sigma$. Moreover, the curves of $C_d$ versus $\sigma$ for the subspaces $L_z = 6$ and $L_z = 8$ intersect around $\sigma = 0.75$, implying the same value of degree of condensation. We find that over the range $0 \leq \sigma \leq 0.9$, the angular momentum state $L_z = 6$ is a fragmented state with more than one macro-scopically large eigenvalues $\lambda_1 \sim \lambda_2$ of the SPRDM in Eq. 1. For example, at $\sigma = 0.75$ in $L_z = 6$ subspace for $N = 4$, the largest two eigenvalues of SPRDM are $\lambda_1 = 0.340$ and $\lambda_2 = 0.310$. On the other hand, the angular momentum state $L_z = 8$ corresponding to a second vortex state for $N = 4$ with $\sigma = 0.75$ have the largest two eigenvalues of SPRDM as $\lambda_1 = 0.338$ and $\lambda_2 = 0.213$.

To examine the effect of quantum statistics, we consider a system of $N = 8$ bosons which appears to be large enough for nucleation of first and second vortex states. We present in Fig. 5 the variation of von Neumann entropy $S_1$ and degree of condensation $C_d$ with the interaction range $\sigma$ for $N = 8$ bosons in different subspaces of $L_z$. It is observed from Fig. 5(a) that $S_1$ decreases with increasing value of $\sigma$ in each subspace.
of $L_z$. This decreasing behavior of $S_1$ with $\sigma$ is found to be steep for $L_z = 0, 8, 16$, moderate for $L_z = 4$ and approximately constant for $L_z = 12$. It is to be noted that for a given value of $\sigma$, the entropy $S_1$ increases with increasing angular momentum $L_z$, except for the first vortex state. The value of $S_1$ is lower for the first vortex state with $L_z = N = 8$ compared to the angular momentum state with $L_z = 4$. This is further supported by the fact that for a given $\sigma$, the degree of condensation $C_d$ decreases with increasing $L_z$, except for the first vortex state $L_z = N = 8$ and the second vortex state $L_z = 12$, as shown in Fig. 5(b). Thus, for small values of $\sigma \leq 0.4$, the $C_d$ versus $\sigma$ curve for $L_z = 8$ and $L_z = 12$ vortical states shift to higher values of $C_d$ compared to $L_z = 4$ state. We also notice that in $L_z = 12$ subspace, the interaction range $\sigma$ of the Gaussian repulsion has hardly any effect on $S_1$ and $C_d$. Further, the $C_d$ versus $\sigma$ curves for $L_z = 12$ and $L_z = 4$ states intersect at $\sigma = 0.4$ and for $L_z = 12$ and $L_z = 16$ states at $\sigma = 0.8$. In the following, now, we discuss the effect of interaction range $\sigma$ on the critical angular velocity of the first vortex with $L_z = N$.

C. First Vortex State

The non-rotating ground state of the system lies in the angular momentum state $L_z = 0$ subspace. As the system is rotated, other (energetically favored) non-zero angular momentum states ($L_z \neq 0$) successively become the ground state of the system. These are obtained by minimizing the free energy in the rotating frame:

$$E^{\text{rot}}(\Omega, L_z; g_2) = E^{\text{lab}}(L_z, g_2) - \Omega L_z$$

where $g_2$ is the interaction parameter. The energy of a vortex-free state $E^{\text{rot}}_0(\Omega)$ in the rotating frame is numerically equal to the energy $E^{\text{lab}}_0$ in the laboratory frame because the angular momentum of a vortex-free state vanishes. A singly quantized vortex along the trap axis has total angular momentum $L_z = N$, therefore, the corresponding energy of the system in the rotating frame is $E^{\text{rot}}_1(\Omega) = E^{\text{lab}}_1 - \Omega N$. The difference between these two energies is the increased energy

$$\Delta E^{\text{rot}}(\Omega) = E^{\text{rot}}_1(\Omega) - E^{\text{rot}}_0(\Omega) = E^{\text{lab}}_1 - \Omega N - E^{\text{lab}}_0$$

associated with the formation of the vortex at an angular velocity $\Omega_{c_1}$. Setting $\Delta E^{\text{rot}}(\Omega) = 0$ gives the corresponding value of the critical angular velocity of the first vortex state with $L_z = N$,

$$\Omega_{c_1} = \frac{E^{\text{lab}}_1 - E^{\text{lab}}_0}{N}$$

expressed solely in terms of the energy $E^{\text{lab}}_1$ of the first centered vortex state ($L_z = N$) as a function of the interaction range $\sigma$ for a rotating system of $N = 4, 8, 12$ and 16 bosons. It is observed from the figure that for a given set of interaction parameters ($g_2$ and $\sigma$) of the repulsive Gaussian potential, the critical angular velocity $\Omega_{c_1}$ of the first vortex state ($L_z = N$) decreases with increase in number of bosons $N$. It is further observed that with increasing $\sigma$, the repulsive Gaussian interaction potential, in general, lowers the critical angular velocity $\Omega_{c_1}$ regardless of the number of bosons $N$. Thus, for a rotating system of $N$ bosons with a given value of interaction parameter $g_2$, there is a value of $\sigma$ for which the critical angular velocity $\Omega_{c_1}$ attains a minimum value. This implies that for an optimal value of $\sigma$ of the Gaussian interaction potential, the nucleation of the first centered vortex may begin at a lower value of rotational angular velocity as compared to the contact
condensed gas. For out a vortex, corresponding to the quantum mechanical vortex state, we determine the difference in von Neumann entropy $\Omega_{c1}$ in Fig. 6(d). The different shape of $\Omega_{c1}$ shifts to larger values of $\sigma$ obtained with repulsive Gaussian interaction potential on the critical angular velocity $\omega_{\perp}$ versus the interaction range $\sigma$ (in units of $a_{\perp}$) of the Gaussian potential (2). With fixed value of interaction parameter $g_2 = 9.151$, the minimum value of $\Omega_{c1}$ is observed (a) for $N = 4$ at $\sigma = 0.4$, (b) for $N = 8$ at $\sigma = 0.65$, (c) for $N = 12$ at $\sigma = 0.7$ and (d) for $N = 16$ at $\sigma = 0.75$ on the system size scale.

For $\sigma \to 0$) interaction potential.

We notice that for small values of $\sigma$ ($< 0.1$), the effect of Gaussian interaction potential on the critical angular velocity $\Omega_{c1}$ is negligible and becomes significant only as the value of $\sigma$ is increased which depends on the number of bosons $N$. For instance, as shown in Fig. 6a for $N = 4$ bosons, the critical angular velocity $\Omega_{c1}$ decreases for small values of $\sigma$ and then increases steeply for large values of $\sigma$. However, as seen in Fig. 6b for $N = 8$ (which may be the least number of particles to produce the first stable vortex state), the decrease in value of $\Omega_{c1}$ with $\sigma$ is steeper than for the $N = 4$ boson system. Similarly, beyond $\sigma = 0.25$, the decrease of $\Omega_{c1}$ with $\sigma$ for $N = 12$ is steeper than for $N = 4$ as shown in Fig. 6c. However, for $N = 16$ bosons, $\Omega_{c1}$ increases with $\sigma$ and a peak appears at $\sigma = 0.45$ in the $\Omega_{c1}$ versus $\sigma$ curve and then falls sharply with a minima at $\sigma = 0.75$ as seen in Fig. 6d. The different shape of $\Omega_{c1}$ versus $\sigma$ curve for $N = 16$ can be attributed to quantum statistics. It is also observed that the critical angular velocity $\Omega_{c1}$ always increases for large values of $\sigma(< 1)$, regardless of the number of bosons considered. Moreover, with increase in number of bosons, the minimum value of $\Omega_{c1}$ obtained with repulsive Gaussian interaction potential shifts to larger values of $\sigma$.

In order to support the above analysis of the first vortex state, we determine the difference in von Neumann entropy of the many-body state with and without a vortex, corresponding to the quantum mechanically stable states (in the co-rotating frame) of the Bose-condensed gas. For $N = 4, 8, 12$ and 16 bosons, Fig. 7 presents the finite-range effect of the Gaussian interaction potential (2) on the change in von Neumann entropy $\Delta S_1 = S_1(L_z = N) - S_1(L_z = 0)$ of the first vortex state $L_z = N$ and the respective ground state $L_z = 0$. We observe a kink at $\sigma = 0.25$ and $\sigma = 0.45$ in the $\Delta S_1$ versus $\sigma$ curve for $N = 12$ and $N = 16$ bosons, respectively, where the effect of quantum statistics is significant, which may be seen as a signature of quantum phase transition.

IV. SUMMARY AND CONCLUSION

In conclusion, we have presented an exact diagonalization study of the finite-range effects of repulsive Gaussian interaction potential, on the rotating system of few ($2 \leq N \leq 16$) harmonically confined bosons in different subspaces of quantized total angular momentum $L_z$. The study considered the variation of experimentally accessible physical quantities such as lowest eigenstate energy, quantum correlation (measured in terms of von Neumann entanglement entropy as well as degree of condensation) and critical angular velocity of the trapped Bose-condensed gas, with interaction range $\sigma$ of the Gaussian potential. For the non-rotating system of $N = 2, 4, 8, 12, 16$ bosons in $L_z = 0$ subspace, the variation of ground state energy with $\sigma$ is obtained. It is found that with small values of $\sigma$, the ground state energy increases for few-bosons $2 \leq N \leq 8$ but decreases for many-bosons $N > 8$, on the other hand with relatively large values of $\sigma < 1$, it exhibits a monotonic decrease regardless of the number of bosons $N$. The effect of quantum (Bose) statistics is observed if more than two-bosons with Gaussian repulsion are considered. The $\sigma$-dependence of the ground state energy of two-boson
trapped system in small $\sigma$ limit, is in good agreement with recent studies \[17\]. For a given $N$, the value of von Neumann entropy decreases and the degree of condensation increases with increase in $\sigma$, leading to an enhanced phase coherence compared to the zero-range ($\delta$-function potential). Thus, the use of repulsive finite-range Gaussian interaction potential leads to Bose-Einstein condensate with relatively lesser value of entropy and higher degree of condensation than the use of zero-range interaction potential \[30\].

For a rotating system with fixed number of bosons $N$ in the angular momentum regime of $0 \leq L_z \leq 2N$, the effect of increasing rotation (with quantized $L_z$) on the ground state energy dominates over the effect of interaction range $\sigma$. The variation of energy versus $\sigma$ for a rotating system, gradually increases for few bosons ($N = 4$) and decreases for $N = 8$ bosons with increase in $L_z > 0$, in contrast to the non-rotating ground state $L_z = 0$. This finding supports the previous notion that when the particle number is increased to $N = 8$, the $\sigma$-dependence of the energy follows trend opposite to that of $N = 4$ boson system and can be attributed to quantum (Bose-Einstein) statistics. For a given $L_z$, the quantum correlation is enhanced with increasing $\sigma$, as the von Neumann entropy decreases and degree of condensation increases, specifically at large values of $\sigma$. However, for a given $\sigma$, von Neumann entropy increases and degree of condensation decreases with increase in $L_z$. The critical role of fragmented state (with more than one macroscopically large eigenvalues of the single-particle reduced density matrix), the first vortex state ($L_z = N$) and the second vortex state are also discussed here.

Further, for a given value of $\sigma$, the critical angular velocity $\Omega_{c1}$ of the first vortex state ($L_z = N$) decreases with increase in number of bosons $N$ \[19\]. However, with increasing $\sigma$, the repulsive Gaussian interaction potential, in general, lowers the critical angular velocity $\Omega_{c1}$ regardless of the number of bosons $N$. Thus, for a rotating system of $N$ bosons with a given interaction strength, there is value of $\sigma$ for which the critical angular velocity $\Omega_{c1}$ attains a minimum value. It indicates that for an optimal value of $\sigma$ of the Gaussian interaction potential, the nucleation of the first centered vortex may begin at lower value of rotational angular velocity as compared to the zero-range interaction potential. With increase in number of bosons $N$, the minimum value of $\Omega_{c1}$ obtained with Gaussian repulsion shifts to the larger values of $\sigma$. The effect of interaction range of the Gaussian repulsion potential on the ground state properties is negligible for small values of $\sigma(<0.1)$, however, the effect becomes significant for large values of $\sigma(>0.1)$ on the system size scale. With the possible experimental realization of quasi-2D few-body quantum system in future and the experimental controllability of the scattering length through Feshbach resonance; one may hope that theoretical results obtained here may prove useful for a meaningful study of rotating quantum many-body systems with more realistic interaction potential in two dimensions.

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