Few-Body Syst
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Anna Okopińska · Przemysław Kościk

Entanglement of Two Charged Bosons in Strongly Anisotropic Traps

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Abstract Examination of the ground-state correlation properties of two Coulombically interacting bosons confined in strongly anisotropic harmonic potentials is carried out within the framework of the single-mode approximation of the transverse components. The linear entropy of the quasi-one dimensional systems is discussed in dependence on the confinement anisotropy and the interaction strength. A comparison with a strictly one-dimensional limit is performed.

1 Introduction

Artificially created effective many-body systems such as quantum dots and trapped atoms or ions, which can be investigated under controllable and tunable experimental conditions, are promising candidates for quantum computing devices. The profound understanding of their strongly correlated regime is of particular importance for the practical applications. The Coulombically interacting particles in a harmonic trap can be used to model a system of ions in an electromagnetic trap. Here we consider a system of two bosons confined in an axially symmetric 3D harmonic potential with trapping frequencies ω_x and $\omega_\perp = \epsilon\omega_x$. The system is described by the Schrödinger equation $H\Psi(\mathbf{r}_1, \mathbf{r}_2) = E\Psi(\mathbf{r}_1, \mathbf{r}_2)$ with a Hamiltonian

$$H = \sum_{i=1}^{2}\left[-\frac{\nabla_i^2}{2} + \frac{1}{2}x_i^2 + \frac{1}{2}\epsilon^2\rho_i^2\right] + \frac{g}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{1}$$

where $\rho_i = \sqrt{y_i^2 + z_i^2}$. In order to reduce the number of parameters the coordinates are measured in terms of the longitudinal oscillator length $\sqrt{\frac{m\omega_x}{\hbar}}$, the energies in terms of $\hbar\omega_x$, and the dimensionless coupling $g = \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{m}{\hbar^3\omega_x}}$ represents the ratio of the Coulomb interaction to the longitudinal trapping energy scale. We focus our attention on experimentally accessible quasi-1D case when the anisotropy parameter $\epsilon \gg 1$ and the particles may be assumed to stay in the lowest energy state of the transverse Hamiltonian $H_\perp = -\frac{\nabla_\rho^2}{2} + \frac{1}{2}\epsilon^2\rho^2$. The two-body wave function in the one-mode approximation takes the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) \cong \psi_{1D}(x_1, x_2)\varphi(y_1)\varphi(z_1)\varphi(y_2)\varphi(z_2), \tag{2}$$

A. Okopińska · P. Kościk (✉)
Institute of Physics, Jan Kochanowski University, Świętokrzyska 15, 25-406 Kielce, Poland
E-mail: koscik@pu.kielce.pl

A. Okopińska
E-mail: okopin@fuw.edu.pl

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where $\varphi(y) = (\frac{\epsilon}{\pi})^{\frac{1}{4}} e^{-\frac{\epsilon y^2}{2}}$ and $\varphi(z) = (\frac{\epsilon}{\pi})^{\frac{1}{4}} e^{-\frac{\epsilon z^2}{2}}$, while ψ_{1D} is a real function that fulfills the approximate Schrödinger equation

$$\left[\sum_{i=1}^{2}\left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2}+\frac{1}{2}x_i^2\right]+gU_{1D}(x_2,x_1)+2\epsilon\right]\psi_{1D}(x_1,x_2)=E_{1D}\psi_{1D}(x_1,x_2). \tag{3}$$

with the effective interaction potential $U_{1D}(x_1, x_2) = \sqrt{\frac{\epsilon\pi}{2}} e^{\frac{\epsilon(x_2-x_1)^2}{2}}(1 - erf[\sqrt{\frac{\epsilon}{2}}|x_2 - x_1|])$, where $erf(x)$ is the error function. The effective potential depends on the anisotropy parameter ϵ and we can notice that the larger is the value of ϵ, the closer to the origin does the effective potential begin to exhibit Coulomb behavior. In the 1D limit of $\epsilon \to \infty$, the effective potential becomes Coulombic, and diverges at $x_1 = x_2$, which causes ultraviolet divergences in the direct calculations of symmetric wave functions. Fortunately, the calculation in the strictly 1D limit may be performed [1] thanks to the Bose–Fermi mapping $\psi^+_{1D}(x_1, x_2) = |\psi^-_{1D}(x_1, x_2)|$, which relates the ground-state wave function $\psi^+_{1D}(x_1, x_2)$ to the lowest energy antisymmetric wave function $\psi^-_{1D}(x_1, x_2)$ whose a relative motion part can be determined through the Rayleigh–Ritz method with a basis of odd eigenfunctions of the 1D harmonic oscillator.

2 Localization of the Particles

Localization of the particles can be studied by analysing the two-particle probability density $\psi^2_{1D}(x, x')$. Another source of information is the one-particle reduced density matrix (RDM) defined as

$$\rho(\mathbf{r}, \mathbf{r}') = \int \Psi(\mathbf{r}, \mathbf{r}_2)\Psi(\mathbf{r}', \mathbf{r}_2)d\mathbf{r}_2, \tag{4}$$

which in the one-mode approximation (2) is given by

$$\rho(\mathbf{r}, \mathbf{r}') \cong \varphi(y)\varphi(y')\varphi(z)\varphi(z')\rho_{1D}(x, x'). \tag{5}$$

The 1D effective RDM can be represented in the Schmidt form

$$\rho_{1D}(x, x') = \int \psi_{1D}(x, x_2)\psi_{1D}(x', x_2)dx_2 = \sum_{l=0}^{\infty} \lambda_l v_l(x)v_l(x'), \tag{6}$$

where $\{v_l(x)\}$ are the natural orbitals and their occupancies $\{\lambda_l\}$. In the case of a two-particle system, the natural orbitals can be determined more easily from the wave function, which being real and symmetric, admits the Schmidt decomposition

$$\psi_{1D}(x_1, x_2) = \sum_{l=0}^{\infty} k_l v_l(x_1)v_l(x_2). \tag{7}$$

It is easy to check that the coefficients $\{k_l\}$ are related to the eigenvalues of the RDM by $\lambda_l = k_l^2$. Below we compare the distributions $\psi^2_{1D}(x, x')$ with $\rho_{1D}(x, x')$ for anisotropically confined systems of two Coulombically interacting bosons.

The plots of the two-particle probability densities $\psi^2_{1D}(x, x')$ calculated for a highly anisotropic system ($\epsilon = 30$) are shown in top row of Fig. 1 at four values of the scaled interaction strength g. Due to repulsive nature of the interaction, the probability of finding the bosons close to each other decreases with increasing g, which explains the widening of the gap of vanishingly small probability which stretches along the diagonal. For comparison the probability densities calculated at the same values of g for the strictly 1D system ($\epsilon \to \infty$) are shown in bottom row of Fig. 1. The differences are visible only at small values of g, where the gap in the probability distribution at anisotropy $\epsilon = 30$ is much narrower than that of the corresponding strictly 1D system. Above $g \approx 2$ the differences disappear and the probability distribution of the system with anisotropy $\epsilon = 30$ reproduces the one calculated in the strictly 1D limit.

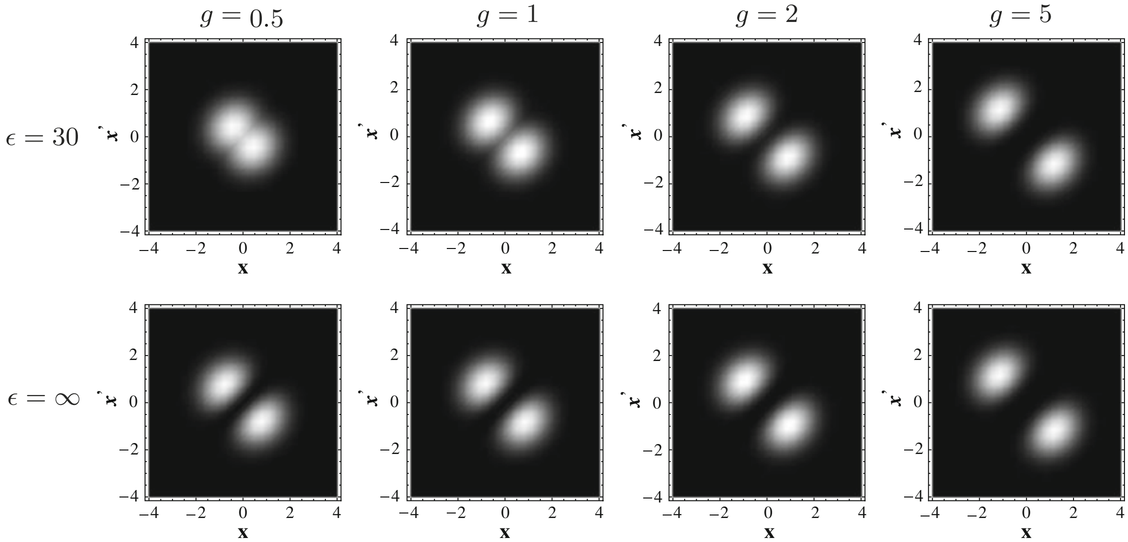

Fig. 1 Two-particle probability density $\psi^2_{1D}(x, x')$ at various interaction strengths $g = 0.5,\ 1,\ 2,\ 5$. The case of anisotropy $\epsilon = 30$ (*top*) compared with the strictly 1D limit of $\epsilon = \infty$ (*bottom*)

In Fig. 2, the plots of the 1D effective RDM $\rho_{1D}(x, x')$ are shown at the same values of g as $\psi^2_{1D}(x, x')$ in Fig. 1. The results for the system with anisotropy $\epsilon = 30$ (top row) are compared with those of the strictly 1D system (bottom row). Similarly as was the case for $\psi^2_{1D}(x, x')$, the differences between RDM at $\epsilon = 30$ and that at $\epsilon \to \infty$ disappear above $g \approx 2$. In the case of $\rho_{1D}(x, x')$, the localization of the particles due to repulsive interaction shows up in diminishing of the off-diagonal contributions with increasing g. It is clearly visible that the off-diagonal parts disappear only above $g \approx 5$ and the particles can be treated as individual entities, which corresponds to a Wigner molecule.

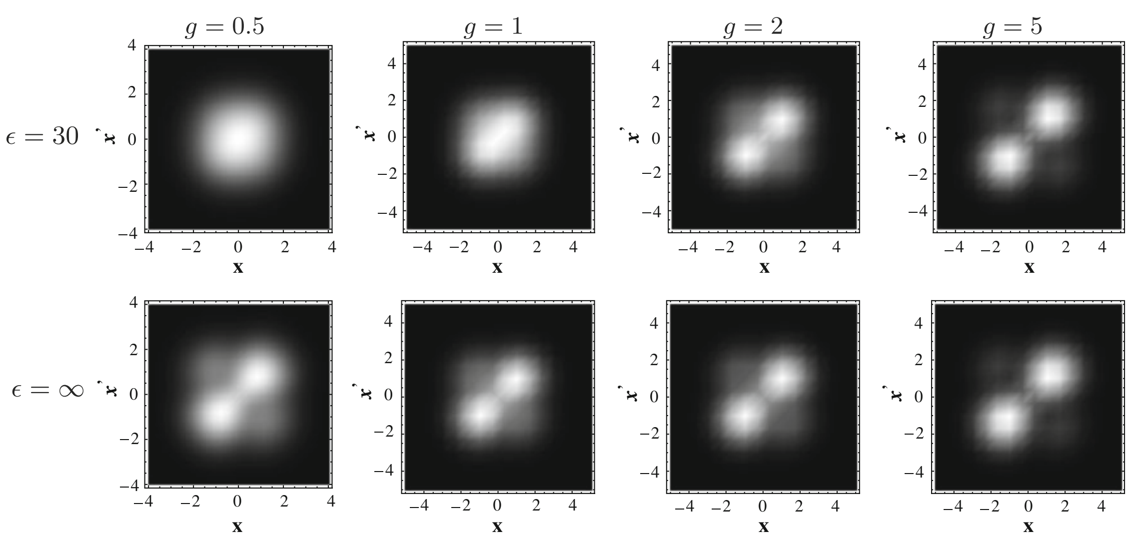

Fig. 2 Effective RDM $\rho_{1D}(x, x')$ at various interaction strengths $g = 0.5,\ 1,\ 2,\ 5$. The case of anisotropy $\epsilon = 30$ (*top*) compared with the strictly 1D limit of $\epsilon = \infty$ (*bottom*)

It is interesting to note that the plots obtained in the strictly 1D limit (bottom rows of Figs. 1, 2) show some similarities to those for the Tonks molecule of two contact interacting bosons in the 1D trap with a barrier of tunable height at the center [2].

3 Entanglement in the Two-Boson System

The entanglement in two-particle systems is fully characterised by the Schmidt decomposition of wave function (7). Popular entanglement measures are constructed as functions of natural orbital occupancies $\{\lambda_l\}$. The easiest to calculate is the linear entropy defined as

$$L = 1 - \int\int \rho_{1D}(x, x')^2 dx' dx = 1 - \sum_l \lambda_l^2. \tag{8}$$

In Fig. 3, we compare our numerical results for the linear entropy of the two Coulombically interacting bosons at various confinement anisotropies with those calculated for the strictly 1D system. The linear entropy increases with g and above $g \approx 5$ saturates at a constant value that does not depend on the anisotropy parameter ϵ.

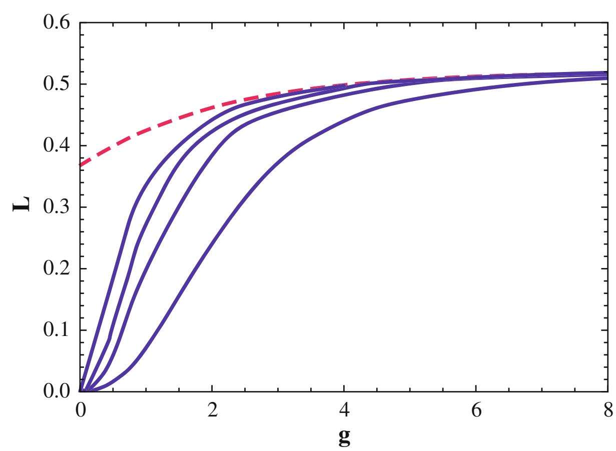

Fig. 3 Linear entropy L as a function of g at different confinement anisotropies $\epsilon = 5,\ 30,\ 100,\ 1,000$. *Dashed line* represents the results for the strictly 1D case

The asymptotics at $g \to \infty$ can be studied analytically, using the harmonic approximation that becomes exact in this limit [3]. The calculation analogous to that performed by us in the 2D case [3] gives $L^{g\to\infty} = 1 - \sqrt{-\frac{3}{2} + \sqrt{3}} \approx 0.518$, which is in agreement with the numerical result. In the limit of $g \to \infty$, we have checked that only two lowest natural orbitals are actively involved in (7), since only their corresponding occupancies have considerable values, namely $k_0^{g\to\infty} \approx -0.7005$, $k_1^{g\to\infty} \approx 0.7005$ ($\lambda_0 = \lambda_1 = 0.4907$), which is reflected by the value of the asymptotic linear entropy. This means that the ground-state of strongly repelling bosons ($g \to \infty$) is represented with a satisfactory accuracy by a single permanent, which implies that the state is almost perfectly fragmented and very weakly entangled [4].

The above calculation can be extended to systems containing more than two particles. The linear entropy in the case of $N = 3$ and $N = 4$ shows a similar behavior [5] to the one shown in Fig. 3. In the systems of ions in linear traps, which provide experimental realization of the discussed model, the values of g are much larger than the value at which we observe the saturation of the entropy. In this regime, the correlation depends very weakly on anisotropy and the strictly one-dimensional approximation is well justified. It would be however interesting to consider systems with larger number of particles and the excited states, where a stronger dependence on the anisotropy is expected. We are also planning to study the time behavior of the entropic correlation measures in quasi-1D systems interacting with external degrees of freedom, which is of vital importance for quantum computing.

We are also planning to study the time behavior of the entropic correlation measures between the external and internal degrees of freedom of the trapped ions, which is of vital importance for quantum computing.

4 Summary

In summary, we investigated the ground-state properties of the system of two bosons that repel by Coulomb interaction in the strongly anisotropic confinement. Within the framework of the single-mode approximation of the transverse component, we calculated the two-particle probability density, the RDM and the linear entropy for several values of the scaled interaction strength g. In the regime of small values of g, the anisotropy parameter ϵ influences the behavior of both the two-particle probability density and the effective 1D RDM, so that increasing anisotropy results in an increase in the interparticle distances. Above $g \approx 2$, there is no appreciable change in the probability distribution and in the RDM with ϵ. The onset of the Wigner crystallization shows up in vanishing of the off-diagonal contributions in the RDM, which happens at $g \gtrsim 5$. The linear entropy of the systems is larger for higher anisotropy and increases with the increase in g. Above $g \approx 5$ the entropy saturates at a constant value that does not depend on the anisotropy, the ground-state of the corresponding system is almost non entangled.

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