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Two-Boson Correlations in Various One-Dimensional Traps

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Abstract A one-dimensional system of two trapped bosons which interact through a contact potential is studied using the optimized configuration interaction method. The rapid convergence of the method is demonstrated for trapping potentials of convex and non-convex shapes. The energy spectra, as well as natural orbitals and their occupation numbers are determined in function of the inter-boson interaction strength. Entanglement characteristics are discussed in dependence on the shape of the confining potential.

1 Introduction

Entanglement as a measure of quantum correlations is investigated in the hope of better understanding the structure of strongly-coupled many-body systems. Recently there is a growing interest in studying few-particle trapped systems, since they became accessible in experiments with ultracold gases in optical lattices and microtraps. The interatomic interaction can be there considered as a contact one. By choosing the transverse confinement much stronger than the longitudinal one, the quasi-one-dimensional systems with an effective interaction $g_{1D}\delta(x_2 - x_1)$ of an adjustable strength g_{1D} may be experimentally realized [1]. In the Tonks–Girardeau (TG) limit of $g_{1D} \rightarrow \infty$ the system is solvable for arbitrary trapping potential [2]. Theoretical consideration of such a system evolution from weak to strong interactions is thus of interest.

We discuss entanglement properties for a system of two bosons interacting through a contact potential and subject to a confining potential $V(x)$. The dimensionless Schrödinger equation takes a form

$$H\phi(x_1, x_2) = E\phi(x_1, x_2), \quad (1)$$

where the Hamiltonian reads

$$H = -\frac{1}{2} \frac{\partial^2}{\partial x_1^2} - \frac{1}{2} \frac{\partial^2}{\partial x_2^2} + V(x_1) + V(x_2) + g_{1D}\delta(x_2 - x_1). \quad (2)$$

Since the two-boson function is symmetric and may be chosen real, there exists an orthonormal real basis $\{v_l\}$ such that

$$\phi(x_1, x_2) = \sum_l k_l v_l(x_1)v_l(x_2), \quad (3)$$

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where the coefficients k_l are real and $\sum_l k_l^2 = 1$. Therefore

$$\int_{-\infty}^{\infty} \phi(x, x') v_l(x') dx' = k_l v_l(x), \quad (4)$$

which means that v_l are eigenvectors of the two-particle function. It may be shown that v_l are also eigenvectors of the density matrix, known as natural orbitals. Density matrix decomposition is given by $\rho(x, x') = \sum \lambda_l v_l(x) v_l(x')$, where the occupancies $\lambda_l = k_l^2$. The number of nonzero coefficients k_l and the distribution of their values characterize the degree of entanglement.

2 Optimized Configuration Interaction Method

The configuration interaction method (CI) consists in choosing the orthogonal basis set in the Rayleigh–Ritz (RR) procedure so as to ensure proper symmetry under exchange of particles [3]. For the two-boson system, the CI expansion reads

$$\phi(x_1, x_2) = \sum a_{ij} \psi_{ij}(x_1, x_2), \quad (5)$$

where $\langle x_1, x_2 | ij \rangle = \psi_{ij}(x_1, x_2) = b_{ij} [\varphi_i(x_1) \varphi_j(x_2) + \varphi_j(x_1) \varphi_i(x_2)]$ with $b_{ij} = 1/2$ for $i = j$ and $b_{ij} = 1/\sqrt{2}$ for $i \neq j$. Exact diagonalization of the infinite Hamiltonian matrix $H_{nmij} = \langle nm | H | ij \rangle$ determines the whole spectrum of the system. Truncated matrices $[H]_{N \times N}$ allow determination of successive approximations to the larger and larger number of states by increasing the order N . We use the one-particle basis of the harmonic oscillator eigenfunctions

$$\varphi_i^\Omega(x) = \left(\frac{\sqrt{\Omega}}{\sqrt{\pi} 2^i i!} \right)^{\frac{1}{2}} H_i(\sqrt{\Omega} x) \exp[-\Omega x^2/2]. \quad (6)$$

Following the optimized RR scheme [4], we adjust the value of the frequency Ω so as to make stationary the approximate sum of N bound-state energies, by requiring

$$\frac{\delta \text{Tr}[H]_{N \times N}}{\delta \Omega} = 0. \quad (7)$$

Such a way of proceeding has been shown to improve strongly the convergence of the RR method [4,5]. The N th order calculation provides approximations to many eigenstates, which enables a direct determination of natural orbitals by representing them in the same basis (6) as $v(x) = \sum p_n \varphi_n^\Omega(x)$. This turns the eigenequation (4) into an algebraic problem

$$\sum (A_{mn} - k_n \delta_{mn}) p_n = 0, \quad (8)$$

$$A_{mn} = \int \psi_m^\Omega(x_1) \phi(x_1, x_2) \psi_n^\Omega(x_1) dx_1 dx_2 = \begin{cases} a_{nn} & \text{for } m = n \\ 2^{-1/2} a_{mn} & \text{for } m \neq n \end{cases}$$

and a_{nm} are determined from diagonalization of $[H]_{N \times N}$. By diagonalization of the matrix $[A]_{N \times N}$, the approximate coefficients k_n may be determined. Due to the fact that $\sum A_{nm}^2 = 1$, their numerical values satisfy $\sum k_n^2 = 1$.

3 Results

In the case of harmonic confinement $V(x) = mx^2/2$ and the contact interaction, the two-particle wave function may be analytically expressed [6]. This allows determination of the occupancies $\lambda_i = k_i^2$ by discretizing (4). The two largest occupancies for the ground state are shown in Fig. 1 in function of g_{1D} . The state is non-entangled ($\lambda_0 = 1$) only if the bosons do not interact. The weakly entangled “condensed” state with only one orbital significantly occupied is realized at very weak interactions, $g_{1D} \lesssim 0.1$. With increasing g_{1D} , the

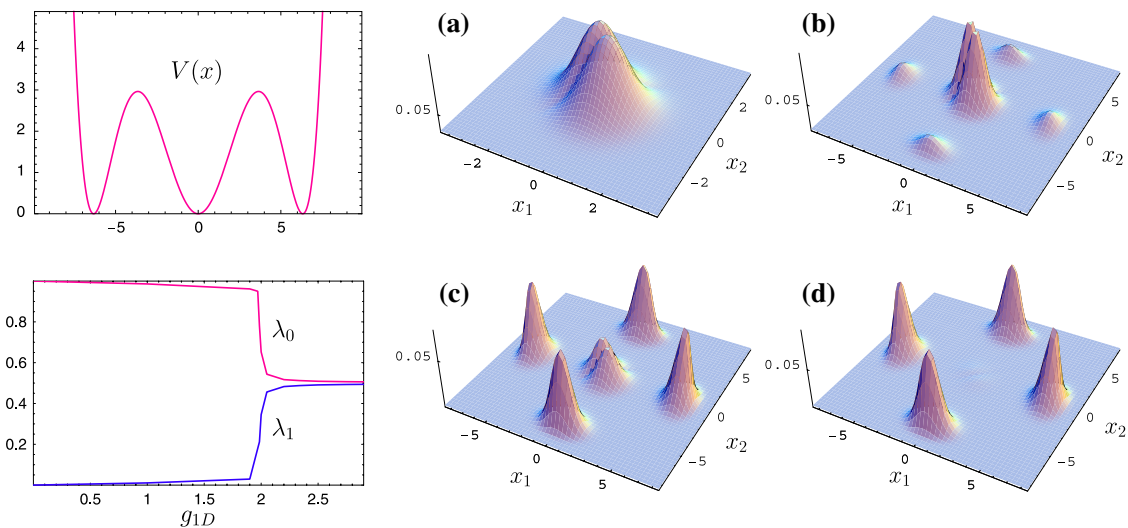


Fig. 3 Same as Fig.2 but for the triple-well potential. The two-boson densities (right) for (a) $g_{1D} = 1$, (b) $g_{1D} = 1.97$, (c) $g_{1D} = 1.985$, (d) $g_{1D} = 2.05$

4 Conclusion

The optimized CI method proves very effective in determining the spectrum and the natural orbitals of the two-particle confined systems.

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