Przemysław Kościk

Quantum Correlations of a Few Bosons within a Harmonic Trap

Abstract We study two one-dimensional atomic models composed of identical bosons trapped in a harmonic trap: one model with a short-range interaction potential and another model with a long-range one, and compare their entanglement features. Properties of the ground-states of two-, three-, and four-particle systems are explored.

1 Introduction

In recent years there has been a growing interest in the physics of ultracold gases due to the ability to control parameters such as the shape of the trapping potential, the interaction strength, and even the number of atoms. Especially, the quasi one-dimensional (1D) systems that are usually created by imposing strong confinement in a 'transversal' direction have attracted much attention [1–12]. The effective interaction potential for such bosons in a 1D system is found to be $U(x_1, x_2) \propto \delta(x_2 - x_1)$[13]. Also, there is a considerable interest in studies of systems composed of bosons interacting via a Coulomb potential [14–16]. Their properties in the 1D limit are, however, rather rarely studied.

In this paper, we consider two models composed of identical bosons confined in a 1D harmonic trap, namely a model with a short-range interaction potential

$$U_\sigma(x) = g \frac{e^{-\frac{x^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma}, \tag{1}$$

which tends to a Dirac delta distribution $g\delta(x)$ as $\sigma \to 0$, and a model with a long-range interaction [17,18]

$$U_\kappa(x) = \frac{\kappa}{\sqrt{x^2 + \gamma}}, \tag{2}$$

which exhibits Coulomb behaviour for large enough $|x|$ ($|x| \gg \gamma$).

We make a detailed investigation of their entanglement properties, and compare them with each other. We base our analysis on the von Neumann (vN) entropy of the one-particle reduced density matrix. For example, the vN entropy in the ground-state of four anyons with δ interaction has been recently investigated in [12]. However, still most of the studies of entanglement properties focus on the two-particle system [2–5,17,18]. Here, we shall discuss the N-body systems with $N = 2, 3, 4$.

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

2 Methods

Many-particle eigenvalue problems are of the form

$$\left\{\sum_{i=1}^{N}\left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2}+\frac{1}{2}x_i^2\right]+\sum_{i<j}U_{\sigma/\kappa}(x_i-x_j)\right\}\psi = E\psi. \tag{3}$$

Since it is rather a time consuming task to solve them by the standard exact diagonalization method, here we calculate the ground-states with the quantum diffusion algorithm [19]. The main results of this paper will be presented for fixed parameters $\sigma = \gamma = 0.05$, without loss of generality. For the sake of brevity, we consider only repulsive interactions ($g > 0, \kappa > 0$).

A tool to investigate two-body correlations is the single-reduced density matrix (RDM) [20]

$$\hat{\rho} = Tr_{2,3,...,N}|\psi\rangle\langle\psi|. \tag{4}$$

We will explore the quantum correlations in the systems by using the vN entropy $S = -Tr[\hat{\rho}Log_2\hat{\rho}]$. The relevant integral eigensystem equation is thus

$$\int_{-\infty}^{\infty}\rho(x,x^{'})v_s(x^{'})dx^{'} = \lambda_s v_s(x), \tag{5}$$

where $\rho(x,x^{'})$ is the RDM expressed in coordinates as

$$\rho(x,x^{'}) = \int \psi(x,x_2,...,x_N)\psi(x^{'},x_2,...,x_N)dx_2...dx_N, \tag{6}$$

where we have assumed ψ to be a real function. In terms of the eigenvalues $\{\lambda_s\}$ (occupancies) and the eigenfunctions $\{v_s(x)\}$ (natural orbitals), the RDM takes the form

$$\rho(x,x^{'}) = \sum_{s=0}^{\infty}\lambda_s v_s(x)v_s(x^{'}), \tag{7}$$

and the vN entropy is given by

$$S = -\sum_{s=0}^{\infty}\lambda_s log_2\lambda_s. \tag{8}$$

Obviously the larger is the value of S, the larger is the number of terms actively involved in the expansion of $\rho(x,x^{'})$ (7).

Discretization of the variables x and $x^{'}$ with equal subintervals of length Δx allows us to turn (5) into an algebraic eigenvalue problem

$$\sum_{i}[B_{ij} - \delta_{ij}\lambda_s]v_s(x_i) = 0, j, \tag{9}$$

where $B_{ij} = [\Delta x\rho(x_i,x_j)]$. Diagonalizing the matrix $[B_{ij}]_{n\times n}$, we get a set of approximations to the N largest eigenvalues of the RDM and then we can obtain an approximation to the entanglement entropy S.

3 Numerical Results

First, we analyse the properties of the systems with (1). Our results are shown in Fig. 1 where the values of S are displayed as a function of the interaction parameter g. For the sake of comparison, in this figure we have also drawn the behaviour of the vN entropy for two-particle systems in the zero-range limit $\sigma \to 0$ of (1), which has been also obtained in [4]. We see that there is a slight difference between the results calculated at $\sigma = 0.05$ and those for the limit $\sigma \to 0$. This becomes more pronounced only at large values of g which we find consistent with the discussion in [6]. One can expect the results presented for three- and four-particle systems to be also quite close to the limit $\sigma \to 0$.

As may be seen, for all cases considered in Fig. 1 an analogous situation occurs, namely the entanglement entropy S has a monotonically increasing behaviour as g increases, and tends to a constant value as $g \to \infty$. Except for the case $g = 0$, the entropy S generally has a higher value for a larger value of N, which is more pronounced at stronger interactions. A transition between the regime of weakly interacting bosons and the strongly correlated *fermionized* regime is manifested by the onset of the plateau in the behaviour of the vN entropy. Interestingly enough, the results of Fig. 1 indicate that the critical interaction parameter at which the fermionic limit is reached is at most weakly sensitive to the number of particles. In fact, the entropies S of two-, three- and four-particle systems make their most rapid variations over the interval $0 < g < 20$ and above $g \approx 20$ reach practically their limiting values.

Now we come to the discussion of the properties of the systems with the long-range interaction (2). The results obtained are presented in Fig. 2. We find that the main entanglement features exhibited by the systems with (2) are similar to those exhibited by the ones with (1). Namely, in the case of (2) the vN entropy also increases both with an increase in the interaction parameter and in the number of particles. It is expected that in the limit of $\kappa \to \infty$, in which the so-called Wigner molecule is formed, the entanglement becomes insensitive to the parameter γ. This is because the average distances between particles tend to infinity as $\kappa \to \infty$,
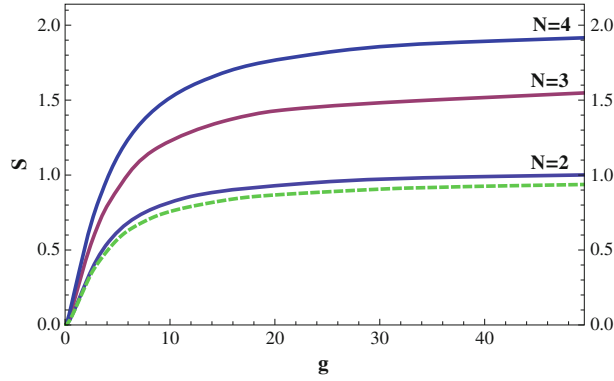

Fig. 1 The vN entropy in the ground-state of the system with (1) at $\sigma = 0.05$, as a function of g for $N = 2, 3, 4$. The *broken curve* corresponds to the vN entropy of the two-particle system in the zero-range limit $\sigma \to 0$ of (1)
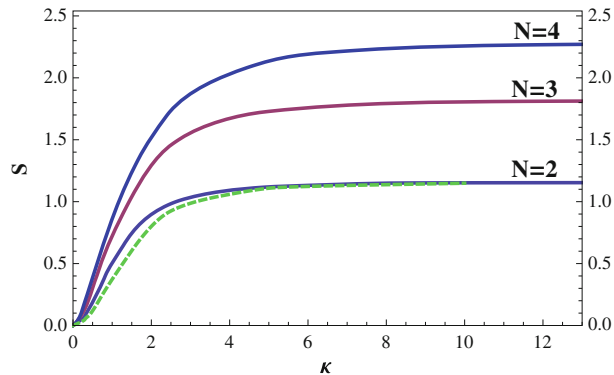

Fig. 2 The vN entropy in the ground-state of the system with (2) at $\gamma = 0.05$, as a function of κ for $N = 2, 3, 4$. The *broken curve* corresponds to the vN entropy of the two-particle system at $\gamma = 0.1$

regardless of γ. We recall here that the interaction potential exhibits a pure Coulomb behavior for $|x| \to \infty$. As an example, in Fig. 2 the behaviour of the entropy S for $N = 2$ is plotted for two different values of γ, which demonstrates that S is indeed insensitive to γ at $\kappa \to \infty$ limit. It is worth noting at this point that at fixed N the vN entropy saturates at a larger value for (2) than for (1).

We have found, for the systems with (2), the value of the occupancy $\lambda_0(N)$ to be of the order N^{-1} as $\kappa \to \infty$, regardless of γ (at least up to $N = 4$). Finally, it is instructive to compare this result with that obtained for the systems with the contact interaction ($\sigma \to 0$) in the case of $g \to \infty$ namely $\lambda_0(N) \approx N^{-0.41}$ [10].

4 Summary

In summary, we investigated the ground-state properties of two atomic models composed of two, three, and four particles. We found that the main entanglement features exhibited by both models are quite similar. Namely, the entropies S of the systems with (1) and (2) increase with the increase in the interaction parameters g and κ, respectively, and tend to constant values as $g \to \infty$ and $\kappa \to \infty$. In both models an effect of the number of particles turned out to be more expressive at large interaction parameters. In particular, the entanglement features of the systems with (2) become in the limit of $\kappa \to \infty$ unaffected by the parameter γ. In this limit we have found for the occupancy of the lowest natural orbital the approximation: $\lambda_0(N) \approx N^{-1}$, valid at least up to $N = 4$. It would still be desirable to obtain the full dependence of λ_0 on N in the case of $\kappa \to \infty$, in particular, and this is an open topic for future investigations.

It would be interesting to check if any of the trends observed for the models with a harmonic well are shared by the models with other confining potentials. This will be the topic of further studies.

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