Monte Carlo study of few-bosons in a one-dimensional trap

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Abstract: We consider a one-dimensional system of few-bosons in a harmonic trap that interact via a contact potential. In addition, we explore a system of non-interacting bosons in the presence of an impurity. The Variational Monte Carlo method is utilised to calculate an upper bound of the ground state energy. Furthermore, we numerically obtain the one-body density matrix, which allows us to determine the occupation numbers and the impurity density profile. The occupation numbers reveal that, in the absence of any impurity, the condensation diminishes as the repulsive interaction strength among bosons increases. Finally, in the presence of an impurity, we show the existence of two distinct regimes: a miscible regime and a non-miscible one.

I. INTRODUCTION

There have been several experimental studies on ultra-cold atomic gases, which demonstrate their potential as quantum simulators for complex systems in the fields of condensed matter and high energy physics [1–3]. To understand and study the phenomenology of ultra-cold atomic gases, various theoretical and numerical methods, such as Monte Carlo simulations, have been developed. Monte Carlo simulations are of great importance as they allow to obtain the ground state properties of many-particles systems [4].

In this work we investigate a one-dimensional system of few bosons confined in a harmonic trap and interacting via a contact potential. Since all particles are identical, we refer to this system as single-component gas. We treat the interaction strength as an independent variable, adjusted by tuning the scattering length. Additionally, we explore a system of non-interacting bosons under the same conditions but in the presence of an impurity. As this system consists of two types of particles, the impurity and the bosons, we refer to it as a two-component gas.

To initiate our analysis, we propose a trial wave function (TWF) that captures relevant properties of the ground state for each system under investigation. Using this TWF, we initially calculate an upper-bound estimate for the ground state energy. Subsequently, we optimise one or more variational parameters within the TWF to lower this upper-bound. Furthermore, by calculating the one body density matrix (OBDM), we obtain density profiles and occupation numbers for further analysis.

We place particular emphasis on two specific configurations. In the absence of interaction and impurity, bosons form a Bose Einstein Condensate (BEC), where they all occupy the same single-particle state [5]. Conversely, when the interaction strength tends towards infinity, bosons behave as impenetrable point particles. This configuration is known as the Tonks-Girardeau gas (TG), and its significance lies in the fact that the squared modulus of its wave function is equivalent to that of a system of non-interacting fermions [6]. Additionally, we explore the behaviour of the impurity density profile as a function of the interaction strength, which is another intriguing phenomenon of interest.

The document is structured as follows. In Sec. II, we introduce and describe the two systems under investigation. Sec. III explains the algorithms and calculations utilised. The results are presented in Sec. IV, where we discuss the two distinct configurations studied in Subsec. IV A and Subsec. IV B. Finally, in Sec. V, we provide the conclusions.

Throughout the document all quantities are expressed in oscillator units: energies in units of $\hbar w$ and distances in units of $a_{\text{osc}} = \sqrt{\hbar/(mw)}$.

II. THE MODEL

A. Single-component gas

The system under study consists of N bosons confined in a one-dimensional harmonic trap. These bosons interact with each other through a contact potential. The system is described by the following Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i^N \Delta_i + \frac{m\omega^2}{2}\sum_i^N x_i^2 + g\sum_{i<j}\delta(x_i - x_j)\,, \quad (1)$$

where $g = \frac{\hbar^2}{m}\frac{(-2)}{a_{\text{o}}}$ characterises the strength interaction, and a_{o} is the scattering length [7]. For $a_{\text{o}} < 0$, corresponding to $g > 0$, the interaction between the particles is repulsive, with the strength increasing as $|\frac{1}{a_{\text{o}}}|$. The TG gas is obtained in the limit $a_{\text{o}} = 0$, while the absence of interaction between bosons results in a BEC when $\frac{1}{a_{\text{o}}} = 0$. To investigate this system under repulsive interactions, we initiate our study by proposing a non-normalised TWF for the particles positions

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$\vec{R} = (x_1, x_2 \dots x_N)$,

$$\psi_T(\vec{R}) = \prod_{i=1}^{N} e^{-\alpha \frac{x_i^2}{a_{\text{osc}}^2}} \prod_{j<k}^{N} \Big(\frac{|x_k - x_j| - a_{\text{o}}}{a_{\text{osc}}} \Big) , \qquad (2)$$

where α is a variational parameter that must be tuned to minimise the energy. The first term introduces the effect of the harmonic trap, while the second term ensures that the wave function cancels if two bosons are at a distance equal to a_{o}. It is important to note that the TWF is symmetric under the permutation of any two bosons. As an initial approach, we set $\alpha = 0.5$. In the BEC and TG limits, Eq. (2) coincides with the exact ground state wave function after proper normalisation [4].

The case of two cold atoms is particularly interesting for testing our methods, as the ground state energy is analytically known for both repulsive and attractive interactions [7]. Therefore, in addition to the TWF proposed for the repulsive interaction regime in Eq. (2), we also propose a TWF for the attractive regime specifically for the case of two particles:

$$\psi_T(x_1, x_2) = e^{-\frac{1}{2}\frac{x_1^2}{a_{\text{osc}}^2}} e^{-\frac{1}{2}\frac{x_2^2}{a_{\text{osc}}^2}} e^{-\frac{|x_1 - x_2|}{a_{\text{o}}}} . \qquad (3)$$

This attractive TWF exhibits exponential decay as the distance between the two bosons increases relative to the scattering length.

B. Two-component gas

In this case, we consider a gas of non-interacting bosons confined in a one-dimensional harmonic trap that interact repulsively with an impurity. The total number of non-interacting bosons, commonly referred to as bath particles, is denoted as $N_B = N - 1$. The system is described by the following Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i}^{N-1} \Delta_i - \frac{\hbar^2}{2m} \Delta_I + \frac{m\omega^2}{2} \sum_{i}^{N-1} x_i^2 + \frac{m\omega^2}{2} x_I^2 + g \sum_{i=1}^{N-1} \delta(x_i - x_I) , \qquad (4)$$

where the position of the impurity is denoted by x_I. We propose the following non-normalised TWF with two variational parameters α_I and α_B:

$$\psi_T(\vec{R}) = e^{-\alpha_I \frac{x_I^2}{a_{\text{osc}}^2}} \prod_{i=1}^{N-1} e^{-\alpha_B \frac{x_i^2}{a_{\text{osc}}^2}} \prod_{i=1}^{N-1} \Big(\frac{|x_i - x_I| - a_{\text{o}}}{a_{\text{osc}}} \Big) , \qquad (5)$$

where the first term introduces the effect of the harmonic trap on all particles, and the second term ensures that, if the impurity and any boson are at a distance equal to a_{o}, the wave function cancels. As an initial approach, we set $\alpha_I = \alpha_B = 0.5$. It should be noted that for $N = 2$ the system is completely equivalent to the one discussed in Sec. II A.

III. METHODS AND OBSERVABLES

Given one of the TWFs presented in Sec. II, $\psi_T(\vec{R})$, its square modulus can be treated as a probability distribution function after proper normalisation. The positions of the particles can then be sampled using the Metropolis algorithm [8]. It is important to note that the TWF itself does not require normalisation for this sampling procedure, as the Metropolis algorithm only involves ratios of probabilities. Once the positions are sampled, we can use Monte Carlo methods to evaluate integrals involving $|\psi_T(\vec{R})|^2$ and derive various properties of the system.

A. Energy computation

According to the variational principle, the expectation value of the Hamiltonian with respect to a TWF provides an upper bound for the ground state energy. This principle can be expressed mathematically as follows,

$$\langle E \rangle = \frac{\int_{-\infty}^{\infty} \psi_T^*(\vec{R}) \hat{H} \psi_T(\vec{R}) d\vec{R}}{\int_{-\infty}^{\infty} \psi_T^*(\vec{R}) \psi_T(\vec{R}) d\vec{R}} > E_{\text{g.s.}} \qquad (6)$$

Thus, to optimise the variational parameters in the TWF, we aim to minimise the energy. For a general Hamiltonian consisting of kinetic and potential terms $U(\vec{R})$, the ground state energy can be estimated using M samples $\vec{R}_j$ as follows,

$$\langle E \rangle = \frac{1}{M} \sum_{j}^{M} \Big(-\frac{\hbar^2}{2m} \frac{\Delta \psi_T(\vec{R}_j)}{\psi_T(\vec{R}_j)} + U(\vec{R}_j) \Big) . \qquad (7)$$

B. One body density matrix

The one body density matrix (OBDM) is defined as,

$$\rho(x, x\prime) = N \int \psi^*(x\prime, x_2 \dots x_N) \psi(x, x_2 \dots x_N) dx_2 \dots dx_N . \qquad (8)$$

It can be estimated as a Monte Carlo integral with M samples with

$$\langle \rho(x, x\prime) \rangle = \frac{N}{M} \sum_{x_{1j} \in (x\prime + \frac{\delta x}{2}, x\prime - \frac{\delta x}{2})}^{M} \frac{\psi_T^*(x, x_{2_j} \dots x_{N_j})}{\psi_T(x_{1_j}, x_{2_j} \dots x_{N_j})} \frac{1}{\delta x} , \qquad (9)$$

where δx is the step used for discretising the space. We can deduce several important properties of the system from the OBDM, such as the density profile, the momentum distribution or the natural orbitals with their occupation numbers. The density of the system corresponds to the diagonal of the OBDM,

$$n(x) = \rho(x, x) . \qquad (10)$$

The occupation numbers of the natural orbitals are given by the eigenvalues of the OBDM.

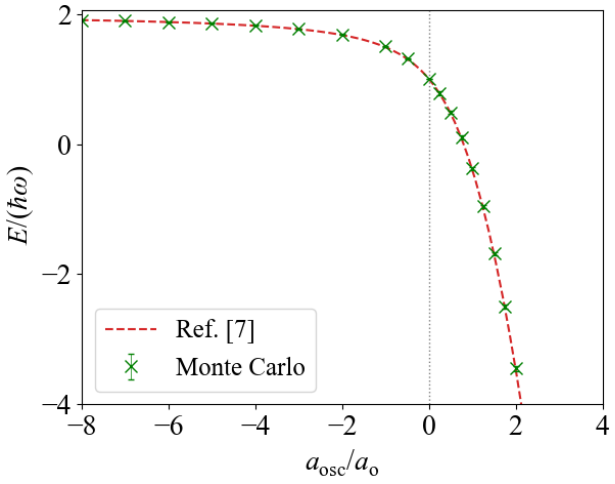

FIG. 1: Energy of two particles as a function of the inverse of the scattering length for both attractive and repulsive interactions in green crosses. The TWFs used are Eq. (2) with $\alpha = 0.5$ and Eq. (3). The analytical energy derived in Ref. [7] is represented in a red dashed line.

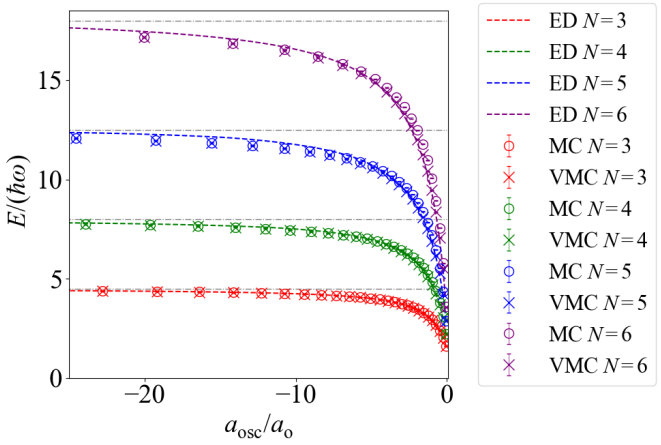

FIG. 2: Energy for N particles as a function of the inverse of the scattering length for the repulsive regime. Both the results obtained with (VMC) and without (MC) optimisation of α are shown by crosses and open circles, respectively. VMC stands for Variational Monte Carlo and MC for Monte Carlo. The obtained energy in Ref. [9] is also plotted with dashed lines (ED). Each colour represents a different N. The TG limits $E = \frac{N^2}{2}\hbar\omega$ are plotted with grey dot-dashed lines.

IV. RESULTS

A. Single-component gas

Energy of the two-particle case. For the simpler case of $N = 2$, we can calculate the energy using TWF (2) for repulsive interactions and TWF (3) for attractive interactions. The computed energy is compared to the analytical energy in Fig. 1. The computed results show a close agreement with the analytical curve. In the repulsive regime, the energy increases as the interaction strength strengthens approaching the TG limit where energy equals $E = N^2\hbar\omega/2 = 2\hbar\omega$ and it corresponds to the energy of a system of N non-interacting fermions in a one-dimensional harmonic trap.

In the repulsive regime, the TWF can be optimised by varying α. Without optimising α, the maximum discrepancy $\Delta_{\max} = \max(|\mathrm{E_{MC}} - \mathrm{E_{exact}}|)$ between the results and the exact value of the energy is $\Delta_{\max} = 0.013 \pm 0.002\ \hbar\omega$. However, by optimising α, a lower upper bound is obtained, reducing the maximum discrepancy to $\Delta_{\max} = 0.006 \pm 0.002\ \hbar\omega$. It is important to note that the computed energy is always an upper bound of the exact energy, as expected from the variational principle. The discrepancies obtained are very small compared to the actual energy value.

Energy of the few-particles case. When $N > 2$, we only focus on the repulsive regime. We can compare our results with the results obtained in Ref. [9] using the exact diagonalization method (ED). In Fig. 2 we observe that both results fit really well, specially for small values of N. Once again, optimising α leads to a lower upper bound for the energy of the system. For weak interactions, the results obtained by ED give a lower upper bound of the ground state energy, while the opposite is true for strong interactions. The maximum discrepancy between both results $\Delta_{\max} = \max(|\mathrm{E_{MC}} - \mathrm{E_{ED}}|)$ increases with the number of particles. For $N = 3$, when α is not optimised, the maximum discrepancy is $\Delta_{\max} = 0.07 \pm 0.01\ \hbar\omega$. After optimising α, the discrepancy significantly decreases to $\Delta_{\max} = 0.02 \pm 0.01\ \hbar\omega$. For $N = 6$, the maximum discrepancy without optimisation is $\Delta_{\max} = 0.76 \pm 0.02\ \hbar\omega$, while after optimisation, the discrepancy is reduced to $\Delta_{\max} = 0.19 \pm 0.02\ \hbar\omega$.

Occupation numbers. The OBDM has been computed for various interaction strengths and number of particles. Then, by diagonalising the computed matrices, we obtain the occupation numbers for different strength interactions and number of particles. The occupation numbers obtained for three particles under different strength interactions are shown in Fig. 3. The sum of all the eigenvalues obtained for a given OBDM is equal to its trace, which is equal to N. In the absence of interaction, bosons form a BEC and we obtain only one non-zero occupation number with a value of $\lambda_0 = N$. As the repulsive interaction increases, condensation diminishes, i.e. the largest occupation number decreases while the other occupation numbers increase. In the TG limit, the behaviour of the largest occupation number λ_{0TG} with respect to N is non-trivial and clearly differs from that of non-interacting fermions, where the OBDM has N non-zero eigenvalues $\lambda_j = 1$. To determine the parameters of a hypothesised power-law relationship $\lambda_{0TG}(N) = cN^b$ for the TG limit, we perform a lineal regression using $\log \lambda_{0TG}$ as the y-coordinate and $\log N$ as the x-coordinate for N ranging from 2 to 10. The

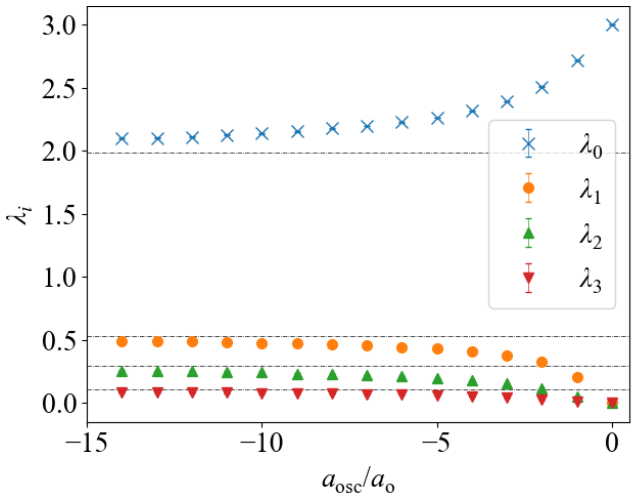

FIG. 3: OBDM eigenvalues of 3 particles as a function of the inverse of the scattering length for the repulsive regime. The dashed lines correspond to the computed value of the eigenvalues at the TG limit.

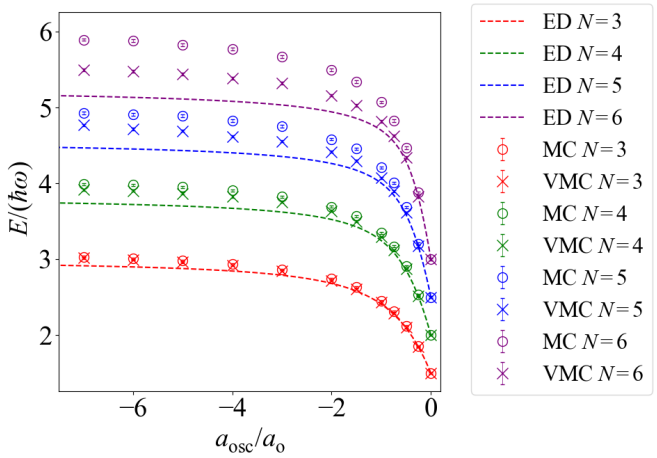

FIG. 4: Energy as a function of the inverse of the scattering length in the repulsive regime for N_B bath particles with one impurity. The data with $\alpha_I = \alpha_B = 0.5$ is plotted with circles (MC). The data optimising α_I and α_B is plotted with crosses (VMC). The obtained energy in Ref. [9] is also plotted with dashed lines (ED). Each colour represents a different N.

coefficient of determination is found to be $R^2 = 0.9996$. The obtained parameters are

$$c = 1.042 \pm 0.008 \qquad b = 0.586 \pm 0.005. \tag{11}$$

These values are in reasonable agreement with the power law obtained in Ref. [10], where they state that $\lambda_{0TG} \approx N^{0.59}$.

B. Two-component gas

Energy of the system. Using the proposed TWF in Eq. (5), we compute the energy of the system as a function of the interaction strength. In Fig. 4, we show the computed energy of the system with and without optimising α_I and α_B, and compare it to the ED results. The energy obtained is always an upper bound of the ED energy. When we optimise α_I and α_B we obtain a significantly lower upper bound, although it is still larger than the energy obtained with ED. In this case, since the system includes an impurity and is more complex, the proposed TWF is not as accurate as the one used for the single-component gas. The discrepancy between the computed energy and the ED energy increases with the total number of particles. Additionally, the discrepancy increases when the interaction becomes stronger, indicating that the proposed TWF is more accurate for weaker interactions.

Impurity density profile. By following the methodology outlined in Sec. III, we have computed the OBDM for the impurity. From it, we can obtain the density profile of the impurity with Eq. (10). In Fig. 5, we show the impurity density profile for a system of 3 particles (two bath particles and the impurity).

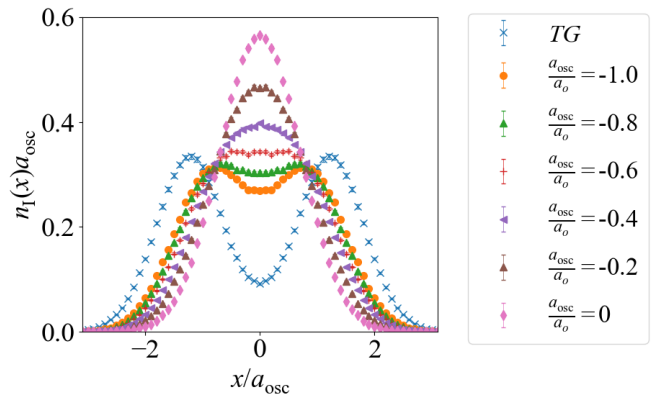

FIG. 5: Impurity density profile for 2 bath particles for different interaction strengths.

For weak interaction strengths, we observe a maximum in the impurity density profile located at the centre of the trap. As the interaction strength increases, this maximum becomes a minimum, and two symmetric maxima appear on each side. These two configurations can be interpreted as a miscible and a non-miscible regime, respectively. In the miscible regime, the impurity is located around the centre of the trap along with the bath particles. In the non-miscible regime, the impurity tends to be located far from the bath particles. The transition between these two regimes occurs at different values of $\frac{1}{a_o}$ for different N_B. To characterise the total interaction strength acting on the impurity, we use $g(N-1) = gN_B$. We can then evaluate the position of the maximum as a function of gN_B. In Fig. 6, we observe that for any number of particles, there is an abrupt transition occurring around the same value of gN_B, approximately $g \approx \frac{1.9}{N_B}\hbar\omega a_{osc}$. When comparing with the ED results,

we find that the actual transition occurs at a higher gN_B. This indicates that our TWF does not accurately predict the critical strength, but it does reveal the existence of this phenomenon.

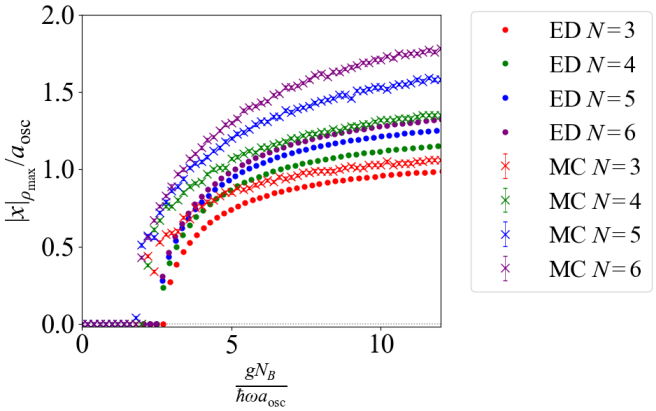

FIG. 6: Position of the impurity density profile maximum value $|x|_{\rho_{max}}$ as a function of gN_B for 3, 4, 5 and 6 particles. The data obtained with Monte Carlo is plotted with crosses while the data obtained with ED is plotted with circles.

V. CONCLUSIONS

In this project, we have investigated a system of many bosons confined in a harmonic trap, both with and without the presence of an impurity. We have proposed and optimised a TWF for the ground state of each system and estimated upper bounds for the ground state energy as a function of the interaction strength. We have also computed the OBDM for different configurations and explored the occupation numbers of the one-component gas as well as the impurity density profile. The main conclusions of our study are:

- The proposed TWF for the system without any impurity is highly accurate. In fact, for strong interactions, it provides a lower upper bound for the ground state energy compared to the ED results.
- The computation of the occupation numbers reveals that the condensation of bosons diminishes when the repulsive interaction between them increases. In the TG limit, the occupation numbers exhibit a distinct behaviour from those of a non-interacting fermionic system. We have confirmed the dependence with N of the largest occupation number in the TG limit, $\lambda_{0TG} \approx N^{0.59}$ as predicted in Ref. [10].
- When an impurity is introduced, the estimated upper bound of the ground state energy significantly deviates from the actual ground state energy, indicating that the TWF is not as accurate as in the case without an impurity. However, the TWF still captures the transition between a miscible and a non-miscible regime.

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