Monte Carlo study of 2D bosonic gases

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Abstract: We consider a bidimensional system of few identical bosons trapped in a harmonic well that interact through a two-body gaussian potential. We discuss the ground state energy using a mean-field approximation and introducing pair correlations. To solve the many-body problem we used Monte Carlo techniques: Variational and Diffusion Monte Carlo. We find that two-body correlations lower significantly the energy per particle of the system in the strong interaction limit.

I. INTRODUCTION

Recent advances allow to study few atom systems, where the atoms are usually confined in a harmonic potential which can be configured in one, two or three dimensions [1][2]. In the ground state of a non-interacting boson system confined in a harmonic trap, atoms populate the same single-particle state. To consider realistic systems one should introduce interactions between the atoms, that usually are short-range [3][4]. We will be interested in computing the ground-state energy and its dependence on the strength of the interaction and the number of atoms.

Monte Carlo methods are based on the use of random distributed numbers to either solve deterministic problems or do simulations. It is an extended powerful tool to solve integrals numerically. When working with random techniques, the statistical error can be reduced using importance sampling, where random numbers are selected following a probability distribution function (pdf) similar to the function to be integrated. In our case the square of the wave function is a good choice as pdf to use in importance sampling.

In this work we are going to face a many-body system composed of a few bosons interacting through a two-body potential and varying the intensity of this interaction. First, we perform a mean-field approach by assuming that all particles in the same single-particle state. In a second step and still in the framework of variational approach, we add two-body correlations to the wave function, to take into account in a direct but approximated way the effects of the interactions on the wave function.

This document is structured in the following way: first we define the model, and the system is described presenting the two-body potential and the total Hamiltonian in Sec. II. In Sec. III the variational method and the correction of the centre of mass are introduced. Then, in Sec. IV the diffusion Monte Carlo (DMC) method is presented to finally show in Sec. V how the ground state energy depends on the number of particles or the intensity of the short range interaction using different methods and discuss some density profiles in Sec. VI.

II. THE MODEL

We consider a system of bosonic atoms confined by a two-dimensional harmonic oscillator potential at zero temperature. Where energy and length are expressed in oscillator units: $\hbar\omega$ for energies and $\sqrt{\frac{\hbar}{m\omega}}$ for distances, being ω the trap frequency and m the mass of the bosons. In these units, the single-particle Hamiltonian reads,

$$\mathcal{H}_{sp} = -\frac{1}{2}\nabla^2 + \frac{1}{2}\vec{r}^2 \quad . \tag{1}$$

Introducing this Hamiltonian in the Schrödinger equation, the single particle ground state (ψ_1), which can be obtained in an analytical way, is a Gaussian Eq. (2),

$$\psi_1(\vec{r}) = \frac{1}{\sqrt{\pi}} \exp\left(-\frac{1}{2}\vec{r}^2\right) \quad , \tag{2}$$

which is normalized as $\int |\psi_1(\vec{r})|^2 d\vec{r} = 1$.

The interactions between particles will be described by a finite Gaussian potential Eq. (3) modelling a two body interaction. Being g and σ the parameters that control the strength and the width of the potential respectively

$$V(\vec{r_i}, \vec{r_j}) = \frac{g}{2\pi\sigma} \exp\left(-\frac{(\vec{r_i} - \vec{r_j})^2}{2\sigma}\right) \quad . \tag{3}$$

For N identical bosons, the total Hamiltonian can be written as a sum of N single particle Hamiltonian Eq. (1), plus the two-body interaction potential between the pairs of particles:

$$\mathcal{H} = \sum_{i=1}^{N} -\frac{1}{2}\nabla^2 + \sum_{i=1}^{N} \frac{1}{2}\vec{r}^2 + \sum_{i<j} \frac{g}{2\pi\sigma} \exp\left(-\frac{(\vec{r_i} - \vec{r_j})^2}{2\sigma}\right) \quad . \tag{4}$$

III. VARIATIONAL METHOD

Given a trial wave function $\Psi_T(r_1, ..., r_N)$, the variational method ensures that the expectation value of the

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Hamiltonian

$$E_T = \frac{\langle\psi_T|H|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \quad , \tag{5}$$

provides an upper-bound of the ground-state energy. The wave function contains variational parameters which are chosen in order to minimize the energy to get the best wave function of the type considered.

A. Correlations

The ψ_T is built as the product of N single-particle states Eq. (2) multiplied with pair correlations to represent the effects of the potential in the wave function. The many-body correlated wave function that we use reads,

$$\psi_T(\bar{r}) = \prod_{i=1}^{N}\psi_i(\alpha,\bar{r})\prod_{i<j}^{N}\left(1-ae^{-b(\vec{r_i}-\vec{r_j})^2}\right) \quad , \tag{6}$$

$$\psi_i(\alpha,\bar{r}) = \sqrt{\frac{\alpha}{\pi}}\exp\left(-\frac{1}{2}\alpha\vec{r}^2\right) \quad . \tag{7}$$

Working with these correlations, the probability of finding two particles very close is reduced. ψ_i is the normalized single particle wave function with a variational parameter α that is related to the cloud size. a and b are also variational parameters that can be easily interpreted. For $a = 0$, the wave function has no correlations, in this case is a mean-field. The parameter a controls the hole in the two-body distribution function produced by the short-range repulsion of the particle. And b is directly related with the correlation length.

B. Centre of Mass

We know that in the ground-state the centre of mass should be in the ground-state of the harmonic oscillator associated to the CM (see below). However, in our wave function, the CM is not in the ground-state. We can therefore calculate the expectation value of the energy of the centre of mass in our trial wave function, subtract this energy and add the energy of the centre of mass in the ground-state.

$$\mathcal{H} = \mathcal{H}_{CM} + \mathcal{H}_{rel} \quad , \tag{8}$$

$$\mathcal{H}_{CM} = \frac{-1}{2N}\nabla^2_{CM} + \frac{N}{2}\vec{R}^2_{CM} \quad , \tag{9}$$

and also the wave function

$$\psi_T = \varphi_{CM}(\vec{R}_{CM})\varphi_{rel}(\vec{r}) \quad , \tag{10}$$

$$\varphi_{CM}(\vec{R}_{CM}) = \sqrt{\frac{\alpha N}{\pi}}\exp(-\frac{1}{2}\alpha N\vec{R}^2_{CM}) \quad ; \tag{11}$$

This correction has a strong dependence on α, is zero for $\alpha = 1$ and smaller α implies large correction, see Eq. (13).

α	ΔE_{CM}
0.3	-0.817
0.4	-0.450
0.5	-0.250
0.6	-0.133
0.7	-0.064
0.8	-0.025
0.9	-0.0056
1	0

TABLE I: Centre of mass corrections as function of α.

In Table I some values that should be subtracted from the energy per particle are presented.

$$\frac{E}{N} = \frac{1}{N}\frac{\langle\psi|\,\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} + \Delta E_{CM} \quad , \tag{12}$$

$$\Delta E_{CM} = -\left(\frac{\alpha}{2}+\frac{1}{2\alpha}\right)+1 \quad . \tag{13}$$

C. Mean-field

In the mean-field approximation all the particles populate the same single-particle state. This wave function will only depend on the variational parameter α.

$$\psi_{mf} = \prod_{i=1}^{N}\sqrt{\frac{\alpha}{\pi}}\exp(-\frac{1}{2}\alpha\vec{r}_i^2) \quad . \tag{14}$$

The energy per particle in the mean-field approximation for the Hamiltonian described in Eq. (4) can be calculated analytically and reads

$$\frac{1}{N}\frac{\langle\psi_{mf}|\mathcal{H}|\psi_{mf}\rangle}{\langle\psi_{mf}|\psi_{mf}\rangle} = \frac{\alpha}{2}+\frac{1}{2\alpha}+\frac{g(N-1)}{4\pi}\frac{\alpha}{\alpha\sigma+1} \quad , \tag{15}$$

where the first term is the kinetic energy, the second one the potential energy of the harmonic oscillator and the last term is the interaction energy of the system. For a given interaction, the minimization of Eq. (15) respect to α provides the best mean-field energy with this type of wave function. The minimization implies values of α smaller than $\alpha = 1$, i.e. the cloud size gets larger increasing the distance between the particles in order to decrease the repulsion. Centre of mass corrections will be important in mean-field approximation (Table I). With $g = 0$ we recover the solution for a 2D non interacting system trapped in a harmonic oscillator ($\alpha = 1$ and $E = 1$) as expected.

D. Variational Monte Carlo

When working with a wave function that includes correlations Eq. (6), the problem becomes non-analytic.

Stochastic techniques as Monte Carlo methods are introduced to numerically evaluate the expectation value of the Hamiltonian for the trial wave function.

The Variational Monte Carlo (VMC) is based on the Metropolis algorithm [5] and provides an upper-bound to the ground-state energy for a given set of variational parameters. From now on, we will refer to VMC when we consider correlations despite we can also calculate the mean-field approximation with this algorithm.

The Metropolis algorithm is used to sample a known probability distribution. We start from an initial position $\bar{X}_i$ with probability $p_i = |\psi(\bar{X}_i)|^2$, here $\bar{X}$ represents all set of coordinates for all the particles. Then a displacement from -step/2 to +step/2 of each coordinate is considered $X_f = X_i$+step*($rand$-0.5), being $rand$ a random number between 0 and 1 uniformly distributed. This new X_f is accepted as the new configuration if $p_f > p_i$ but if $p_f < p_i$, is also accepted with probability p_f/p_i. In the case that the new configuration is discarded we remain at the same position ($X_f = X_i$) and the local energy is calculated again with the same configuration. The step should be adjusted to have an acceptance between 50% and 60% which is the usually admitted as appropriate [5]. A small value of the step, will imply a large acceptance needing a lot of movements to cover all the space. On the other hand, a low acceptance means that we remain at the same configuration for a long time.

The optimum parameters that minimize the ground state energy are obtained using the *Minuit* package [7] which provides algorithms that work calling several times the function to be minimized. In this paper we used *Simplex* routine [7]. It can not provide errors of the output parameters but it requires less calls and converges almost all the computations. In Fig. 1, variational parameters for the case $N = 2$ are shown for different g. In VMC, the values of α of the minimization stay between 0.9 and 1. Although in these cases CM corrections are almost zero, they are considered.

The increase of a, indicates that bosons correlate in order to minimize their energy. In the non-interacting case ($g = 0$), $a = 0$ and the parameter b becomes irrelevant, Eq. (6), being the same wave function as in the mean-field.

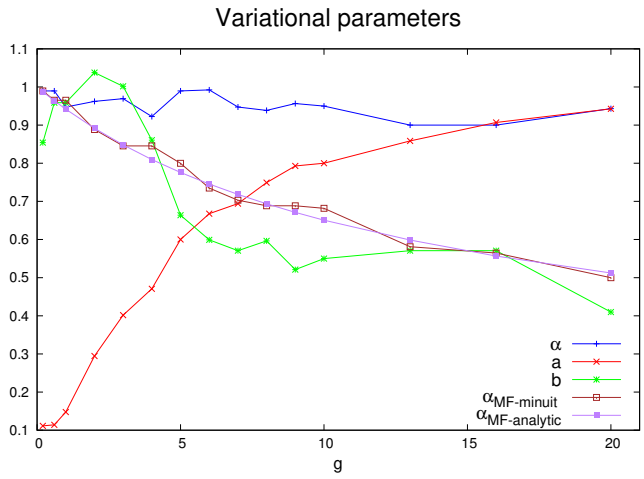

FIG. 1: Variacional parameters obtained using *Simplex* for N=2 and σ=0.125. A comparative between the exact mean-field parameter is showed to see *Simplex* performance. For $g = 0$ mean-field and VMC coincide has the same wave function (b is not relevant if $a = 0$)

IV. DIFFUSION MONTE CARLO

The Diffusion Monte Carlo (DMC) method [6] is non-variational, and tries to obtain the exact solution of the many-body Schrödinger equation which is considered in imaginary time. The wave function is represented by a set of random vectors (also called walkers). And their time evolution represent the evolution of the wave function and is given by what is called *Green Function*

$$\psi(\vec{R}, t) = \exp\left(-(\mathcal{H} - E)t\right)\psi(\vec{R}, 0) \quad , \qquad (16)$$

where $\vec{R}$ represents all the atom coordinates and E is an energy shift which should be near the ground state. One can see by expressing the wave function in the basis of their stationary states of the Hamiltonian ϕ_ν, that for an infinite time and $E = E_{g.s.}$ the only remaining amplitude will correspond to the ground state. If $E \approx E_{g.s.}$ there would be other amplitudes but the larger will still be the ground state one

$$\psi(\vec{R}, t) = \sum_\nu e^{-(E_\nu - E)t} C_\nu \phi_\nu(\vec{R}) \quad . \qquad (17)$$

One can obtain the Green Function calculated for a short time interval dt using a linear approximation [6] which is only valid in the case $dt \to 0$.

To find the right value for the ground state energy, one should calculate the energy for different time steps and then find a linear region and extrapolate the energy to $dt = 0$. An example for $N = 5$ is shown in Fig. 2.

V. GROUND STATE ENERGY

Besides the methods mentioned above, Fig. 3 also shows results from the exact diagonalization method[8]. It should be remarked that the DMC has no variational character and therefore does not provide an upper-bound.

VMC is calculated using 1.000.000 movements, the step size is varied depending on N to obtain an acceptance around 50-60%. For example, to calculate the $N = 2$ system, we used an step of 1.6 getting an acceptance of 59% but if we use the same step for $N = 7$ the acceptance is only of the 21%. So a small step is required, like 0.8, to have a reasonable acceptance of 55%.

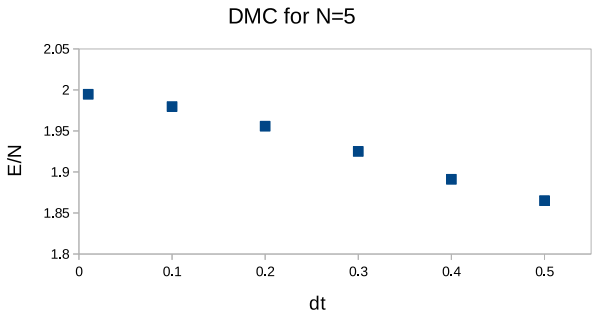

FIG. 2: Diffusion Monte Carlo values of the Energy per particle for $N = 5$, $g = 10$, $\sigma = 0.125$ and 200 walkers. The energy calculated for different steps of time dt should be extrapolated to $dt = 0$ to find the ground state energy. In this case using least squares it is obtained $E_{g.s} = 2.004$.

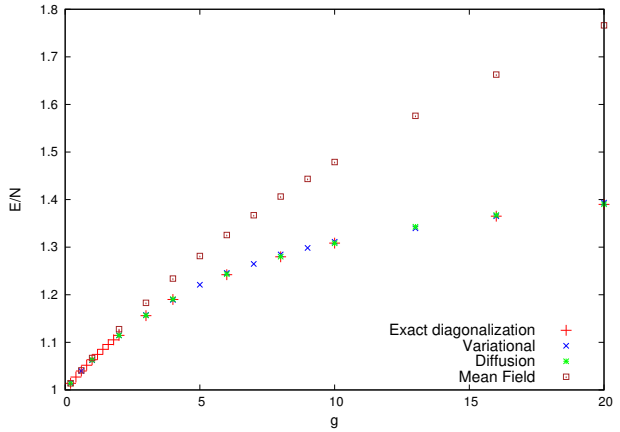

FIG. 3: Energy per particle, calculated with different methods, $N = 2$, $\sigma = 0.125$ and different values of the interaction strength.

DMC requires to calculate the energy for different time steps dt. First we spend around 5000 movements to equilibrate the system discarding these energies. After that, the energy is calculated in 15000 movements. DMC uses what we called walkers and the amount of walkers should remain stable during the calculations. Starting far away from the ground state, the number of walkers may diverge. We used 200 walkers but this election is arbitrary. For instance, in Table II we show that there is no significant variation on the energy for a number of walkers bigger than 50 for $N = 2$.

In Fig. 3 we compare the energies obtained with different methods. As the interaction becomes stronger, the mean-field approximation largely overestimates the energy, providing an upper-bound but far away from the exact result. VMC, DMC and exact diagonalization provide nearly the same results. Despite it can not be appreciated in the scale of this figure, exact diagonalization and DMC are always below VMC.

Fig. 4 shows the dependence on N of the energy for a given g and σ. The mean-field is above VCM and DMC except, of course, in the single-particle case. For a fixed interaction, as N is increased, mean-field and Monte Carlo methods approach each other.

# walkers	$E_{g.s}/N$
10	1.31057
50	1.31580
100	1.31576
150	1.31522
200	1.31538
250	1.31535
300	1.31557
350	1.31587

TABLE II: VMC for $N = 2$, $\sigma = 0.125$, $g = 10$. Energy per particle as a function of the number of walkers.

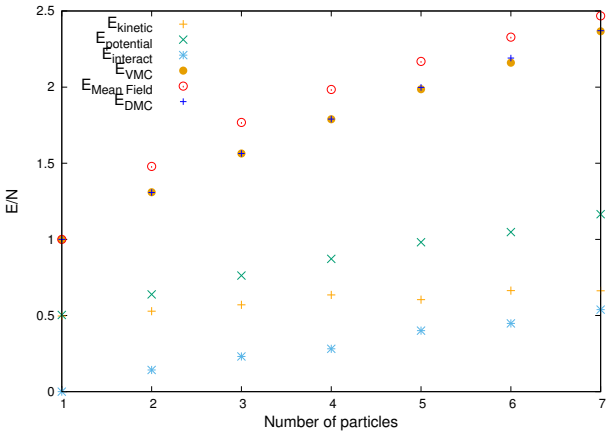

FIG. 4: Energy per particle of a system of N particles trapped in a 2D harmonic potential for $g = 10$ and $\sigma = 0.125$. The kinetic,potential, and interaction energy, are for the variational MC method. For one particle the harmonic oscillator results are recovered.

VI. DENSITY PROFILES

It is also interesting to show the density profiles. Due to the symmetry of the harmonic trap it can be represented depending on the radial distance r. These profiles are calculated counting the number of times that particles are found in a surface $2\pi r dr$ during the sampling process. Error bars correspond to the statistical error considering that falling inside or outside these surface, follows a binomial distribution.

In Fig. 5 densities for $N = 2$ and a fixed $\sigma = 0.125$ for different values of g are presented. For large values of g, the profiles present a plateau that becomes shorter as the interaction is reduced (g approaches to 0). For $g = 0$ we recover a Gaussian profile. Interestingly all curves meet at the same point for $r = 1$, this behaviour does not appear for $N = 3$ and $N = 4$.

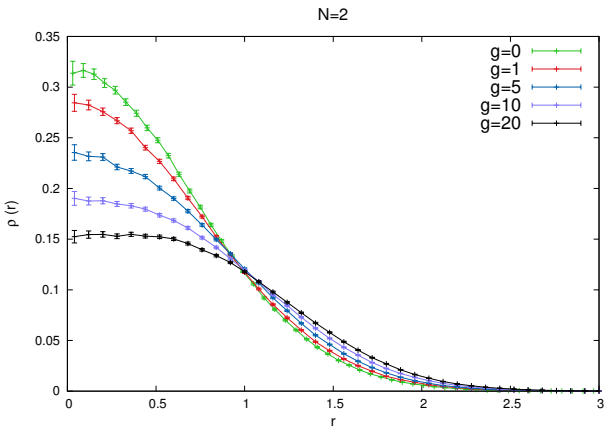

FIG. 5: Probability density normalized as $\int 2\pi r\rho(r)dr = 1$ using the variational Monte Carlo for $\sigma = 0.125$, $N = 2$ and different values of g.

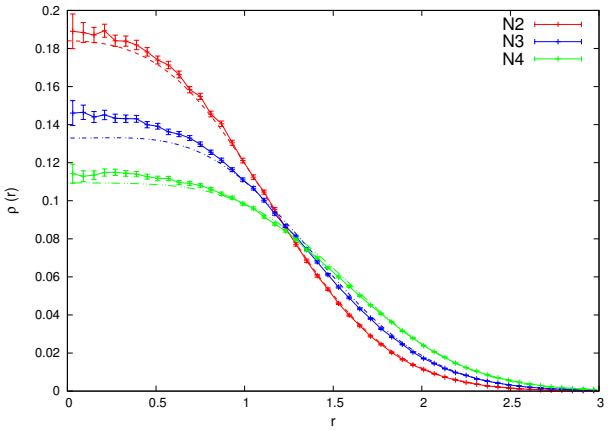

FIG. 6: Probability density normalized to $\int 2\pi r\rho(r)dr = 1$ for different number of particles, g=10 and σ=0.125 . The points with error bars refer to variational Monte Carlo data and discontinuous lines are from the exact diagonalization method.

In Fig. 6 our data is compared with the density profile obtained using the exact diagonalization method. And it can be observed that the flat region becomes larger for higher N.

VII. SUMMARY AND CONCLUSIONS

In this work we have considered a 2-dimensional many-body boson system confined in a harmonic potential where particles interact via two-body potential. We have analysed the mean-field approximation using a simple single-particle wave function of Gaussian type. In a second step, we have introduced a more sophisticated wave function which incorporates two-body correlations and calculated the energy by a Variational Monte Carlo method. Finally, using DMC methods we have determined the ground-state energy. The conclusions are:

- Mean-field approximation is valid when the interaction is weak. However, for a fixed interaction, the mean-field approximation seems to produce reasonable results when the number of particles is increased.
- when the interaction strength between the particles, g, is increased, bosons tend to correlate in order to reduce the energy.
- The correlated many-body wave function proposed provides very good results, comparable in most cases with exact diagonalisation methods or diffusion Monte Carlo ones.

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