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Quantum Monte Carlo study of one-dimensional bosons with finite range interactions

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Abstract. We have studied how the ground state and the one-body density distribution of a one-dimensional system of bosons trapped by a harmonic oscillator potential depend on the repulsive interaction between the bosons. This study has been done using two numerical methods: Variational Monte Carlo and Diffusion Monte Carlo to retrieve information about the ground state energy and the one-body density distribution. We have covered the full range of interaction from the non-interacting regime, where the mean field approximation is a suitable way to describe our system, to the strongly interacting regime where we have reproduced approximately the behavior of a Tonks-Girardeau gas. As the repulsive interaction strength is increased, the system builds pair correlations. We have also proposed a correlated wave function to characterise these correlations.

Keywords: 1D gas of bosons, ground state energy, VMC, DMC

1. Introduction

In recent years, there has been an important effort to understand the quantum many body states appearing in 1D bosonic systems. The main reason to develop the physics of 1D bosons are the recent improvements in the field of ultra-cold atomic gases [1, 2]. Bosonic atoms can be trapped in 1D, 2D and 3D traps of different geometries and their interactions can be tuned in many cases by means of suitable Feshbach resonances [3]. This allows one to consider the transition from the non-interacting regime to the strongly interacting one in 1D systems, which has actually being explored experimentally [4, 5], observing features of the well-known Tonks-Girardeau gas [6].

The aim of this master thesis is the study of a one-dimensional system of N bosons trapped in a parabolic trap, $V_{\text{trap}} = (1/2)m\omega^2 x^2$, in which the bosons interact with each other through a repulsive interaction potential. More specifically, we will concentrate on the properties of the ground state of the system, which will drastically change as we increase the repulsion between the particles.

The system we consider is described by the following Hamiltonian in first quantization,

$$H = \sum_{i=1}^{N} -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x_i^2} + \sum_{i=1}^{N} V_{\text{trap}}(x_i) + \sum_{i<j}^{N} V_{\text{int}}(x_{ij}), \tag{1}$$

where x_i for $i = 1, 2, \ldots, N$ are the positions of the particles in harmonic oscillator units $\sqrt{\hbar/(m\omega)}$ with m the mass of the particles and ω the frequency of the oscillator. $V_{\text{int}}(x_{ij})$ is the interaction potential between pairs of particles ij where $x_{ij} = |x_i - x_j|$, in units of $\hbar\omega$. We consider an atom-atom interaction potential of the form

$$V_{\text{int}}(x_{ij}) = \frac{g}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\frac{x_{ij}^2}{\sigma^2}}, \tag{2}$$

where $g > 0$ characterises the repulsive strength of the interaction and σ^2 defines the interaction range. Note that this finite range potential tends to a contact δ-interaction in the limit $\sigma^2 \to 0$.

There are three well-defined regimes in this problem. The first one, is a weakly interacting regime, $g \ll 1$. In this case, we expect that the mean field approximation should work well. The second one is found by further increasing the interaction, $g \gg 1$. In this case, the system starts to build non-trivial correlations among the particles. The mean field description fails. We will show that a correlated wave function is able to capture the correlations appearing in the system. Finally, when $g \to \infty$, with $\sigma^2 \to 0$ we have the well known Tonks-Girardeau regime for which we can derive analytical expressions.

This work is organized as follows. In Section 2 we introduce the variational method and the different families of wave functions considered. In Section 3 we describe the variational Monte Carlo (VMC) strategy, which allows us to go to larger number of particles. In Section 4 we present the main tools of the Diffusion Monte Carlo (DMC), a method aimed to provide the exact ground state energy. In Section 5, we discuss the main results we have obtained with the different methods and in Section 6 we present the conclusions of this master thesis.

2. Variational Methods

Our first approach will be to find upper bounds to the energy of the many-body system by means of the variational approach. That is, we will consider a parametric many-body wave function $|\Psi_\lambda\rangle$ and find upper bounds for the energy by minimizing the expected value of the Hamiltonian, $\partial E_\lambda / \partial \lambda = 0$, with,

$$E_\lambda = \frac{\langle \Psi_\lambda | H | \Psi_\lambda \rangle}{\langle \Psi_\lambda | \Psi_\lambda \rangle}. \tag{3}$$

2.1. Mean field approximation: weak interacting regime

For a system of N non-interacting bosons at zero temperature, all the particles are assumed to be in the same single particle state. The total wave function of the system is then written as $\psi(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N} \phi(x_i)$. As starting point, we can consider a simple Gaussian wave function

$$\phi(x_i) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha^2 x_i^2}, \tag{4}$$

where $\alpha > 0$ is a variational parameter. This ansatz should work for weak interactions. The variational energy of the system corresponding to this wave function is given by

$$E(\alpha^2) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = N\left(\frac{\alpha^2}{4} + \frac{1}{4\alpha^2}\right) + \frac{N(N-1)}{2}\frac{g}{\sqrt{2\pi}}\sqrt{\frac{\alpha^2}{\alpha^2\sigma^2 + 1}}. \tag{5}$$

For the simplest, non-interacting, case $g = 0$, $\alpha^2 = 1$ minimizes the energy and one recovers the harmonic oscillator energy $N/2$. The minimization of $E(\alpha^2)$ with respect to α provides the best energy in this family of wave functions.

The best mean field description of the problem can be obtained solving the Hartree-Bose equations, which are obtained by imposing that the energy of the system is stationary with respect to small functional variations of ϕ. The energy reads,

$$E = \langle \psi | H | \psi \rangle = N\left\langle \phi \left| -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 \right| \phi \right\rangle + \frac{N(N-1)}{2}\langle \phi\phi | V_{int} | \phi\phi \rangle, \tag{6}$$
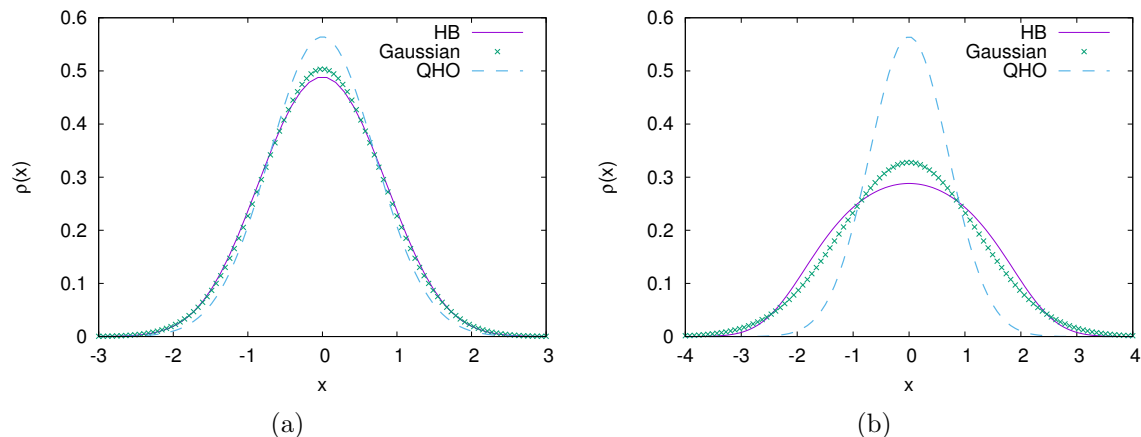
Figure 1: One-body density distribution normalized to unity for a system of $N = 4$ particles with $g = 0.5$ (a) and $g = 4$ (b), both for $\sigma^2 = 0.125$. The solid line corresponds to the solution of the Hartree-Bose equations, the cross dotted line to the Gaussian wave function (4) and the dashed line to the non-interacting harmonic oscillator wave function (QHO).

where $\langle \phi\phi \, | V_{int} | \, \phi\phi \rangle$ is a two-body matrix element. This requirement is expressed by means of

$$\frac{\delta}{\delta\phi} \left[\langle \psi \, | H | \, \psi \rangle - \lambda \langle \psi | \psi \rangle \right] = 0, \tag{7}$$

where λ is a Lagrange multiplier to ensure the normalization of $|\psi\rangle$. The result of this minimization process yields the following Hartree-Bose equation

$$\lambda\phi(x) = -\frac{1}{2}\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} + \frac{x^2}{2}\phi(x) + (N-1)\left[\int \mathrm{d}x' V_{\mathrm{int}}(x - x')|\phi(x')|^2 \right]\phi(x), \tag{8}$$

where

$$\lambda = \left\langle \phi \left| -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2 \right| \phi \right\rangle + (N-1)\langle \phi\phi \, | V_{\mathrm{int}} | \, \phi\phi \rangle, \tag{9}$$

defines the chemical potential. The two equations, (8) and (9), define a self-consistent procedure. Finally, the Hartree-Bose mean field energy is given as

$$E_{HB} = \langle \psi \, | H | \, \psi \rangle = N\lambda - \frac{N(N-1)}{2}\langle \phi\phi \, | V_{\mathrm{int}} | \, \phi\phi \rangle. \tag{10}$$

In table 1 we report the values of the ground state energy for $N = 4$ comparing both approaches. As expected, the Hartree-Bose solution gives a better lower bound for the energy of the ground state as compared to the simple gaussian mean field ansatz. The differences between the simple ansatz and the Hartree-Bose are larger as we increase the strength of the interaction. Correspondingly, the density associated to the single particle orbital obtained with the Hartree-Bose is broader than the one obtained with the simple gaussian ansatz as can be seen in figure 1. For small g the shapes are very similar, but as g is increased, the shape obtained with the Hartree-Bose is much broader and closer to the Thomas-Fermi limit [2], which would correspond to an inverted parabola. In both cases the results are clearly different from the non-interacting case.

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Table 1: Values of the energy for a simple gaussian variational wave function (E_{G}) and the one obtained solving the Hartree-Bose equations (E_{HB}). We consider $N = 4$ and two different values of the interaction strength, $g = 0.5$ and $g = 10$. The range of the interaction is the same in both cases. The value of α^2 corresponding to the simple Gaussian ansatz is also provided.

N	g	σ^2	E_{HB}	E_{G}	α^2
4	0.5	0.125	3.06561	3.070618	0.7964824
4	4	0.125	8.59706	8.749062	0.3376884

2.2. Introduction of correlations between the particles of the system

As the interaction strength is increased there are two competing effects. On one side the system gets larger, reducing the atom-atom interactions. On the other side, the system builds up suitable pair correlations to avoid the atom-atom interaction. The mean field only captures the first effect, to incorporate the second we need to take into account correlations. We propose the following correlated wave function,

$$\psi(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N} \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha^2 x_i^2} \prod_{i<j} \left(1 - ae^{-bx_{ij}^2}\right), \qquad (11)$$

where a and b are the parameters which characterize the correlations between the particles. The three parameters α, a and b will be used as variational parameters. The parameter a has a very clear physical interpretation. If $a = 0$ the wave function reduces to the simple mean field Gaussian of (4). If $a = 1$ the wave function has zeros whenever two atoms are at the same position, thus reducing the atom-atom interaction.

2.2.1. Case of two particles. The $N = 2$ case can be evaluated analytically. We express the Hamiltonian in terms of the centre of mass position $X = \frac{x_1 + x_2}{2}$ and the relative coordinate $x_r = x_1 - x_2$,

$$H = H_{\mathrm{CM}} + H_r = -\frac{1}{4}\frac{d^2}{dX^2} + X^2 - \frac{d^2}{dx_r^2} + \frac{1}{4}x_r^2 + g\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\frac{x_r^2}{\sigma^2}}, \qquad (12)$$

where H_{CM} is the Hamiltonian of the centre of mass and H_r is the relative Hamiltonian between the two particles which also includes the interaction term. The wave function of the system using these coordinates can be expressed as:

$$\psi(X, x_r) = \phi_{CM}(X) \cdot \phi_r(x_r) \propto e^{-\alpha^2 X} e^{-\frac{\alpha^2}{4}x_r^2}\left(1 - ae^{-bx_r^2}\right). \qquad (13)$$

The variational energy is computed by means of

$$E_{N=2} = \frac{1}{4B^2}\left[\sqrt{\frac{2\pi}{\alpha^2}}\frac{1}{\alpha^2} - 2a\sqrt{\frac{2\pi}{\alpha^2 + 2b}}\frac{1}{\alpha^2 + 2b} + a^2\sqrt{\frac{2\pi}{\alpha^2 + 4b}}\frac{1}{\alpha^2 + 4b}\right] + \frac{\alpha^2}{4} + \frac{1}{4\alpha^2} +$$

$$+ \frac{1}{B^2}\left[\frac{\sqrt{2\pi}\alpha^2}{4} - \left(\frac{1}{2}a\alpha^4 + 2ab\alpha^2\right)\frac{\sqrt{2\pi}}{(\alpha^2 + 2b)^{3/2}} + \left(\frac{1}{4}\alpha^4 a^2 + 4a^2 b^2 + 2a^2 b\alpha^2\right)\frac{\sqrt{2\pi}}{(\alpha^2 + 4b)^{3/2}}\right] +$$

$$+ \frac{1}{B^2}\frac{g}{\sqrt{2\pi\sigma^2}}\left[\sqrt{\frac{2\pi\sigma^2}{\alpha^2\sigma^2 + 1}} - 2a\sqrt{\frac{2\pi\sigma^2}{\alpha^2\sigma^2 + 2b\sigma^2 + 1}} + a^2\sqrt{\frac{2\pi\sigma^2}{\alpha^2\sigma^2 + 4b\sigma^2 + 1}}\right], \qquad (14)$$

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where B^2 is a normalization constant whose value is

$$B^2 = \sqrt{\frac{2\pi}{\alpha^2}} - 2a\sqrt{\frac{2\pi}{\alpha^2 + 2b}} + a^2\sqrt{\frac{2\pi}{\alpha^2 + 4b}}. \tag{15}$$

This analytical expression can be minimized numerically in order to obtain the value of the ground state energy. We have used it to test the results of the energies obtained later with VMC and DMC for $N = 2$.

3. Variational Monte Carlo

The Variational Monte Carlo Method evaluates the average value of the Hamiltonian, (3), with the proposed wave function. The upper bound is found performing the following average,

$$E_{\mathrm{GS}}^{\mathrm{upper}} = \frac{1}{N_{\mathrm{iter}}} \sum_{i=1}^{N_{\mathrm{iter}}} E_L^i, \tag{16}$$

where E_L is the local energy of the system

$$E_L = \frac{1}{\psi_T} H\psi_T = \sum_{i=1}^{N} \left(-\frac{1}{\psi_T}\frac{1}{2}\frac{\mathrm{d}^2\psi_T}{\mathrm{d}x_i^2} + \frac{1}{2}x_i^2 \right) + \sum_{i<j} g\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\frac{x_{ij}^2}{\sigma^2}}, \tag{17}$$

where ψ_T is a trial wave function which characterises the system. In our case it corresponds to the correlated wave function (11). E_L has to be computed a large enough number of times N_{iter} because (16) is exact in the limit $N_{\mathrm{iter}} \to \infty$. The local energy has to be computed for different positions of the particles, these positions should describe the correlated wave function. To achieve this, we use the Metropolis algorithm which provides sets of positions for the particles describing the probability density distribution of the system.

We consider that initially all the particles are distributed at random inside a given volume. Then, we start a series of random movements following the Metropolis algorithm which is implemented in the following way:

1.− Each particle is moved to a new trial position $x_{\mathrm{new}} = x_{\mathrm{old}} + \mathrm{SCAL} \cdot (\zeta - 0.5)$ where SCAL is an arbitrary distance. The new wave function is then computed, $\psi_T(x_1^{\mathrm{new}}, x_2^{\mathrm{new}}, \ldots, x_N^{\mathrm{new}})$.

2.− We compute, $\frac{\left|\psi_T(x_1^{\mathrm{new}}, x_2^{\mathrm{new}}, \ldots, x_N^{\mathrm{new}})\right|^2}{\left|\psi_T(x_1^{\mathrm{old}}, x_2^{\mathrm{old}}, \ldots, x_N^{\mathrm{old}})\right|^2}$. If this value is smaller than a random number between zero and one, the new positions are rejected and the particles remain in the old positions. Otherwise, the new positions are accepted and the particles are moved to the new positions.

3.− The local energy corresponding to the current positions of the particles is computed.

We repeat this iterative process adding the different local energies obtained with the different sets of positions generated by means of the Metropolis algorithm. Then, the upper bound of the ground state energy is computed by means of (16).

We have to choose properly the SCAL distance, a large value implies that the wave functions in the old and in the new position could be quite different. So, the number of accepted new positions will decrease which means that the particles will remain a larger number of iterations in the same positions. If the SCAL distance is too small, the number of accepted trial moves would be higher but it would require a large number of iterations to avoid that the particles remain in an small region. A reasonable number of accepted movements is normally accepted to be between 50-70% [10].

The Variational Monte Carlo provides an upper bound of the ground state energy for a given set of values of the variational parameters α^2, a and b. However, we can

not know how far away this upper bound is from the actual ground state energy. To determine the best upper bound, we have assembled the VMC calculations with a package of FORTRAN subroutines called MINUIT [11]. This package finds the values of the variational parameters for which the upper bound of the ground state energy is minimized.

3.1. Centre of mass correction

Similarly to what we have done to compute the variational energy (14) for $N = 2$, the Hamiltonian for the N-particle system can be also decomposed in two pieces: $H = H_{CM} + H_r$ and the same happens with the correlated wave function. Therefore, the expectation value of the total Hamiltonian can be separated in two contributions:

$$\langle \psi | H | \psi \rangle = \langle \phi_{CM} | H_{CM} | \phi_{CM} \rangle + \langle \phi_r | H_r | \phi_r \rangle \tag{18}$$

with $\langle \phi_{CM} | H_{CM} | \phi_{CM} \rangle = \frac{\alpha^2}{4} + \frac{1}{4\alpha^2}$. Then we define a new upper bound for the ground state energy as

$$\tilde{E}_{\text{GS}}^{\text{upper}} = E_{\text{GS}}^{\text{upper}} - \left(\frac{\alpha^2}{4} + \frac{1}{4\alpha^2} \right) + \frac{1}{2}, \tag{19}$$

which is equivalent to assume that the centre of mass is in the ground state of the system. Both expressions (16) and (19) are upper bounds of the ground state energy but $\tilde{E}_{\text{GS}}^{\text{upper}} < E_{\text{GS}}^{\text{upper}}$ so $\tilde{E}_{\text{GS}}^{\text{upper}}$ is a smaller upper bound.

4. Diffusion Monte Carlo

In this section we go one step further and consider a method to compute the exact ground state energy of the system. The Diffusion Monte Carlo method provides the value of the ground state energy by solving the time dependent Schrödinger equation in imaginary time

$$- \frac{\delta \psi(\vec{x}, t)}{\delta t} = [H(\vec{x}) - E_T] \psi(\vec{x}, t), \tag{20}$$

whose formal solution is

$$\psi(\vec{x}, t) = e^{-[H - E_T]t} \psi(\vec{x}, t = 0), \tag{21}$$

where $\vec{x} \equiv \{x_1, x_2, \ldots, x_N\}$ defines the positions of the N particles and E_T is a trial energy. The wave function of the system is represented by a set of walkers, each walker is made of N particles. The time evolution of the wave function, which is done in small time steps $dt = t/n_{steps}$, is represented by the time evolution of these walkers. We can express the starting state $\psi(\vec{x}, t = 0)$ in the base of the stationary states of the Hamiltonian

$$\psi(\vec{x}, t) = \sum_{n=0} e^{-[E_n - E_T]t} C_n \phi_n(\vec{x}), \tag{22}$$

where C_n is the amplitude of the stationary state ϕ_n. So if, we let the system evolve for a large time, $t \to \infty$, only the ground state component will survive. This is the basic idea behind DMC.

To efficiently implement DMC, one introduces an importance sampling wave function which improves the variance of the ground state energy as well as reducing the computational time. We define $f(\vec{x}, t) = \psi_T(\vec{x})\psi(\vec{x}, t)$, where $\psi_T(\vec{x})$ is a time independent trial wave function which in our case is the correlated wave function (11).

The Diffusion Monte Carlo method is an iterative algorithm repeated N_{times} consisting in the next steps:

1.− For a given value of dt, the N walkers are initialized to describe $f(\vec{x}, t = 0)$. This is done using a previous VMC calculation. The trial energy E_T is computed as the mean value of the local energy (17) of each walker.

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2.− Each walker is moved to a new position representing a time step dt.

$$\vec{x}_{\text{new}} = \vec{x}_{\text{old}} + \frac{1}{2}dtF(\vec{x}_{\text{old}}) + \xi, \tag{23}$$

where ξ is a random number sampled from a multivariate gaussian distribution with null mean and $\sigma = dt$. $F(\vec{x})$ is a drift term whose function is to displace the walkers towards the region where the trial wave function ψ_T is larger [10].

3.− At time step j, the number of walkers is modified by means of the replication factor

$$n_j = e^{dt(E_j^{\text{old}}/2 + E_j^{\text{new}}/2 - E_T)}, \tag{24}$$

where E_j^{old} and E_j^{new} are the local energies of each walker in the previous and in the current positions. We create n_j copies of each walker obtaining a new set of walkers for the next iteration. The energy of this iteration, $E^{N_{\text{final}}}$, is computed as the mean value of the local energies of this new set of walkers.

We repeat this process N_{times} to represent the time evolution of the wave function in a time $t \to \infty$. We add the different $E^{N_{\text{final}}}$ obtained to compute the ground state energy for this time step dt as $E_{\text{GS}}^{dt} = (\sum_{i=1}^{N_{\text{times}}} E^{N_{\text{final}}})/N_{\text{times}}$. With this algorithm, we obtain the value of the ground state energy for a given dt. To obtain the ground state energy we have to compute E_{GS}^{dt} for different values of dt and compute the least-square extrapolation of E_{GS}^{dt} to $dt \to 0$ [10], this can be seen in figure 2.
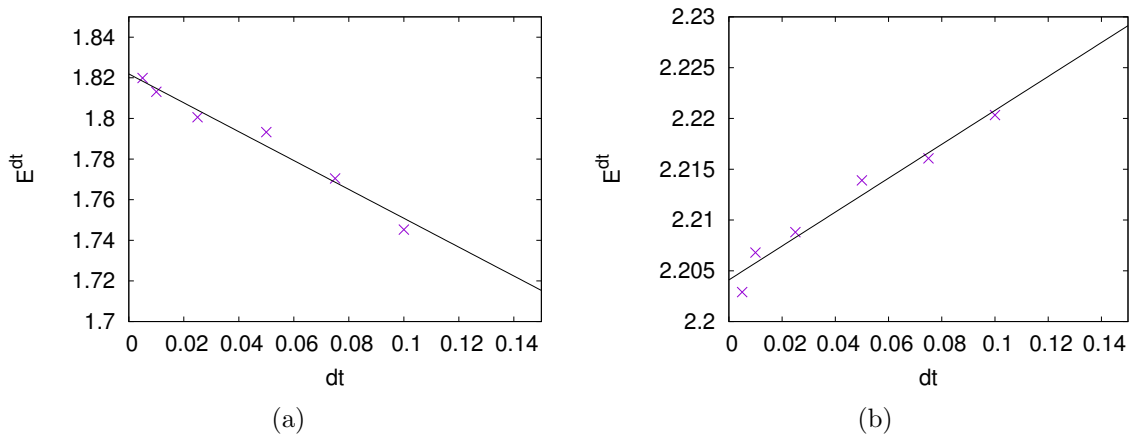

(a)　　　　　　　　　　　　　　(b)

Figure 2: Values of E_{GS}^{dt} obtained for different dt, the black line is the least-square extrapolation of E_{GS}^{dt} to $dt \to 0$. (a) $N = 2$ with $g = 3$ and $\sigma^2 = 0.5$. (b) $N = 2$ with $g = 10$ and $\sigma^2 = 0.125$. The extrapolated values $E_{\text{GS}}^{dt \to 0}$ are given in table 2.

5. Results: Interplay between interactions and correlations

5.1. Evolution of the ground state energy

Some features of the transition from the non-interacting to the strongly interacting limit can be illustrated even with $N = 2$. In figure 3 we depict the evolution of the different terms of the Hamiltonian as a function of the interaction strength g. The numbers are obtained with a fairly small range, $\sigma^2 = 0.001$.

First we observe that the total energy increases from $E_T \simeq 1$ for $g = 0$, as expected for two bosons in a 1D harmonic potential, to a value slightly above 2 for $g \simeq 20$. The total energy is seen to saturate as g is increased. The kinetic and potential energies follow a similar trend: they increase with g for small g but then saturate as g is further increased. The interaction energy follows a very different fate. For small values of g it

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increases, as predicted also by the simple mean field approach. At a certain value of $g \simeq 3$ the interaction energy reaches its maximum value and then decreases as g is increased. This is due to the development of correlations among the particles which reduce the interaction energy. Moreover, for $g = 20$ the value of the interaction energy is nearly zero as it is expected in the strongly interacting regime (with zero range) in which we have a Tonks-Girardeau gas.
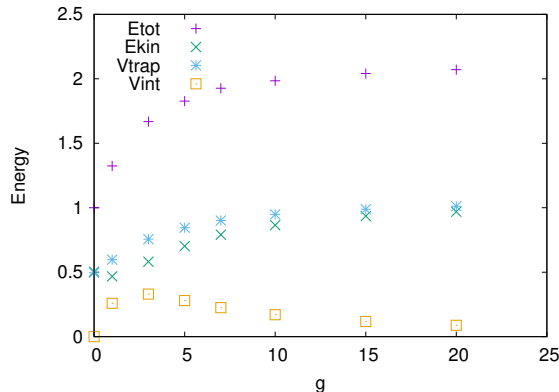

Figure 3: Values of the total energy (E_{tot}), the kinetic energy (E_{kin}), the parabolic trapping potential (V_{trap}) and the interaction energy (V_{int}) for a system of $N = 2$ as a function of the repulsive strength g and $\sigma^2 = 0.001$.

The results obtained with the correlated VMC are in general of similar quality to those obtained with DMC. This basically means that our correlated variational wave function captures well the exact solution. In table 2 we report some results obtained with DMC compared to VMC also for $N = 2$ bosons and different values of the interaction strength. In all cases, the DMC results are slightly smaller than the VMC ones, as expected.

Table 2: Values of the energies for a system of $N = 2$ obtained using VMC (E_{VMC}), DMC (E_{DMC}) and minimizing numerically (14) ($E_{\text{variational}}$) for different values of g and σ^2.

N	g	σ^2	$E_{\text{variational}}$	E_{DMC}	E_{VMC}
2	10	0.125	2.212031	2.2071	2.2122
2	3	0.500	1.823598	1.8220	1.8237
2	2	0.125	1.581950	1.5791	1.5821

The density distribution of the system changes substantially as g is varied. In figure 4 we compare the one-body density distributions obtained using a mean field approximation, panel (a), with the ones resulting from the correlated wave function of (11), panel (b). As expected, for small values of g both approximations agree. As we increase g the mean field does not predict a qualitative change in the density while the correlated wave function starts to develop a two peak structure.

5.2. Study of the strong interacting regime

In the limit case $g \to \infty$ and $\sigma^2 \to 0$ the bosonic gas in 1D becomes the so-called Tonks-Girardeau gas [6]. In this limit, the Fermi-Bose mapping allows one to obtain the analytical wave function of the system [6, 9]. The wave function of the ground state of a system made of N interacting bosons can be written as the absolute value of the wave function of a system of N non-interacting fermions in the same trap:

$$\psi_{\text{bosons}}^{g=\infty}(x_1, x_2, \ldots, x_N) = |\psi_{\text{fermions}}^{g=0}(x_1, x_2, \ldots, x_N)|. \tag{25}$$
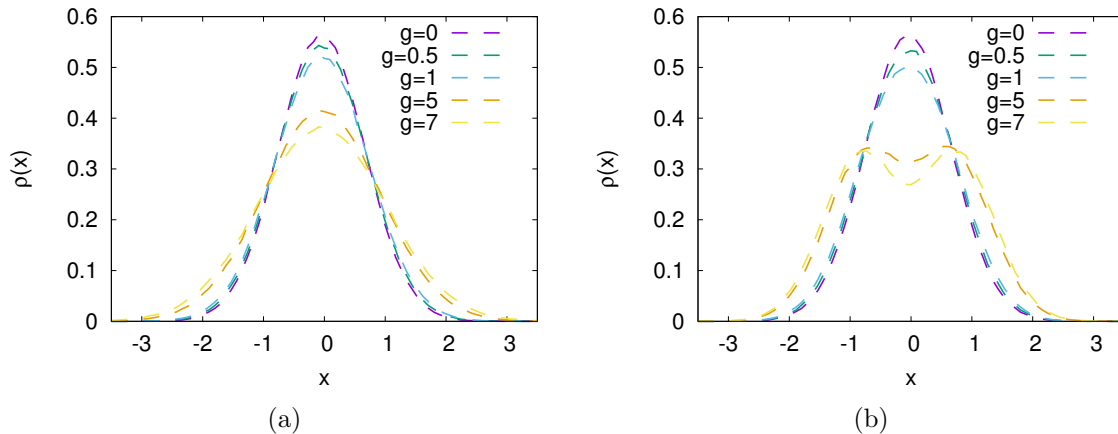
Figure 4: One-body density distributions for $N = 2$ and different g's and a constant value of $\sigma^2 = 0.125$. (a) mean field approximation, (b) correlated wave function (11).

The density of the system can then be readily written as,

$$\left|\rho_{\text{bosons}}^{g=\infty}(x)\right|^2 = \left|\rho_{\text{fermions}}^{g=0}(x)\right|^2 = \sum_{n=0}^{N-1}\left|\left(\frac{1}{\pi}\right)^{1/4}\frac{H_n(x)}{\sqrt{2^n n!}}e^{-x^2/2}\right|^2, \tag{26}$$

where H_n are the Hermite polynomials. The corresponding ground state energy is $E = \sum_{n=0}^{N-1}(2n + 1)/2$.

In order to study our system of N bosons in the limit $g \to \infty$ and $\sigma^2 \to 0$, we have used the correlated wave function (11) and large enough values of g and small enough values of σ^2. As it is shown in the table 3, for the case of $N = 2$ the interaction energy is nearly zero and the ground state energy is nearly equal to the fermionized value $E = 2$.

For the case of $N = 5$ the interaction energy has not a value near to zero but is quite smaller than the kinetic energy and the parabolic trapping potential. The total energy is 12.75 while the expected one is 12.5. So, we can say that in both cases the systems are in the very strong interacting regime.

Table 3: Values of the total energy for a system of N bosons (E), the kinetic energy (E_{kin}), the parabolic trapping potential (V_{trap}) and the interaction energy (V_{int}), for given values of g and σ^2.

N	g	σ^2	E	E_{kin}	V_{trap}	V_{int}
2	20	0.001	2.076	0.0982	1.0031	0.082
5	15	0.0001	12.75	4.791	6.772	1.12

Moreover, figure 5 shows the one-body density distributions obtained with the values of N, g and σ^2 of table 3. As it can be seen, the one-body density distribution of a system of N bosons can be approximately mapped with the one-body density distribution of a system of non-interacting fermions with the same number of particles (26).

6. Summary and Conclusions

We have studied the energy and the one-body density distribution of a one-dimensional system of N bosons trapped by an harmonic oscillator potential in which the bosons interact through a repulsive interaction of gaussian type, characterised by its strength g and its range σ^2. For weak interactions, $g \ll 1$, the system is well described by a mean

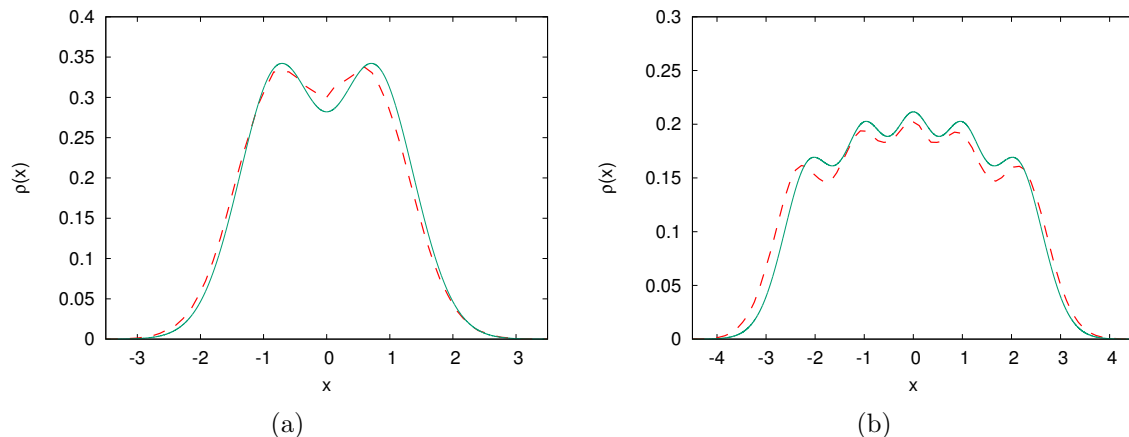Quantum Monte Carlo study of one-dimensional bosons

Figure 5: One-body density distribution for a system of $N = 2$ bosons, $g = 20$ and $\sigma^2 = 0.001$ in panel (a) and for $N = 5$, $g = 15$ and $\sigma^2 = 0.0001$ in panel (b). In both panels the dashed line represents the density distribution calculated with the correlated wave function (11) and the solid line corresponds to the distribution calculated with (26).

field wave function. We have solved the Hartree-Bose equations to determine the best mean field wave function. As the strength of the interaction increases, the system builds up pair correlations to decrease the interaction energy. As, by definition, the mean field can not incorporate these correlations we have proposed a correlated wave function which reduces to the mean field one for certain values of the parameters defining the variational wave function. The VMC method has been used to calculate the variational energy. The case of $N = 2$ can be calculated analytically and has been used as a benchmark for the VMC method. To test the quality of the proposed wave function we have compared the outcomes with DMC results.

Finally, using the same correlated wave function we have satisfactorily explored the case in which the strength of the interaction goes to $g \to \infty$ and $\sigma^2 \to 0$ which is equivalent to the Tonks-Girardeau gas.

We can conclude, that the proposed variational wave function provides a global accurate description of the energy and structure of the ground state in the full range of the interactions.

Acknowledgments

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