Variational study of trapped bosonic systems in one dimension

Author: Jesus Sono
*Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.**

Advisor: Artur Polls

Abstract: The aim of this work is to study the ground-state energy of trapped bosonic systems in one-dimension. The bosons interact through a finite range interaction. Different variational wave functions are proposed and their range of application is explored depending on the intensity of the interaction. The Tonks-Girardeau limit is also analyzed.

I. INTRODUCTION

The recent improvements in the field of ultra-cold atomic gases have motivated an important effort to study quantum bosonic systems in 1D [1]. These systems can be experimentally realized in ultracold gases confined in cigar-shaped traps [2]. One of the main peculiarities of one-dimensional systems is that the reduced geometry has important consequences on the wave function. For instance, the only way to exchange two particles is passing one through the other [3]. Usually, the interaction between the particles is described by means of a δ-contact interaction with strength g. When the strength of the interaction becomes large, $g \to \infty$, one obtains the Tonks-Girardeau (TG) gas [4]. In this situation many of the properties of the system are identical to the case of non-interacting fermions.

In this work, we will perform a variational study of the ground-state energy and density profiles of one-dimensional bosonic systems trapped by a 1D harmonic oscillator (HO) potential with finite range interactions between them. When the range of these interactions tend to zero they are reduced to contact interactions. We are interested in the behavior of different observables, mainly the energy of the ground state, when the finite range force evolves into a contact interaction. To this end, we will propose different variational wave functions and explore their validity depending on the strength of the interaction. We will see that for strong interactions the system develops interparticle correlations that should be incorporated to the trial wave function.

This TFG is organized as follows. In section II we introduce the model Hamiltonian and the finite range interactions considered in this study. In section III we discuss the different variational methods used to calculate the energy and also propose the variational wave functions. In section IV we present and discuss the results. In section V we summarize the conclusions of the work.

*Electronic address: jesonora@gmail.com

II. THE MODEL HAMILTONIAN

We consider N non-relativistic bosons of mass m trapped in a HO potential, with frequency ω, which interact through a two-body finite range interaction $V_{int}(x_{ij})$, where x_{ij} is the interparticle distance. Using the energy and length units associated to the HO trapping potential, the system is described by the following Hamiltonian,

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

Along this work, we consider two finite-range interactions of Gaussian and Lorentzian type respectively:

$$V_1(x_{ij}) = \frac{g}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{x_{ij}^2}{\sigma^2}} \qquad V_2(x_{ij}) = \frac{g}{\pi}\frac{\sigma}{x_{ij}^2+\sigma^2}\,, \quad (2)$$

both of them normalized to g, which measures the strength of the interaction. The σ^2 measures the range of the potential and when it tends to zero, they become a δ-contact interaction . We will be mainly concerned with the Gaussian potential but we will also discuss their differences when they approach the δ interaction.

III. VARIATIONAL METHOD

The main idea of the variational method is to obtain upper bounds to the ground-state energy of the many-body system by evaluating the expectation value of the Hamiltonian in a parametric wave-function,

$$E_\alpha = \frac{\langle\Psi_\alpha|H|\Psi_\alpha\rangle}{\langle\Psi_\alpha|\Psi_\alpha\rangle}\,. \qquad (3)$$

The minimization of the energy with respect to the variational parameters ($\partial E_\alpha/\partial\alpha = 0$) defines the lowest upper bound in the considered set of functions. In the case that the functional space defined by the variational parameters contains the ground state wave function, the minimization procedure should provide the exact ground-state energy.

A. Mean field

Our first approach is to use the mean field approximation, in which all the particles are assumed to be in the same single-particle state, $\Psi(x_1, x_2, ...x_n) = \prod_{i=1}^{n} \phi(x_i)$. This approximation is useful in weak interacting regimes.

1. *Variational Gaussian single-particle wave function*

As a starting point, we propose a family of simple Gaussian single-particle wave functions, that depend on the variational parameter α,

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

The corresponding variational energy of the system reads,

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

In the limit $\sigma \to 0$ the energy reduces to

$$E(\alpha) = N\left(\frac{\alpha^2}{4} + \frac{1}{4\alpha^2}\right) + \frac{N(N-1)}{2}\frac{g}{\sqrt{2\pi}}\alpha\,. \tag{6}$$

The minimization of $E(\alpha)$ with respect to α provides the best energy within this family of many-body wave functions.

2. *Hartree-Bose*

To derive the Hartree-Bose (HB) equations, we propose a mean field wave function, $\Psi(x_1, x_2, ...x_n) = \prod_{i=1}^{n} \phi(x_i)$, built with a generic single-particle wave function. Then we require the energy to be stationary for small variations of the single-particle wave function,

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

where, λ is a Lagrange multiplier introduced to perform the functional variations preserving the norm. From this condition, we get the HB equation:

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

where λ can be identified with the chemical potential μ. In the case that the interaction is a $\delta-$contact interaction, one obtains the Gross-Pitaevskii equation,

$$\mu\phi(x) = -\frac{1}{2}\frac{d^2\phi(x)}{dx^2} + \frac{x^2}{2}\phi(x) + (N-1)g|\phi(x)|^2\phi(x)\,. \tag{9}$$

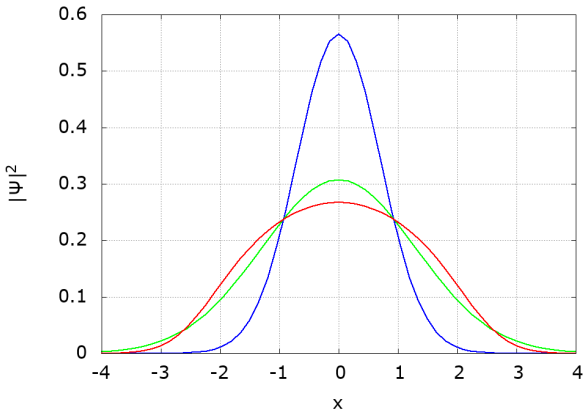

FIG. 1: Comparison of the different single-particle wave functions used to construct the mean field wave function for $N = 4$ and the gaussian interaction with $g = 4.0$ and $\sigma^2 = 0.5$. The ground-state wave function of the HO (blue-line) is compared with the best gaussian wave function (green-line) and with the best single-particle wave function solution of the HB equation (red-line)

B. Beyond the Mean Field Approximation

When the strength of the interaction increases, there is an emergence of two-body correlations in the wave function. These correlations try to minimize the energy by avoiding the atom-atom interaction, i.e. they attempt to keep the particles apart. Taking all that into account, we propose the following correlated wave function:

$$\Psi(x_1, ..., x_N) = \prod_{i=1}^{N}\left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha^2 x_i^2}\prod_{i<j}\left(1 - a\,e^{-bx_{ij}^2}\right)\,, \tag{10}$$

where α, a and b are the variational parameters.

Notice also that the Hamiltonian can be separated in two pieces, $H = H_{CM} + H_r$, which correspond to the center of mass (H_{CM}) and the relative (H_r) motion. Actually, the proposed correlated wave function can also be factorized in two pieces: one for the center of mass and the other describing the relative motion of the particles. In the exact wave function the center of mass should be in the ground state of H_{cm}. On the other hand, we know how to calculate the average value of H_{CM} in the trial variational wave function. Therefore, we can easily incorporate this improvement to our variational energy by subtracting this expectation value to the variational energy and adding the ground-state energy of H_{CM}:

$$\hat{E} = E - \left(\frac{\alpha^2}{4} + \frac{1}{4\alpha^2}\right) + \frac{1}{2}\,. \tag{11}$$

This correction is valid for any number of particles, for both the mean field approach built with gaussians and also for the correlated wave function. In the case of two-particles, the expectation value of the Hamiltonian with

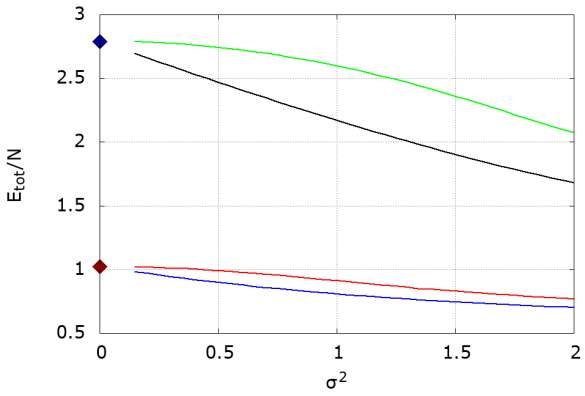

FIG. 2: Total energy per particle for a $N = 4$ as a function of the range of the interaction. The two-top lines correspond to $g = 6.0$, and the two-bottom lines to $g = 1.0$. The blue and black lines correspond to the results provided by the Gaussian and the green and red lines correspond to the Lorentzian potentials. The two rhombus at the $y-$axis are the energies for the $\delta-$contact interaction limit.

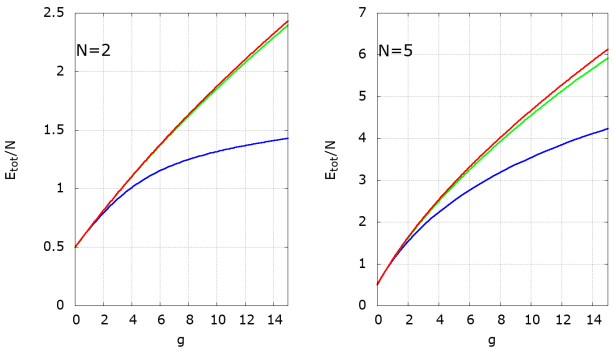

FIG. 3: Total energy per particle for $N = 2$ (left) and $N = 5$ (right) as a function of g for the Gaussian potential with a range $\sigma^2 = 0.5$. The red-line corresponds to the variational method with we Gaussian family, the green line to the Hartree-Bose, the blue line refers to the energy corresponding to the correlated wave function, Eq.(11). In all cases, the energy has been minimized.

this correlated wave function can be evaluated analytically. The expression is rather lengthly and has been given in Ref. [5].

Variational Monte Carlo

The aim of this method is to evaluate multidimensional integrals using the Monte Carlo numerical integration[6]. In this case the energy associated with the Hamiltonian is,

$$E_{VMC} = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\int d\mathbf{X}\Psi(\mathbf{X})^2 E_L(\mathbf{X})}{\int d\mathbf{X}|\Psi(\mathbf{X})|^2} = \\ = \int \rho(\mathbf{X}) E_L(\mathbf{X}) d\mathbf{X} \qquad (12)$$

where $\mathbf{X} = (x_1, ...x_N)$ are the bosons positions, E_L the local energy and $\rho(\mathbf{X})$ a normalized probability density. We can estimate the energy as an average value of E_L using the Metropolis algorithm to sample the probability density $\rho(\mathbf{X})$, $E_{VMC} \approx (1/M)\sum_{k=1}^{M} E_L(\mathbf{X}_k)$.

At this point, we have a method to evaluate the expectation value of the Hamiltonian for the variational wave function, which will depend on the three variational parameters. To obtain the lowest upper-bound energy we must optimize the variational parameters.

IV. RESULTS

We start by minimizing the variational energy provided by the mean field wave function built with the gaussian single-particle wave functions. In a second step, we find the best single-particle wave function by solving iteratively the HB equation. Firstly, we take as a starting single-particle wave function the ground-state wave function of the HO. Then, we calculate the mean field potential associated to this wave function and solve the corresponding Schrödinger equation to obtain the next single-particle wave function, which will be used for the next iteration until convergence is reached.

The different single-particle wave functions are reported in Fig. 1 for $N = 4$. The best gaussian single particle wave function (green-line) and the HB solution (red-line) are very similar and both are very different from the HO wave-function (blue-line). The repulsive interaction between the particles translates in wider single-particle wave functions. As expected, the best ground-state energy per particle is provided by the HB approach: $E_{HB} = 2.078$. However the gaussian wave function provides a rather close upper bound, $E_{var} = 2.105$, while the energy associated to the HO wave function is $E_{HO} = 2.454$ which would coincide with the energy provided by first order perturbation theory.

The dependence of the energy on the range of the potential calculated in the HB approach for the two types of interactions considered in this work is shown in Fig. 2. We also report the energies provided by the $\delta-$contact interaction with the same strength, obtained by solving the Gross-Pitaevskii equation. For all ranges of the potentials, the energy of the Gaussian potential is more repulsive than the Lorentzian ones and, as expected, both tend to the same result for zero-range interaction. The differences between the Gaussian and Lorentzian interactions are larger for stronger interactions ($g = 6$ compared with $g = 1$).

In the next step, we start to explore the need of correlations when the interaction is stronger. Fig. 3 reports the total energy per particle for $N = 2$ and $N = 5$ particles as a function of the strength of the interaction, using the gaussian potential with the range $\sigma^2 = 0.5$.

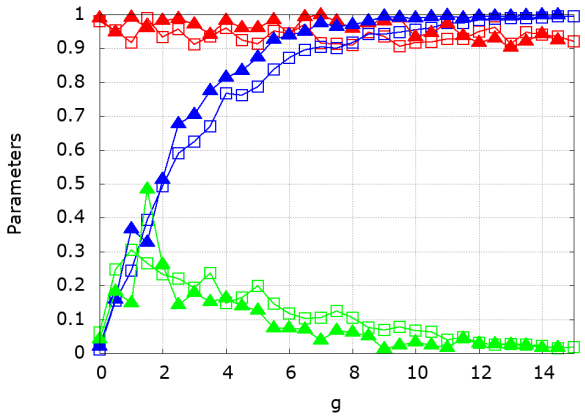

FIG. 4: Dependence of the optimal parameters for the correlation function on the strength of the interaction for the case $N = 2$ (solid triangles) and $N = 5$ (empty squares) with $\sigma^2 = 0.5$. The red, blue and green lines correspond to α^2, a and b parameters respectively.

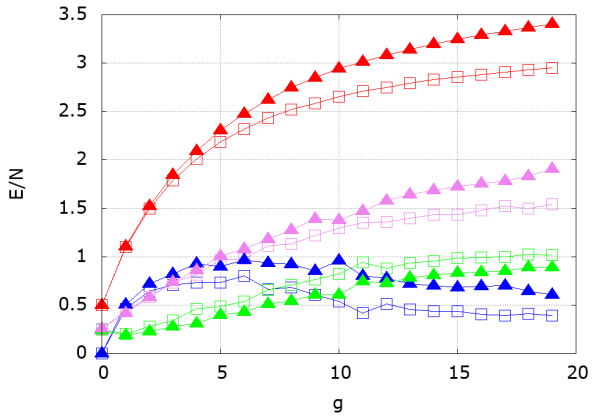

FIG. 5: Total energy per particle (red lines) for $N = 5$ as a function of g, the solid triangles correspond to $\sigma^2 = 0.125$ and the empty squares to $\sigma^2 = 0.05$. The energy is decomposed in the HO energy (pink lines), the kinetic energy (green lines) and the interaction energies (blue lines).

For all strengths, the HB and the variational energies of the gaussian family are very close. For weak interactions, up to g equal 3, the effect of correlations is negligible but when the strength of the interaction increases they become crucial to decrease the energy. In any case, we should keep in mind that the correlated wave function is not the exact wave function but we are sure that it provides an upper bound.

The energies corresponding to the correlated wave function have been calculated using the VMC method. The case $N = 2$, for which exist the analytical results, has been used as a test for the Monte Carlo procedures. The energies reported in the Fig. 3 are the result of a minimization procedure which determine the optimal variational parameters at each case. The optimal variational parameters for the gaussian interaction, are reported in Fig. 4, for $N = 2$ and $N = 5$ as a function of the strength of the interaction, for the range $\sigma^2 = 0.5$. Independently of the number of particles, when the strength of the interaction increases, the a parameter approaches unity. In this way, the particles avoid being at the same point. The behavior of the variational parameters is very similar for $N = 2$ and $N = 5$. That may suggest the possibility to fix the two-body correlation at the two-body system and minimize only with respect to α for the systems with $N > 2$.

The VMC method is implemented using Fortran77. However the minimization method is built on a SciPy library. The bridge between the fortran program and the minimization Python library is provided by the Python library F2PY which translates the Monte Carlo code in a function depending on the three variational parameters. This procedure for the Monte Carlo calculation and for the minimization is tested in the case $N = 2$ for which analytical results exists.

As shown in the Fig. 5, the interaction energy has a maximum in the interval from $g = 5$ to $g = 10$. After this point it decreases due to the two-body correlations, as can be seen comparing with Fig. 3, where we can see that the correlated wave function result deviates substantially from the mean-field one. In Table 1, we report the energies obtained with the different methods for $N = 2$ and $N = 5$ for $g = 5$.

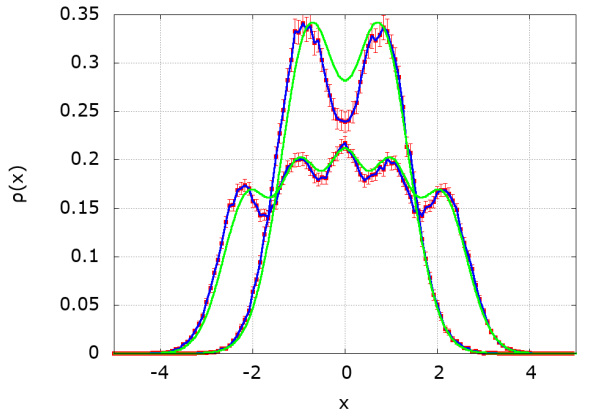

FIG. 6: Density profile for $N = 2$ and $N = 5$ particles produced with the gaussian interaction potential with $g = 19$ and $\sigma^2 = 0.05$. The green line represents the analytical result for N non-interacting fermions enclosed in the same HO potential while the blue line is provided by the VMC.

In the strong interaction limit and for small range of the interaction the many-body wave function should resemble the one of the TG gas. This can be seen in Fig. 6 where we compare the density profiles produced by a strong interaction ($g = 19$) with a range $\sigma^2 = 0.05$ for $N = 2$ and $N = 5$, corresponding to the correlated wave function (Eq. 10), with the ones of a free Fermi system trapped in the same HO potential (which can be analytically calculated). As expected from the fermionic result, the density profile develops a number of bumps equal to

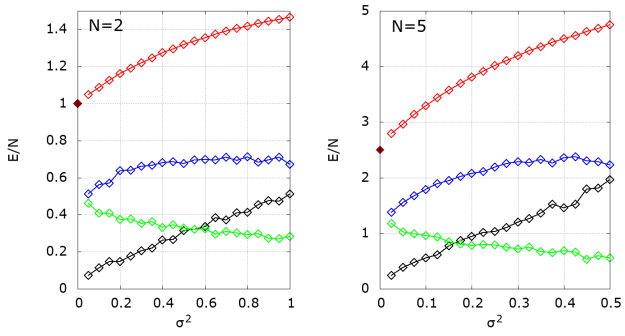

FIG. 7: Energies per particle for $N = 2$ (left) and $N = 5$ (right): total energy (red line), interaction energy (black line), kinetic energy (green line) and potential energy (blue line) for $g = 10$. The red full dots ($\sigma^2 \to 0$) correspond to non-interacting fermions trapped in the same HO potential at each case.

N	g	E_{var}	E_{HB}	E_{VMC}	$\hat{E}_{VMC}$
2	5.0	1.244	1.238	1.091	1.076
5	5.0	2.939	2.884	2.513	2.504

TABLE I: Energy per particle for $\sigma^2 = 0.5$ obtained with different methods for $g = 5$ and $N = 2$ and $N = 5$. The energy $\hat{E}_{VMC}$ takes into account the center of mass correction.

the number of particles.

In Fig. 7 , we report the dependence on the range of the interaction of the total energy per particle for $g = 10$ and $N = 2$ and $N = 5$. The figure also shows the potential HO, the kinetic and the interaction energies. It is worth to notice that for this strength of the interaction the system already approaches the TG limit when $\sigma^2 \to 0$ and the total energy tends to 1 in the case of $N = 2$ and to 2.5 for $N = 5$.

In this way, Fig. 8 exemplifies the TG behavior, when we let $\sigma^2 \to 0$ but the g is not large enough $g = 2$ in the figure, the energy does not go to the fermionic result (green lines). On the other hand, for strong interactions, $g = 10$ and $g = 20$, we get the same limit, i.e., the TG limit, when the interaction approaches a δ-interaction.

V. CONCLUSIONS

We have analyzed different variational methods to calculate the ground-state energy and the one-body density profile of a one-dimensional system of N bosons trapped by an HO potential. The bosons interact through a repulsive finite range interaction, characterized by its strength g and range σ^2. First of all, we have proposed a very simple mean field wave function of gaussian type which provides energy results in very good agreement with the best mean-field wave function obtained by solving the Hartree-Bose equations. As expected, the mean field approach gives satisfactory results only at weak interaction

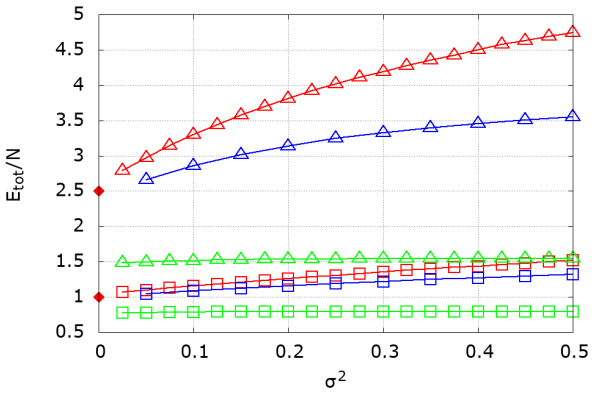

FIG. 8: Total energy per particle for $N = 5$ (triangles) and $N = 2$ (squares) for different g. The red-lines are for $g = 20$, the blue-lines are for $g = 10$ and the green-lines are for $g = 2$.

regimes. For stronger regimes it is necessary to go beyond the mean field approach and introduce two-particle correlations in the wave function. We have proposed a physically founded correlated wave function and calculated the expectation value of the Hamiltonian by Monte Carlo techniques. By analyzing the dependence of the energy on the strength and range of the interaction we have seen that the proposed variational wave function provides a good description of the Tonks-Girardeau limit.

Acknowledgments

I would like to thank my advisors Artur Polls and Bruno Juliá-Díaz for their guidance and dedication as well as my parents and friends, specially to J. C. Rivera and G. Giralt for their infinite patience.

[1] T. Kinoshita, T. Wenger, and D.S. Weiss, Nature **440**, 900 (2006).
[2] N. Matveeva, G. E. Astrakharchik, New J. Phys. **18**, 065009 (2016).
[3] A. I. Gudyma, G. E. Astrakharchik, and M. B. Zvonarev, Phys. Rev. A **92**, 021601 (2015).
[4] M. Girardeau, J. Math. Phys. **1**, 516 (1960).
[5] V. Cami in *Quantum Monte Carlo study of one-dimensional bosons with finite range interactions*, TFM Photonics (2017).
[6] J. Toulouse, R. Assaraf, C. J. Umrigar *Introduction to the variational and diffusion Monte Carlo methods*, (2015).