

Bose-Einstein condensation in trapped bosons with a Diffusion Monte Carlo approach

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1 Introduction

The aim of the project is to reproduce some results obtained in the theoretical and numerical study of Bose-Einstein condensation in systems of trapped bosons. In particular it is interesting to understand if a system constituted by a gas of N confined bosons interacting between each other just through a hard core potential sustains BEC.

We restrict our attention to the study of $N = 128$ Rubidium atoms confined within a spherically symmetric harmonic trap. The scattering length of Rubidium is taken as the radius of the hard core potential and its ratio with respect to the typical length of the harmonic trap is given by $a_{Rb}/a_{ho} = 4.33 \times 10^{-3}$.

We only consider the vanishing temperature case $T = 0K$. The properties of the system are investigated through a Diffusion Monte Carlo (DMC) analysis: this method is based on the imaginary time propagation of the wavefunction. The idea behind is that if we start from a guess of the wavefunction having a non-vanishing overlap with the ground state, then after a sufficiently long propagation in imaginary time the ground state will be the leading term of the evolution. The implementation consists in building up many different replicas (walkers) of the system, each describing a “snapshot” of the many-body wavefunction in real space at a given time instant. At every time-step the evolution of the wavefunction is described through a gaussian diffusion of all the particles for each single walker, after which the effect of the potential is applied through birth and death processes of the walkers.

The DMC method here implemented is valid only for real and positive definite wavefunctions.

2 Monte Carlo Formulation of the Problem

The Hamiltonian which describes the many-body problem is given by

$$\mathcal{H} = \sum_i^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{i < j}^N V_{int}(\mathbf{r}_i, \mathbf{r}_j; a), \quad (1)$$

with a spherically symmetric harmonic potential

$$V_{ext}(\mathbf{r}) = \frac{1}{2} m \omega_{ho}^2 r^2, \quad (2)$$

and the interaction between particles is described by a hard core potential

$$V_{int}(\mathbf{r}_i, \mathbf{r}_j; a) = \begin{cases} \infty, & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0, & |\mathbf{r}_i - \mathbf{r}_j| \geq a, \end{cases} \quad (3)$$

where a is the scattering length of the atoms we are considering.

To implement the problem in a way which is numerically meaningful we choose as natural

units of the problem three constants given by the typical trap length a_{ho} as unit of length, Planck's constant \hbar as unit of angular momentum and the particle mass m as unit of mass. From this it follows automatically that the trap frequency in these units is given by $\omega_{ho} = \hbar/(ma_{ho}^2) = 1$. Another advantage is that the scattering length which enters the function f is now a/a_{ho} so that for Rubidium we can use $a_{Rb} = 4.33 \times 10^{-3}$.

To describe the ground state of the boson gas we start from a trial many-body wavefunction depending on two variational parameters b_0 and b_1 . The trial variational wavefunction of the N bosons system is given by

$$\Psi_T(\mathbf{r}_1, \dots, \mathbf{r}_N; b_0, b_1) = \prod_i^N g(\mathbf{r}_i; b_0, b_1) \prod_{i < j}^N f(\mathbf{r}_i, \mathbf{r}_j; a). \quad (4)$$

Here the function g contains the solution of the Schrödinger equation in the case of the non-interacting system, which is given by a gaussian centered at the center of the trap, plus a correction in r^4 . The function is controlled by the two variational parameters b_0 and b_1 :

$$g(\mathbf{r}; b_0, b_1) = \exp[-(b_0 r^2 + b_1 r^4)]. \quad (5)$$

On the other side the function f is given by the solution of the hard core scattering problem in the s -wave limit

$$f(r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|; a) = \begin{cases} 1 - a/r_{ij} & , \quad r_{ij} > a \\ 0 & , \quad r_{ij} \leq a \end{cases}. \quad (6)$$

This choice of f is particularly suitable because it prevents automatically two particles to come too near to each other at a distance $r < a$ so that the hard-core prescription is automatically taken into account. In this way we don't have to introduce explicitly the V_{int} term within the numerical implementation of the Hamiltonian. It is however stressed here that we lack any variational parameter controlling the inter-particle interaction.

The space of configurations of the atoms grows as \mathbb{R}^{3N} with the number N of atoms in the trap. It is then important to drive the diffusion sampling of the wavefunction towards regions of the configuration space which describe better the behavior of the ground state. This can be achieved by implementing an importance sampling which exploits a guiding function that controls the diffusion of the walkers during the DMC process. In our case we choose as guiding function the trial wavefunction $\Psi_T(\bar{b}_0, \bar{b}_1)$ with parameters \bar{b}_0 and \bar{b}_1 that minimize the ground state energy. The guiding function is thus determined through a variational procedure involving a Variational Monte Carlo (VMC) approach.

2.1 Determining the guiding function through VMC

In order to determine the guiding function we need to minimize the energy of the system with respect to the variational parameters b_0 and b_1 . The expectation value of the energy is given by

$$\langle E(b_0, b_1) \rangle = \frac{\langle \Psi_T(b_0, b_1) | \mathcal{H} | \Psi_T(b_0, b_1) \rangle}{\langle \Psi_T(b_0, b_1) | \Psi_T(b_0, b_1) \rangle}. \quad (7)$$

We introduce the collective label R representing all atoms coordinates in a compact form, in such a way that $\int dR = \int d^3r_1 \int d^3r_2 \dots \int d^3r_N$. By introducing the local energy

$$E_L(b_0, b_1) = \frac{\mathcal{H}\Psi_T(R; b_0, b_1)}{\Psi_T(R; b_0, b_1)}, \quad (8)$$

we can rewrite the expectation value as

$$\langle E(b_0, b_1) \rangle = \frac{\int dR \Psi_T^2(R; b_0, b_1) E_L(b_0, b_1)}{\int dR \Psi_T^2(R; b_0, b_1)}. \quad (9)$$

As the bosonic wavefunction is real and everywhere positive on its domain $\Psi_T^2(R; b_0, b_1)$ represents a probability density function and we can evaluate the expectation value of the energy by sampling the local energy E_L through the Metropolis algorithm using $\Psi_T^2(R)$ as the asymptotic probability density. The value of the energy will then be given by

$$\langle E(b_0, b_1) \rangle = \frac{1}{N_{step}} \sum_{n=1}^{N_{step}} E_L(R^{(n)}; b_0, b_1), \quad (10)$$

where N_{step} is the number of steps during the Metropolis algorithm and $R^{(n)}$ is the configuration of atoms sampled at the n -th step. In order to reduce the fluctuations around the energy we consider the evolution of different walkers starting all from the same initial configuration and then we also average on the walkers at each step:

$$\langle E(b_0, b_1) \rangle = \frac{1}{N_{step}} \frac{1}{N_{walk}} \sum_{i=1}^{N_{step}} \sum_{j=1}^{N_{walk}} E_L(R^{(i,j)}; b_0, b_1), \quad (11)$$

where N_{walk} is the number of walkers, while $R^{(i,j)}$ is the configuration of the atoms sampled at the i -th step for the j -th walker. At each step an atom is chosen randomly for each walker and displaced by a random vector whose components live in the interval $[-d, d]$, where d is the maximum displacement allowed for a single component.

$$R_{trial}^{(i,j)} = (R^{(i-1,j)} + \xi^{(i,j)}) \quad (12)$$

After the displacement the probability that the move is accepted is evaluated as the ratio

$$P_A^{(i,j)} = \frac{\Psi_T^2(R_{trial}^{(i,j)})}{\Psi_T^2(R^{(i-1,j)})}. \quad (13)$$

In order to determine numerically if the move is accepted or not another random number $\eta^{(i,j)}$ is extracted for each walker within the uniform distribution from the interval $[0, 1]$. If $\eta^{(i,j)} < P_A^{(i,j)}$ then the move is accepted and we set $R^{(i,j)} = R_{trial}^{(i,j)}$, otherwise the move is rejected and the configuration is replicated $R^{(i,j)} = R^{(i-1,j)}$. This way a Markov chain of configurations is generated with the asymptotic probability distribution given by $\Psi_T(R; b_0, b_1)$ and can be used to evaluate the expectation value given in eq. 11.

It must be stressed that the chosen family of wavefunctions which can be described as a product of single particle functions plus a product of symmetric interaction terms is particularly suitable for the numerical implementation: if we change only one atom at each trial move (consider for instance the atom at position \mathbf{r}_m) then the only terms that change in $\Psi_T(R_{trial}^{(i,j)})$ with respect to $\Psi_T(R^{(i-1,j)})$ are the single particle term $g(\mathbf{r}_m)$ and all the interaction terms $f(r_{mn})$ with $n \neq m$, while the unchanged terms cancel out in the ratio. The acceptance probability assumes then the form

$$P_A^{(i,j)} = \frac{g(\mathbf{r}_m + \xi^{(i,j)})}{g(\mathbf{r}_m)} \prod_{n \neq m} \frac{f(|\mathbf{r}_m + \xi^{(i,j)} - \mathbf{r}_n|)}{f(|\mathbf{r}_m - \mathbf{r}_n|)}, \quad (14)$$

where we have to consider the ratio of N terms, being N the number of atoms in the trap. The local energy is then evaluated for each configuration as

$$E_L(R) = - \sum_{i=1}^N \frac{1}{2} \frac{\nabla_i^2 \Psi_T(R)}{\Psi_T(R)} + \sum_{i=1}^N V_{ext}(\mathbf{r}_i). \quad (15)$$

While the part of the local energy associated to the harmonic potential V_{ext} can be determined trivially as the sum of the potential evaluated for each single particle, the kinetic

term is slightly more difficult to determine. In this implementation we decide to evaluate it numerically using the finite difference method. Again, as the laplacian is evaluated on one single particle at a time, we can exploit the fact that a shift of the atom in one direction causes only N terms to change within the building blocks of the many-body wavefunction. The kinetic term associated to a single particle is then given by

$$\Delta K_{i,\alpha}^{(\pm)} = \frac{g(\mathbf{r}_i \pm \Delta \mathbf{x}_\alpha)}{g(\mathbf{r}_i)} \prod_{j \neq i} \frac{f(|\mathbf{r}_i \pm \Delta \mathbf{x}_\alpha - \mathbf{r}_j|)}{f(|\mathbf{r}_i - \mathbf{r}_j|)} \quad (16)$$

$$K_i = -\frac{1}{2} \frac{\nabla_i^2 \Psi_T(R)}{\Psi_T(R)} = -\frac{1}{2} \sum_{\alpha=1}^3 \frac{K_{i,\alpha}^{(+)} - 2 + K_{i,\alpha}^{(-)}}{\Delta x^2}, \quad (17)$$

where Δx is the variation of a coordinate considered in the finite difference method (here we take $\Delta x = 10^{-4}$) and α labels the cartesian coordinate direction in space (x, y or z axis). In order to maintain a compact notation we indicated $\Delta \mathbf{x}_\alpha$ as the three dimensional vector having only one non-vanishing component on the α axis of magnitude Δx (e.g. $\Delta \mathbf{x}_1 = (\Delta x, 0, 0)^T$).

With this implementation the kinetic term of each atom can be evaluated in $\mathcal{O}(N)$ function calls; the overall cost of evaluating the total kinetic term is then given by $\mathcal{O}(N^2)$ function calls. In this case the chosen form of the wavefunction allows also for the exact evaluation of the kinetic terms, which involves first and second derivatives of the wavefunction. The number of terms in this case grows however as $\mathcal{O}(N^2)$ for a single atom, making the numerical procedure more efficient with respect to the number of operations involved.

2.2 Diffusion Monte Carlo

A detailed description of the standard DMC method can be found in [3], while here we focus on the adjustments we need in order to implement an importance sampling procedure. After the variational procedure has been completed we take as guiding function $\Psi_G(R)$ the wavefunction $\Psi_T(R; \bar{b}_0, \bar{b}_1)$ whose parameters \bar{b}_0 and \bar{b}_1 minimize the expectation value of the energy. The guiding function allows to implement an importance sampling procedure when investigating the configuration space of the system, making the algorithm more effective. The DMC algorithm requires to start from an initial wavefunction that should have meaningful overlap with that of the ground state of the system. For our purpose we initialize a given number of walkers N_{walk} and we sample the initial configuration as in the VMC procedure, using the Metropolis algorithm with $\Psi_G(R)$ as asymptotic distribution. This way each walker is initialized with a configuration sampled directly from $\Psi_G(R)$. We then proceed with the diffusion-branching procedure. At each time-step each walker updates the coordinates of the atoms of its configuration as

$$R' = R + \frac{1}{2} F(R) \Delta t + \xi \sqrt{\Delta t}, \quad (18)$$

where Δt is the time-step we are considering, ξ is a gaussian random number sampled from a configuration with mean value $\mu = 0$ and standard deviation $\sigma = 1$, while $F(R)$ is the driving force and it is defined as

$$F(R) = 2 \frac{\nabla \Psi_G(R)}{\Psi_G(R)} \quad (19)$$

Following Ceperley [4] we introduce also an improved propagation, with the possibility of rejecting moves that do not satisfy the detailed balance condition. We evaluate the quantity

$$\mathcal{G}(R \rightarrow R') \propto \exp \left[-\frac{(R' - R - \frac{1}{2} \Delta t F(R))^2}{2 \Delta t} - \Delta t (E_L(R) - E_T) \right], \quad (20)$$

where E_L is the local energy evaluated as in eq. 15 using the guiding function, while E_T is the value taken as reference of the energy scale. The probability of accepting the move is defined as

$$P_A = \frac{\mathcal{G}(R' \rightarrow R)\Psi_G(R')^2}{\mathcal{G}(R \rightarrow R')\Psi_G(R)^2}. \quad (21)$$

As in the variational procedure we then extract a random variable η uniformly distributed within the interval $[0, 1)$ and the move is accepted if $\eta < P_A$. With this improved propagation we reduce the accumulation of errors due to the finite timestep Δt used within the propagation.

Then the branching step takes place. For each walker we evaluate the corresponding branching factor taking into account also the local energy of the former step (see [4]):

$$w = \left\lfloor \exp\left(-\frac{1}{2}\Delta t(E_L(R) - E_L(R') - 2E_T)\right) + u \right\rfloor, \quad (22)$$

where u is a random number extracted uniformly from $[0, 1)$ that allows to randomly increase by one unit the branching factor. In order to avoid an excessive growth in the number of walkers we decide to allow only for the production of at most three extra walkers for each branching walker ($w_{max} = 4$).

In order to stabilize the number of walkers which are generated or removed we also implement an active population control through the adjustment in runtime of the energy scale E_T which controls the branching factor. The energy scale is updated periodically with

$$E_T^{(n)} = \langle E_L \rangle + \frac{\ln(P^{(0)}/P^{(n)})}{k\Delta t}, \quad (23)$$

where $P^{(n)}$ is the number of walkers at step n , while k is a problem dependent constant that we explain how to set in the next section.

The diffusion-branching procedure allows to explore the configuration space, sampling “snapshots” of the many-body wavefunction that can be used in the evaluation of different physical quantities.

2.3 Determining the condensate fraction

As we are studying a gas of bosons at zero temperature we are interested in determining if BEC is present for this system and which is the fraction of atoms that would take part in the condensation. In order to determine this fraction we follow a procedure presented in [1].

The key ingredient in the calculation is the one-body density matrix (OBDM) defined as

$$\rho(\mathbf{r}, \mathbf{r}') = \int d^3r_2 \dots \int d^3r_N \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N). \quad (24)$$

The OBDM can then be expanded in terms of the natural orbitals (NO) $\{\phi_i(\mathbf{r})\}$, which are single-particle states defined as the eigenstates of the OBDM.

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{ij} \delta_{ij} \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}') N_i, \quad (25)$$

with N_i the eigenvalue of the OBDM associated to the NO ϕ_i . If the overall potential, including the interaction term, is assumed to be spherically symmetric then the NO wavefunction can be factorized in a radial and in an angular part as

$$\phi_i(\mathbf{r}) = \phi_{nl}(r) Y_{lm}(\theta, \varphi), \quad (26)$$

where $Y_{lm}(\theta, \varphi)$ is the spherical harmonic with eigenvalue of total orbital angular momentum l and orbital momentum along the z -axis m , while n is the quantum number labeling the eigenvalue of the energy. It is shown in [1] that also the OBDM can be expanded in radial components and that those components, labeled with value of angular momentum l are defined as

$$\rho_l(r_1, r'_1) = \int d\Omega_1 \int d^3r_2 \dots \int d^3r_N \Psi^*(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}'_1, \mathbf{r}_2, \dots, \mathbf{r}_N) P_l(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}'_1), \quad (27)$$

where $P_l(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}'_1)$ is the Legendre polynomial of order l . By introducing the function $u_{nl}(r) = r\phi_{nl}(r)$, the radial terms of the OBDM satisfy the following matrix relation

$$\int dr' [r\rho_l(r, r')r'] u_{nl}(r') = N_{nl}u_{nl}(r). \quad (28)$$

This last equation can be casted into a 1D matrix equation by discretization of the space and can be solved numerically as an eigenvalue equation. The condensate orbital is defined as the orbital with the lowest quantum numbers $\phi_{00}(r)$ and its corresponding eigenvalue N_{00} is the fraction of atoms in that orbital. If the system supports BEC than after solving the eigenvalue problem we should find an orbital with an occupation number $N \simeq 1$, while all other eigenvalues are suppressed by orders of magnitude.

In order to determine numerically the structure of $\rho_0(r, r')$ we observe that if the many-body wavefunction were built out of non interacting single-particle states $\psi(r_i)$ than eq. 27 reduces to

$$\rho_0^{non-int}(r, r') = 4\pi\psi^*(r)\psi(r') = 4\pi\psi(r)\psi(r'), \quad (29)$$

where the last equality holds as we are considering only real and positive wavefunctions. This suggests to evaluate numerically the OBDM as the joint probability amplitude of simultaneously finding one particle at radial distance r from the origin and another one at distance r' . By discretizing the radial distance and integrating using spherical shells, the number of particles N_{ij} such that one is within a distance $[r_i, r_i + \Delta r]$ from the origin and the other one is at distance $[r_j, r_j + \Delta r]$ is given by

$$N_{ij} = \sum_n (4\pi\Delta r)r_i^2 |\phi_{n0}(r_i)|^2 (4\pi\Delta r)r_j^2 |\phi_{n0}(r_j)|^2 = N_{at}^2 (\Delta r)^2 (r_i \rho_0(r_i, r_j) r_j)^2, \quad (30)$$

where the last equality is assumed to hold if we neglect higher orders of l in the expansion and N_{at} is the total number of atoms.

The OBDM is then numerically determined by discretizing the radial distance on a grid and counting the number of particles N_{ij} as

$$r_i \rho_0(r_i, r_j) r_j = \frac{\sqrt{N_{ij}}}{N_{at} \Delta r} \quad (31)$$

3 Results

In this section we discuss the details of the numerical implementation and the obtained results.

3.1 VMC Results

In the VMC procedure we fix a given number of walkers and randomly generate the same initial configuration, enforcing spherical symmetry and satisfying the hard core condition, for all walkers. This configuration is then used as the starting point of the metropolis

algorithm to generate a Markov chain of configurations for the many-body system; in this case each walker evolves in a different way during the Metropolis procedure, in order to increase the overall number of samplings and reduce the fluctuations around the mean value of the energy. In order to have acceptance ratios $a_{acc} > 50\%$ we need to set the virtual displacement amplitude d as defined in Sec. 2.1 as $d = 1.0$ (in units of the trap length a_{ho}).

As the number of coordinates of the trial wavefunction increases as $3N_{at}$ it is convenient to evaluate the energy at runtime and update the coordinates configuration for each walker, more than saving all configurations and then evaluate the energy later.

During the VMC procedure we observe as expected that an initial number of step is required to equilibrate the local energy E_L , after which it starts fluctuating around an almost constant mean value. The number of equilibration steps needed is observed to be around $N_{steps}^{eq} \simeq 10^4$. In order to reduce the computational cost it is useful to have a long VMC run of a single walker, save the final coordinates produced at the end of the run and use them as the initial condition in future runs. This “equilibrated coordinates” still depends on the pair of variational parameters (b_0, b_1) of the trial wavefunction, but using them as a starting point for future VMC calculations reduces the number of equilibration steps to $N_{step}^{eq} \simeq 10^3$.

In order to find the pair of parameters (b_0, b_1) minimizing the energy we decide to discretize them taking for each of them 11 values uniformly distributed in the intervals $b_0 \in [0.46, 0.5]$ and $b_1 \in [0.0, 0.002]$, thus defining a meshgrid of 11×11 points. The reason behind the choice of the interval is to sample values of the variational parameters near those that solve the non interacting many-body problem, which are given by $b_0^{N.I.} = 0.5$ and $b_1^{N.I.} = 0.0$.

For each pair of parameters (b_0, b_1) we perform a VMC run using $N_{walk} = 200$ and with a total of $N_{step} = 10^5$ steps for each walker. The energy is then evaluated according to eq. 15, taking as error the standard deviation. Results of the minimization procedure are shown in Fig. 1.

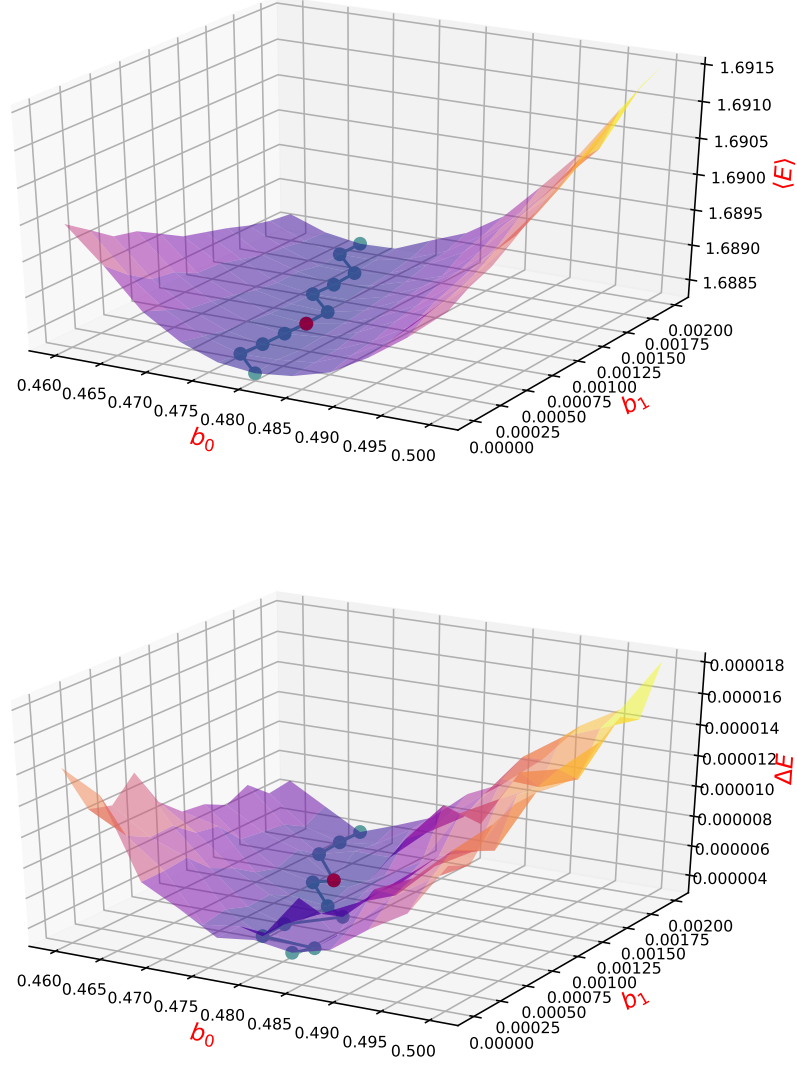


Figure 1: (Above) VMC expectation value of the ground state energy as a function of the variational parameters (b_0, b_1) and (Below) the error associated to it. A solid blue line shows the minimum of $\langle E \rangle$ and ΔE for each value of the parameter b_1 , while the red marker signals the position of the minimum for both the energy and the error. $\langle E \rangle_{min} = 1.6883113$ with $(b_0, b_1) = (0.476, 0.0008)$, while $(\Delta E)_{min} = 3 \times 10^{-6}$ with $(b_0, b_1) = (0.472, 0.0014)$.

We find the following values for the minima of the energy per atom and the error associated to it :

$$\langle E \rangle_{min} = 1.6883113 \quad (\bar{b}_0, \bar{b}_1)_{\langle E \rangle} = (0.0476, 0.0008) \quad (32)$$

$$(\Delta E)_{min} = 3 \times 10^{-6} \quad (\bar{b}_0, \bar{b}_1)_{\Delta E} = (0.0472, 0.0014). \quad (33)$$

It is interesting to notice that in this case the VMC procedure produces two different values for the position of the minima of the energy and the error. We observe though that with the chosen number of steps and walkers $\langle E \rangle$ appears to be a smooth function of the

variational parameters, while ΔE presents significant fluctuations. In this case we decide then to keep as pair of parameters (\bar{b}_0, \bar{b}_1) those that minimize the energy. The value of ΔE serves still as an indication that the region of the minimum of $\langle E \rangle$ has been determined correctly, as when we approach the true ground state with the variational procedure we should minimize both the expectation value of the energy and the fluctuations around it. It is also important to notice that the minimum is found to live in a flat region of the parameter space. In the VMC procedure the minima of the energy as evaluated on the blue line of Fig. 1 differ by more than $10^{-5}/10^{-6}$, which is the typical order of magnitude of ΔE , so that the position of the minimum returned by the VMC calculation should be stable. However if the DMC procedure returns an error with an higher order of magnitude we should keep in mind that the pair of parameters (\bar{b}_0, \bar{b}_1) which define the guiding function may have an influence on the value of the energy returned by the DMC procedure. The energy per atom returned by the VMC is also meaningful by the physical point of view. In absence of interaction we should have $\langle E \rangle^{(N.I.)} = 1.5$, so that we understand that the hard-core interaction has the effect of increasing the ground state energy with a small correction of order 10^{-1} .

3.2 DMC Results

We implement the DMC procedure using as guiding function $\Psi_G(R) = \Psi_T(R; b_0 = 0.0476, b_1 = 0.0008)$. In this case we initialize a set of $N_{walk} = 1000$ walkers. Each walker is initialized with a coordinate configuration obtained through the metropolis procedure using Ψ_G as the trial wavefunction. In this case the number of walkers will vary during the numerical procedure, so that we define an overall array of walkers containing $N_{walk}^{max} = 2000$ possible entries. The entries on the tail will be removed or added according to the branching of the existing walkers.

We decide to take as timestep $\Delta t = 10^{-4}$: this is the larger timestep that produces an acceptance probability of $P_A \simeq 90\%$ for the moves during the diffusion step (see eq. 21). It is observed that taking a smaller timestep improves both the acceptance probability and the fluctuations around the value of the energy, but makes the convergence extremely slow.

Taking as reference value of the energy the one produced by the VMC procedure in eq. 32, with the timestep Δt , has the effect of producing no branching at all for the walkers, due to the structure of the branching factor described in eq. 22. We then deliberately increase the value of it to $E_T = 5$ in order to force branching of walkers in the first part of the procedure. To tune the population control we also set the constant k defined in eq. 23 as $k = P(0)$, where $P(0)$ is the initial population of walkers. This value is seen to prevent large fluctuations in the number of walkers that will eventually kill all of them or produce too many to exceed the limit of memory. The value of the reference energy E_T is then updated as in eq. 23 every 100 steps.

The first part of the procedure is dedicated to the equilibration of the system for which we consider a run of $N_{step} = 3 \times 10^4$, so that the diffusion-branching steps take place until the value of the energy and the population of walkers fluctuate around their mean values. Results of the equilibration procedure are shown in Fig. (2).

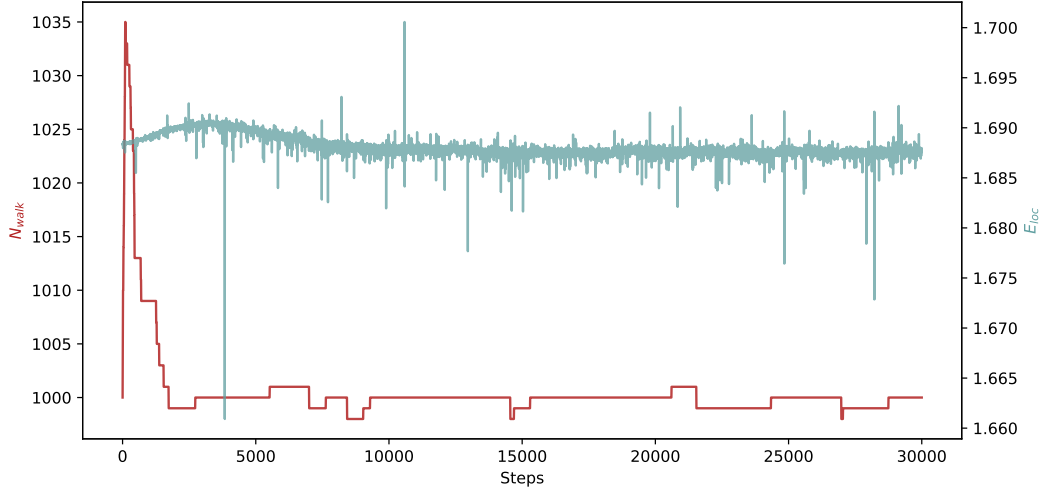


Figure 2: Equilibration of the energy and of the population of walkers during the DMC procedure. Both values stabilize around a mean value and start fluctuating after $N_{step} = 10^4$ steps. The population control implemented through eq. 23 have the population of walkers fluctuating around the initial population $P(0)$ after the equilibration is concluded.

We can observe that after the equilibration the ground state energy fluctuates around a fixed value, while the population of walkers fluctuates around the initial number of walkers, thanks to the population control implemented through eq. 23. We can also observe that both branching of walkers and variations in the value of the energy have a significant effect for $\simeq 10^3$ steps, while after 10^4 steps the procedure is stable.

After the equilibration is concluded we continue the diffusion-branching procedure, but we start sampling the OBDM as described in eq. 31. We discretize the radial distance and we consider a total of 5000 samples of the wavefunction and for each one of them we evaluate the numerical OBDM through the coordinates configurations stored into the walkers. At each sample the OBDM is averaged with the number of walkers present for that given step of the DMC procedure. Eventually we average on the total number of samples. In order to reduce the correlation from one sample to the other the many-body wavefunction is sampled every 100 steps. The energy instead is evaluated at every step, for a total of 5×10^5 observations, as it is observed from the equilibration procedure that there are consistent fluctuations.

At the end of the sampling procedure we determine the DMC value for the ground state energy with an associated value given again by the standard deviation around the mean value.

$$\langle E \rangle = 1.6876 \pm 0.0002 \quad (34)$$

The OBDM obtained through eq. 31 is then diagonalized following the matrix equation associated to eq. 28. The diagonalization of the OBDM as evaluated from eq. 31 does not produce any macroscopically occupied orbital¹. As expected all eigenvalues take values in $[0,1]$. However the diagonalization procedure considered evaluates the eigenvalues from the smaller to the greater one, which may cause difficulties in the computation. A careful redefinition of the eigenvalue problem as

$$\tilde{\rho}_{ij} = r_i(\rho_0)_{ij}r_j \quad (35)$$

$$\tilde{\rho}_{ij} \rightarrow \tilde{\rho}'_{ij} = \delta_{ij} - \tilde{\rho}_{ij} \quad (36)$$

$$\tilde{\rho}_{ij}\phi_j = N\phi_i \rightarrow \tilde{\rho}'_{ij}\phi_j = (1 - N)\phi_i \quad (37)$$

¹We are using *dsyev* routine within the LAPACK package.

allows to have the greater eigenvalue becoming the smaller one and viceversa, helping the convergence of the calculation. Indeed by evaluating the eigenvalues N' of ρ' and then recasting them into eigenvalues of ρ as $N = 1 - N'$ gives one eigenvalue $N_0 \simeq 0.95$, while all others eigenvalues are suppressed by orders of magnitude ($N_{i>0} \simeq 10^{-3}$). This result is compatible with the trapped atoms undergoing BEC with the condensate orbital given by the eigenstate associated to the eigenvalue N_0 representing the condensate fraction. The value of the condensate fraction obtained with this procedure is

$$N_0 = 0.966676 \pm 0.000005, \quad (38)$$

while the condensate orbital ϕ_{00} associated to u_{00} as described in eq. 27 is shown in Fig. 3. The uncertainty is associated by determining which significant digit varies when repeating the numerical experiment multiple times. With a spatial discretization of 25 points we observe variations on the sixth significant digit.

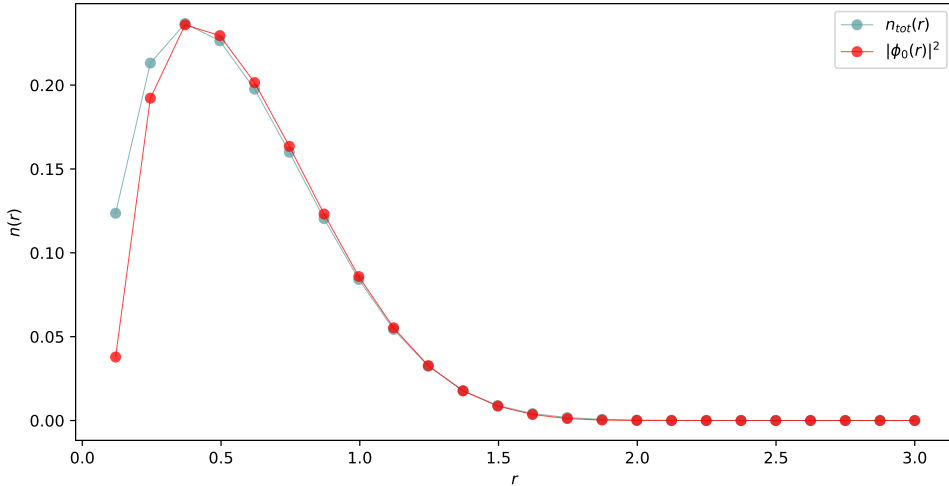


Figure 3: Plot of the condensate orbital $\phi_0(r)$ obtained from the $l = 0$ component of the OBDM, compared with the radial density $n(r)$. The radial distance $r \in [0, 3]$ is discretized in 25 subintervals. The agreement between $n(r)$ and $\phi_0(r)$ is almost perfect, which is a hint that a large fraction of atoms is taking part into the condensate. The condensate fraction here is given by $N_0 = 0.966676$.

It also useful to sample the radial distribution $n(r)$ of particles during the sampling procedure. This gives a way to determine if the OBDM has been sampled correctly as we should have $\rho(r, r) = n(r)$. In Fig. 3 we also compare the radial distribution function with the condensate orbital.

We observe that while the value of the condensate fraction in eq. 38 is compatible with those evaluated in the limit of small number of particles in [2], we have difficulties in sampling the number of particles near the center of the trap. The orbital shown in Fig. 3 is expected to be flat from the value of its maximum towards the center of the trap for $r \rightarrow 0$, as shown in [1] where a VMC procedure is used. In our case instead it reaches a maximum and then drops to zero for $r \rightarrow 0$. This behavior, which is replicated also by the radial density, can be a symptom of the fact that the integration over spherical shells undersamples the particles distribution for small values of r , as the volume of the shell tends towards zero in this case.

It is also pointed out in [2] that a higher packaging of atoms at the centre of the trap can be obtained by having a proper inter-particle function f (see eq. 4) depending on some variational parameter.

4 Conclusion

In this project we have used a DMC procedure to study the ground state energy and BEC of a gas of $N_{at} = 128$ Rubidium atoms trapped in a harmonic potential with a hard core interaction potential at zero temperature.

The result for the energy is given by

$$\langle E \rangle = 1.6876 \pm 0.0002, \quad (39)$$

where the energy is expressed in units of the trap length $\Delta E = \hbar\omega$.

This energy is lower compared to that of eq. 32, proving that the DMC implementation has effectively obtained a better description of the Ground State with respect to the variational procedure. In the VMC procedure the error on the energy, which brought to the choice of the variational parameters defining the guiding function of the DMC procedure is of $\mathcal{O}(10^{-6})$. In this case the DMC value for the energy returns an error of $\mathcal{O}(10^{-4})$. Indeed there is still a dependence of the energy on the choice of the parameters entering the guiding function. Exploring several options we find that the minimum value recorded in our numerical experiments is reached for $b_0 = 0.474$ and $b_1 = 0$, leading to

$$\langle E^* \rangle = 1.6793 \pm 0.0002.$$

The error on the energy should then be overall corrected, including an uncertainty due to the choice of the parameters of the guiding function, and leading to

$$\langle E \rangle = 1.68 \pm 0.01. \quad (40)$$

We manage to observe BEC for this system, with a fraction of atoms taking part into the condensate given by

$$N_0 = 0.966676 \pm (5 \times 10^{-6}). \quad (41)$$

As described in [1] and [2] the effect of the inter-particle interaction is to deplete part of the atoms from the condensate, as for a non-interacting gas the expected condensate fraction at zero temperature is $N_0^{N.I.} = 1.0$. The system size is however compatible with having a small depletion as $N_0^{N.I.} - N_0 \simeq \mathcal{O}(10^{-2})$.

This result is also compatible with the fact that the condensate orbital $\phi_0(r)$ shown in Fig. 3 overlaps almost exactly with the radial particle density. The value of the orbital at the centre of the trap is however small compared with what one would expect from [1] and [2]. This may be due to having integrated the particle density using spherical shells, whose volume tends to vanish when approaching the centre of the trap. In [2] it is also shown that introducing other variational parameters can bring the particles to pack more closely at the centre of the trap.

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