Bose-Einstein condensate in traps: 
A Diffusion Monte Carlo analysis

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1. INTRODUCTION

The first demonstration of Bose-Einstein condensation in gases of alkali atoms in magnetic traps in 1995 ignited a dramatic increase in interest in finite sized Bose systems [1-3]. In the initial experiments (e.g. $^{87}$Rb in harmonic traps) the Bose gas was dilute. However, trapped Bose systems with higher densities are now being investigated [4-5]. As the density or interaction strength is increased, condensate depletion increases and effects of interaction between the condensate and non-condensate become important.

In this paper we explore the properties of trapped Bose gases over a wide range of densities using Monte Carlo (MC) methods. We evaluate the total energy, the distribution of Bosons in the trap, the condensate fraction, the distribution of the condensate throughout the trap and other properties as a function of density. We go from the dilute gas limit to densities comparable to liquid $^4$He densities. We compare the MC results with mean field theories (e.g. Gross-Pitaevskii (GP) theory of the condensate, the Bogoliubov expression for the condensate fraction) and determine the densities at which MC and mean field results begin to differ. We find that the condensate moves from the center of the trap in the dilute limit to the outer surface of the gas at high densities. We present particularly new Diffusion Monte Carlo (DMC) results and discuss some technical problems that arise in DMC applied to a finite sized system in a central potential.

The density of Bosons in a trap and the importance of interatomic interactions is conveniently characterized by the parameter, $n(0)a^3 = N(0)a^3/V$. Here $n(0) = N(0)/V$ is the number density at the center of the trap and $a$ is the scattering length (or hard sphere diameter in a hard sphere model of the atom). In a uniform system, the $na^3$ is the ratio of the volume occupied by the Bosons, $Na^3$, to the total volume ($V$) of the gas. At $a \rightarrow 0$, the gas is ideal. In the dilute limit (e.g. $^{87}$Rb in a trap) where $n(0)a^3 \approx 10^{-5}$, the interaction between Bosons is important. However, it can
be reliably treated using mean field theories (e.g. GP theory). At these densities, depletion of the condensate by the interaction is negligible (≤ 1%). Liquid \( ^4 \text{He} \) at SVP, \( na^3 = 0.21 \), is, in contrast, a strongly interacting liquid requiring full treatment of correlations induced by the interaction. The range of densities of trapped Bose systems investigated to date is displayed in Fig. 1. Of special interest is \(^{85}\text{Rb}\) for which the scattering length, \( a \), can be adjusted to large positive and negative values by using a Feshbach resonance [4-5]. With this technique trapped Bosons of variable density can be created.

To sketch the physical properties of trapped Bosons, we note that the energy of a single particle in a typical harmonic trap (e.g. \(^{87}\text{Rb}\)) is \((3/2)\hbar \omega_{ho} \approx 10 \, nK\). Since the mean square vibrational amplitude of a particle in a trap with trap frequency \( \omega_{ho} \) is \( \langle u^2 \rangle = (\hbar/2m\omega_{ho}) \), a useful measure of the gas size or "trap length" is \( a_{ho} \equiv (\hbar/m\omega_{ho})^{1/2} \). The scattering length of \(^{87}\text{Rb}\) is \( a \approx 50 \, \text{Å} \approx 100 \, a_0 \), where \( a_0 = 0.529 \, \text{Å} \) is the Bohr radius. In this work we will sometimes use a ratio of scattering length to trap length which corresponds to the initial experiments of Anderson et. al [1] (\( a_{Rb}/a_{ho} = 4.33 \times 10^{-3} \)) as a benchmark. Introducing the mean distance between Bosons, \( n = N/V = \bar{r}^{-3} \), we have, \( a \ll \bar{r} \ll a_{ho} \) in the dilute limit and \( a \approx \bar{r} \ll a_{ho} \) in the dense limit. In the dilute limit, \( a \ll \bar{r} \), the interatomic interaction is weak and the trap potential dominates. In the dense limit \( a \approx \bar{r} \), the interatomic interaction dominates, the trap potential is negligible and the gas exhibits properties comparable to a self bound liquid (e.g. a liquid \(^4\text{He}\) droplet). To achieve BEC, the thermal de Broglie wavelength \( \lambda_T = (\hbar^2/2\pi mkT)^{1/2} \) must be large enough so that \( n\lambda_T^3 \gtrsim 2.616 \). That is, \( \lambda_R \approx \bar{r} \). The critical temperature of BEC determined by \( n\lambda_T^3 \approx 2.616 \) is \( T_c \approx 75 \times 10^4 (na^3) \, nK \). For \( na^3 = 10^{-4} \) and \( T = 0.1 \, T_c \), a temperature \( T = 7.5 \, nK \) similar to the trap energy is required. We consider only \( T = 0K \) here.

2. Bosons in Traps: Monte Carlo Formulation

We consider \( N \) Bosons of mass \( m \) confined in an external trapping potential,
\( V_{\text{ext}}(\mathbf{r}), \) and interacting via a two-body potential, \( V_{\text{int}}(\mathbf{r}_1, \mathbf{r}_2). \) The Hamiltonian for this system is:

\[
H = \sum_i N \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) \right) + \sum_{i<j} N V_{\text{int}}(\mathbf{r}_i, \mathbf{r}_j),
\]

(1)

where the trapping potential is spherically symmetric and harmonic,

\[
V_{\text{ext}}(\mathbf{r}) = \frac{1}{2} m \omega_{ho}^2 r^2.
\]

(2)

Here \( \omega_{ho}^2 \) defines the trap potential strength. We have chosen to represent the inter-Boson interaction by a pairwise, hard sphere potential with diameter \( a. \) \( V_{\text{int}}(r) \) is zero if the Bosons are separated by a distance \( r > a \) but infinite if they attempt to come within a distance \( r \leq a. \) In the low energy limit, the scattering length between a pair of particles interacting via a hard core potential is purely s-wave with scattering length \( a. \) Similarly, in this limit the scattering between a pair of particles interacting via the contact potential

\[
v(r) = g\delta(r) = \frac{4\pi\hbar^2a}{m} \delta(r)
\]

is also purely s-wave with scattering length \( a. \) Thus properties of \( H \) defined in (1-2) and evaluated using MC can be compared directly with properties calculated using (3) and the GP equation in the limit where the s-wave approximation is valid.

Systems of \( N = 128 \) to \( N = 1024 \) particles with varying values of \( a \) are considered. We express lengths in units of the trap length, \( a_{ho}, \) and energies in units of the trap energy, \( \hbar\omega_{ho}, \) introduced above.

As a trial variational wave-function we use

\[
\Psi_T = \prod_{i=1}^N \phi(\mathbf{r}_i) \prod_{i<j} f(|\mathbf{r}_i - \mathbf{r}_j|).
\]

(4)

The single Bosons component with variational parameters, \( \alpha_0, \) and \( \alpha_1 \) is

\[
\phi(\mathbf{r}) = e^{-(\alpha_0 r^2 + \alpha_1 r^4)}.
\]

(5)

We used two pair Jastrow functions,

\[
f_0(\mathbf{r}_{ij}) = (1 - a/r_{ij})
\]

(6)

denoted VMC0 and

\[
f_1(\mathbf{r}_{ij}) = (1 - a/r_{ij}) \exp[\beta_0 \exp((r_{ij} - a)^2/\beta_1)]
\]

(7)

denoted VMC1. The \( f_0(\mathbf{r}_{ij}) \) is the exact solution for a pair of particles at low energy interacting via a hard core potential. The \( f_1(\mathbf{r}_{ij}) \) contains a correction term which improves this and has two variational parameters, \( \beta_0 \) and \( \beta_1. \)
The variational MC energy is, using (4),
\[ E_{\text{VMC}} = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}. \]

\( E_{\text{DMC}} \) is the usual Diffusion MC energy obtained using \( \Psi_T \) as the initial and guiding function [6]. We wish to compare MC energies with mean field energies. For example, the energy of a uniform hard core Bose gas (\( V_{\text{ext}} = 0 \)) at \( T = 0 \) K is [7],
\[ E/N = 4\pi na^3 \left( \frac{\hbar^2}{2ma^2} \right) \left[ 1 + \frac{128}{15\sqrt{\pi}} (na^3)^{\frac{1}{2}} + \ldots \right]. \] (8)

Here \( 4\pi na^3 \) is the energy per Boson of the condensate (in units of \( \hbar^2/2ma^2 \)). The term in \((na^3)\) represents the increase in \( E/N \) arising from Bosons excited out of (or depleted from) the condensate by interactions. This “depletion” term can also be incorporated into the GP energy functional’s interaction term in a local density approximation. The resulting modified Gross-Pitaevskii (MGP) equation gives an \( E/N \) for Bosons in a trap in the large \( Na \) (Thomas-Fermi) limit of
\[ E_{\text{MGP}}/N = \frac{5}{7} \mu_{TF} \left[ 1 + \frac{7}{8} (\pi n_{TF}(0)a^3)^{1/2} \right] \] (9)
where \( \mu_{TF} = gn_{TF}(0) \) [7]. Here \( n_{TF}(0) \) is the number density of the Bosons at the center of the trap in the Thomas Fermi limit. The difference between \( E_{\text{MGP}} \) and \( E_{\text{GP}} = 5/7\mu_{TF} \) arising from depletion is,
\[ (E_{\text{MGP}} - E_{\text{GP}})/N\hbar\omega_h = \frac{35}{112} \frac{(15)^{3/5}}{\sqrt{8}} N^{3/5} \left( \frac{a}{a_{ho}} \right)^{8/5} \] (10)

Particularly we note that the increase in \( E \) arising from depletion is proportional to \( N^{3/5} (a/a_{ho})^{8/5} \).

Condensate properties are obtained by diagonalizing the one-body density matrix (OBDM) as described in ref [8]. The OBDM is [9]
\[ \rho(r', r) = \langle \hat{\Psi}^{\dagger}(r'), \hat{\Psi}(r) \rangle, \] (11)
where \( \hat{\Psi}(r) \) is the field operator that annihilates a single particle at the point \( r \) in the system. The OBDM, \( \rho(r', r) \), characterizes the correlations which exist between the points \( r \) and \( r' \) in a many-body state. We consider spherically symmetric traps only. For a spherically symmetric system, the OBDM may be expanded in terms of the Legendre polynomials, \( P_l \), as
\[ \rho(r, r') = \sum_l \frac{(2l + 1)}{4\pi} P_l(\hat{r} \cdot \hat{r}') \rho_l(r, r'). \] (12)

Here, \( \rho_l(r_1, r'_1) \) may be approximated in terms of the optimized trial wave-function, \( \Psi_\nu \), as
\[ \rho_l(r_1, r'_1) = \int d\Omega r_2 \ldots d\Omega r_N \Psi_\nu^\dagger(r_1 \ldots r_N) P_l(\hat{r}_1 \cdot \hat{r}_1') \Psi_\nu(r_1' \ldots r_N). \] (13)

Each \( \rho_l(r_1, r'_1) \) is a matrix and may be diagonalized to obtain the orbitals \( \phi_{ln}(r) \) and their corresponding occupation numbers \( n_{ln} \). In principle any orbital which
Figure 2. Comparison of energy per particle obtained from Diffusion Monte-Carlo, $E_{DMC}$, Variational Monte-Carlo, $E_{VMC}$, and Gross-Pitaevskii, $E_{GP}$, for hard sphere Bosons in a spherically symmetric harmonic trap as a function of the number of Bosons, $N$, in the trap. Energies are presented in units of the trap energy, $\hbar \omega_{ho}$. The ratio of hard core diameter to the characteristic trap length, $a_{ho} = (\hbar/m\omega_{ho})^{1/2}$, is $a/a_{ho} = 8 \times a_{Rb}/a_{ho}$ where $a_{Rb}$ is the scattering length $^{87}$Rb. At $N = 1024$, $E_{GP}$ lies $2.6\%$ below $E_{DMC}$, while $E_{DMC}$ and $E_{VMC}$ agree to within $0.01\%$.

satisfies $n_{\nu_0} \gg 1/N$ may be considered a macroscopically occupied pseudo-particle state – i.e. the equivalent of a Bose-Einstein condensate. A Bose system with more than one macroscopically occupied state would represent a fragmented condensate [10]. In the systems studied in this work, only a single orbital was found to have macroscopic occupation for each system. We refer to this orbital as the condensate "wave-function", $\phi_0(r)$, and its occupation as the condensate fraction, $n_0 = N_0/N$, respectively.

For a weakly interacting homogeneous BEC, Bogoliubov theory predicts the density of the non-condensate atoms that coexist with the condensate. The $T = 0$ non-condensate fraction for a uniform system reads

$$f = 1 - n_0 = \frac{8}{3} \sqrt{\frac{n a^3}{\pi}},$$

where $n$ is the atom density and $a$ is the s-wave scattering length. Therefore, for
Figure 3. Plots of the One-Body Density Matrix in arbitrary units obtained from: 1) A Variational Monte Carlo calculation using the VMC0 Jastrow (6), $\rho_{VMC}$ 2) Mixed estimator obtained from a Diffusion Monte Carlo calculation using VMC0 as a guiding function, $\rho_M$, 3) First order correction to the Mixed estimator $\rho_M + T(\rho_M) - \rho_{VMC}$. Darker regions have higher statistical error.

$na^3 \ll 1$ the non-condensate fraction goes like $\sqrt{na^3}$. The Bogoliubov expression for a uniform system (14) may be used to determine the non-condensate fraction in a harmonic well within a local density approximation (Bogoliubov-LDA) [11]. By integrating

$$1 - n_0 = \int n_{TF}(r)f(n_{TF}(r))4\pi r^2 dr$$

where $n_{TF}(r)$ is the mean field (GP) density distribution in the large $Na/a_{ho}$ limit,

$$1 - n_0 \approx 0.3798(Na/a_{ho})^{6/5}$$

is obtained.

3. RESULTS

Fig. 2. shows a comparison of the energy per particle obtained from Diffusion Monte-Carlo, $E_{DMC}$, Variational Monte-Carlo using the VMC1 Jastrow (7), $E_{VMC}$, and Gross-Pitaevskii, $E_{GP}$, of trapped hard sphere Bosons as a function of the number of particles, $N$, in the trap. The ratio of hard core scattering length to the characteristic length of the trap in this figure is, $a/a_{ho} = 8 \times a_{Rb}/a_{ho}$. For small $N$, $E_{DMC}$ (open circles), $E_{VMC}$ (filled circles), and $E_{GP}$ (open triangles) are nearly indistinguishable. As $N$ increases, the trap density increases as well with $n(0)a^3 \approx 6 \times 10^{-4}$ for $N = 1024$. The increase of the DMC energy over the GP result begins to become apparent with larger $N$, $\approx 2.6\%$ at $N = 1024$. The VMC1 energies agree well with the DMC results with a difference of only .01% at $N = 1024$. The difference between the DMC and GP energies, $(E_{DMC} - E_{GP})$, scales with $N$ as $N^{3/5}$ as expected from (10). The present DMC results also indicate that $E_{DMC} - E_{GP}$ scales with $a/a_{ho}$ as $(a/a_{ho})^{8/5}$ which is again consistent with (10).
Figure 4. VMC density profiles $n(r)a^3$ for a system with $N = 128$ particles and scattering length $a = 64 \times a_{Rb}$. By allowing particles to pack more closely together near the center of the trap the VMC1 (7) Jastrow function is more successful than VMC0 (6) at optimizing the trade-off between kinetic and potential energy. The resulting difference in energy is only $\delta E \approx .5\%$ while the difference in central density $\delta n(0)$ is $\approx 18\%$.

Fig. 3. shows three plots of the one-body density matrix for a system with $N = 128$ particles, and ratio of hard core diameter to trap length of $a/a_{ho} = 256 \times a_{Rb}$. The first frame in the figure was obtained from a VMC calculation based on an optimized VMC0 Jastrow function. The second frame is the mixed estimator obtained from a DMC calculation using the same VMC0 function as a guiding function. Note the asymmetry in the mixed estimate of the OBDM. This is a direct consequence of the bias induced by the VMC0 guiding function. The third frame shows the first order correction to the mixed estimator, $\rho_M + T(\rho_M) - \rho_{VMC}$. Clearly, in this example, the first order correction to the mixed estimator is not successful in removing the guiding function bias. This figure provides a dramatic demonstration of mixed estimator bias and the inadequacy of the VMC0 Jastrow function (6) to effectively describe the condensate properties of a system with these parameters. Our solution to this problem was to use the improved VMC1 Jastrow function (7) for all DMC calculations of condensate properties.

The simple VMC0 Jastrow (6) forces all particles to interact according to the zero energy solution of the two body scattering problem. This makes the trial function
limited in its ability to optimize the trade off between kinetic and potential energy of particles in the trap. This limitation in the VMC0 wave function is apparent when looking at the density profile, \( n(r) \), for systems at higher densities. Fig. 4. shows a comparison of the density profiles obtained using optimized VMC0 and VMC1 trial functions. The VMC1 wave function allows the particles to pack more closely together near the center of the trap than VMC0. The higher number density results in an increase in the kinetic energy caused by pair correlations but the decrease in potential energy more than makes up the difference. VMC1 is therefore more successful than VMC0 at optimizing the trade-off between kinetic and potential energy. The resulting difference in energy is only \( \delta E \approx 0.5\% \) while the difference in central density \( \delta n(0) \) is \( \approx 18\% \).

In Fig. 5, results for the condensate fraction, \( n_0 \), as a function of the gas density \( n(0)a^3 \) for the ground state of trapped hard sphere Bosons are presented. The filled circles are from the mean-field Bogoliubov expression for a uniform dilute bose gas integrated over the Thomas-Fermi density (16). The down-facing triangles are the VMC results obtained from diagonalizing the OBDM. Up-facing triangles are the DMC results. In the highly dilute regime, \( n(0)a^3 < 10^{-4} \), all three methods agree to within 1%.

4. DISCUSSION

The above results show that reliable values of the energy, the density distribution and condensate fraction of Bosons in traps can be calculated using MC methods. Particularly, if an accurate trial function, \( \Psi_T \), is used, Variational MC and diffusion MC results for all properties up to liquid \( ^4\text{He} \) densities agree well. The energy \( E \) itself is not very sensitive to \( \Psi_T \). However, other properties such as the density distribution, the One-Body Density Matrix and condensate fraction, \( n_0 \), are highly sensitive to \( \Psi_T \). Thus simple minimization of \( E \) to obtain \( \Psi_T \) is not adequate and procedures such as minimizing the variance of \( E \) are needed to obtain \( \Psi_T \) accurately enough to compute other properties such as the OBDM reliably. Once this is done, very reliable results are obtained. Specifically, given the dependence of the OBDM on \( \Psi_T \) even in DMC, an accurate \( \Psi_T \) is needed to compute \( n_0 \).

We have compared the total energy per Boson in the trap with the energy per Boson of the condensate alone calculated using the GP theory (e.g. \( E_{GP} \)). The two agree well in the dilute limit \( (na^3 \leq 10^{-5}) \). This shows that essentially all the Bosons are in the condensate in the dilute limit and that the GP theory of the condensate is accurate. As the density increases some difference appears. For \( N = 1024 \) and atoms having 8 times the scattering length of \( ^{87}\text{Rb} \) \( (na^3 \approx 6 \times 10^{-4}) \), we find \( E_{DMC} \) and \( E_{GP} \) differ by 2.6\%. We also find that the difference in \( E_{DMC} \) and \( E_{GP} \) scales with \( N \) as \( N^{3/5} \) and with \( a/a_{ho} \) as \( (a/a_{ho})^{8/5} \). This is exactly the scaling expected if the energy difference arises from depletion of the condensate by the interaction as \( N \) and \( a \) increase. This suggests that the GP description of the condensate is still accurate at higher densities – but a significant fraction of the Bosons are above the condensate. This was a conclusion in an earlier publication [8] and is confirmed by the present DMC results.

The DMC and VMC results of the condensate fraction agree well over the en-
Figure 5. Condensate fraction, $n_0$, as a function of the gas density $n(0)a^3$ for the ground state of trapped hard sphere Bosons. Here $n(0)$ is the number density at the center of the trap and $a$ is the scattering length. The filled circles are from the mean-field Bogoliubov expression for a uniform dilute bose gas integrated over the Thomas-Fermi density. The down-facing triangles are the VMC results obtained from diagonalizing the OBDM. Up-facing triangles are the DMC results. In the highly dilute regime, $n(0)a^3 < 10^{-4}$, all three methods agree to within 1%.

tire density range $10^{-6} \leq na^3 \leq 0.5$ if an accurate $\Psi_T$ is used. The Bogoliubov-LDA estimate (16) of the condensate fraction, $n_0$, agrees with these MC values for $na^3 \lesssim 10^{-3}$. The Bogoliubov value of $n_0$ lies 10% above the MC value at $na^3 \approx 10^{-2}$. At $na^3 \approx 10^{-2}$, the density distribution $n(r)$ begins to show peaks and valleys which reflect correlations in the density induced by the hard core. The appearance of these local correlations signals a clear departure from mean field properties. At higher density, the inter-Boson interaction dominates the properties and the trap potential plays only a minor role. At higher densities, the Bosons behave more like a liquid $^4$He droplet or self bound system. In this regime the condensate moves from the center of the trap to the surface of the gas. The condensate fraction is 100% at the surface of the Bose fluid at high densities.
5. FUTURE PROSPECTS

The combination of VMC and DMC methods with the OBDM framework for describing Bose-Einstein condensation provide a powerful framework for the study of Bose systems and BEC. An example of a future application of this framework is in the evaluation of BEC in confined geometries using “realistic” interatomic potentials. The QMC method is in no way limited to a particular choice of the interaction potential. As experimental studies of trapped Bosons become able to measure the properties of these systems with greater and greater accuracy, a more detailed understanding of the microscopic interactions between atoms will be required. As densities increase, the form of the interaction potential becomes more important as well since higher terms than the s-wave term in the scattering expansion begin to play a role. Future QMC studies could make a direct connection with specific physical systems by incorporating an appropriately detailed interatomic potential.

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