Stochastic method for calculating the ground state reduced density matrix of trapped Bose particles in one dimension

Omri Buchman\(^1\) and Roi Baer\(^1\)[isci]

\(^1\)Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The reduced density matrix (RDM) is a fundamental contraction of the Bose-Einstein condensate wave function, encapsulating its one-body properties. It serves as a major analysis tool with which the condensed component of the density can be identified. Despite its cardinal importance, calculating the ground-state RDM of trapped interacting bosons is challenging and has been fully achieved only for specific models or when the pairwise interaction is weak. In this paper we discuss a new approach to compute the RDM based on a double-walker diffusion Monte Carlo random walk coupled with a stochastic permanent calculation. We here describe the new method and study some of its statistical convergence and properties applying it to some model systems.

I. INTRODUCTION

Despite its importance for determining the structure and properties of trapped boson systems, calculation of the ground state RDM proves to be a daunting task. It has been calculated exactly (near-analytically) only for hard-core particles in harmonic traps\(\[1,2\]\) and numerically-exactly for weakly interacting systems.\(\[3\]\) The ground state RDM of 3D trapped particles based on diffusion Monte Carlo (DMC) with a variational Monte Carlo guiding function has been used for studying systems of hard core bosons in 3D at various densities with interactions of intermediate strength.\(\[4,5\]\) The RDM in these approaches is evaluated by an approximate expression, involving the variational and mixed estimators of the RDM but relying quite significantly on the quality of the guiding function. This makes the method inappropriate for strong interactions, where the approach also tends to suffer from instabilities in the population control resulting from singularities in the local energy under the guiding function.\(\[6\]\)

In this paper, we present a new stochastic approach for the calculation of the ground-state RDM for trapped strongly interacting bosons. The formalism seems applicable to any number of dimensions but in this paper we describe and study the implementation to 1D bosons, which are challenging systems due to their strong correlation effects.\(\[7,8\]\) The method is based on a DMC random walk and employs a stochastic method for estimating the permanents required to calculate the RDM. In section II we describe the basic formalism, definitions and techniques, in section III we apply the method to systems of bosons trapped in a harmonic well where interaction strength is increased while keeping the the trap potential fixed and then in double-well traps where interaction strength is increased while keeping the density of the system (nearly) fixed; summary and conclusions are given in Section IV.

II. METHOD

A. Basic notions

For \(D\) bosons of mass \(m_b\) in a trap potential \(v(q)\) (\(q\) is the Cartesian position coordinate of a particle) interacting through a pairwise potential \(u(q_{12})\), the Hamiltonian is written as a sum of kinetic and potential energies:

\[
\hat{H} = \hat{T} + \hat{V},
\]

\[
\hat{T} = -\frac{\hbar^2}{2m_b} \sum_{n=1}^{D} \nabla_n^2
\]

\[
\hat{V} = \sum_{n=1}^{D} v(q_n) + \sum_{m<n}^{D} u(|q_n - q_m|)
\]

where \(\hat{V}\) is a sum of one-body and two-body interactions. Although the formalism we develop is not limited to any specific form of the trap potential or two body interactions, we will use, for demonstration purposes, the following even-symmetric trap which combining a harmonic well with a gaussian shaped barrier in its center:

\[
v(q) = \frac{1}{2} m_b \omega^2 q^2 + V_b e^{-\frac{q^2}{2r^2}}.
\]

Here \(\omega, V_b\) and \(\sigma_b\) are, respectively, the harmonic frequency, barrier height and barrier width. The interaction we consider is a pairwise Gaussian repulsion of the form,

\[
u(q_{12}) = \frac{c}{\sqrt{2\pi}\sigma_r} e^{-\frac{q_{12}^2}{2\sigma_r^2}},
\]

where \(c\) is the repulsion strength and \(\sigma_r\) the interaction range. When addressing the purely harmonic trap \((V_b = 0)\) we will use two pure quantities for characterizing the trap:

\[
\alpha_0 = \frac{c}{E_{01}},
\]

\[
\alpha_1 = \frac{\sigma_r}{\ell},
\]
where $E_0 = \hbar \omega$ and $l = \sqrt{\frac{\hbar}{m \omega}}$ are the energy and length scales of the single particle non-interacting harmonic ground-state.

The ground-state reduced density matrix (RDM) for $D$ bosons is defined up to a constant factor as an expectation value of a nonlocal operator:

$$\Gamma_1(q, \tilde{q}) \propto \int dx d\tilde{x} \Psi(x) \Psi(\tilde{x}) \times$$

$$\delta(x_1 - q) \delta(\tilde{x}_1 - \tilde{q}) \prod_{j=2}^{D} \delta(x_j - \tilde{x}_j),$$

where $\Psi(x) \equiv \Psi(x_1, \ldots, x_D)$ is the ground-state, symmetric to particle exchange and normalization $\int \Gamma_1(q, q) dq = D$ can be imposed a posteriori. Singling out particle 1 in this definition is arbitrary as all particles are identical. In fact, we can take advantage of the wave function exchange symmetry and write the RDM in an equivalent but explicitly fully symmetric way:

$$\Gamma_1(q, \tilde{q}) \propto \int dx d\tilde{x} \Psi(x) \Psi(\tilde{x}) \times$$

$$\sum_j w(y(x|j), y(\tilde{x}|j)) \delta(x_j - q) \delta(\tilde{x}_j - \tilde{q}),$$

where $y(x|j) \equiv (y_1, \ldots, y_{D-1}) = (\ldots, x_{j-1}, x_j, \ldots)$ is the vector of $D - 1$ coordinates obtained from the vector $x$ by removing the $j$th coordinate. The weight $w(y, \tilde{y})$ of each double configuration $y, \tilde{y}$ is the number of permutations $P$ of the $\tilde{y}$ coordinates having the property that simultaneously for all $k$, the position $\tilde{y}_k$ is located in an infinitesimal volume element surrounding the position of $y_k$. Mathematically this is expressed as the following sum of products of delta-functions: $w(y, \tilde{y}) \equiv \sum_p \prod_k \delta(y_k - \tilde{y}_k)$.

For a numerical implementations, we coarse-grain the delta functions. First, we introduce a $q$-axis grid containing $2N_G$ bins, each of width $h$, centered on the grid points $y_g = gh$, where $g = -N_G$, $-N_G + 1, \ldots, N_G$ is an integer. The coarse-grained RDM is then a histogram on a $2N_G \times 2N_G$ lattice derived from the exact RDM as an integral over the bins:

$$\Gamma_1^{cg} \equiv h^{-2} \int \Gamma_1(q, \tilde{q}) \theta_h(q - y_g) \theta_h(\tilde{q} - y_g) dq d\tilde{q},$$

where $\theta_h(\xi)$ equals 1 if $\xi \in \left[\frac{-h}{2}, \frac{h}{2}\right]$ and zero otherwise.

Next we introduce the DMC random walk as a means for calculating the coarse grained RDM. Regular DMC produces a trajectory of length $N_T$ time steps made by $M$ walkers, giving $M \times N_T$ $D$-dimensional vectors $x$ distributed as the ground state wave function $\Psi(x)$. However, this is not what we need for the RDM of Eq. (10) where the integral is over $\Psi(x) \Psi(\tilde{x})$. Hence we apply the standard DMC procedure not on a single but on a double-walker system corresponding to $2 \times D$ particles under the Hamiltonian $H = H(x) + H(\tilde{x})$, producing a random walk trajectory of $M \times N_T$ $2D$-dimensional vectors $(x, \tilde{x})$ distributed as the product of ground-state wave functions $\Psi(x) \Psi(\tilde{x})$. The coarse-grained RDM histogram then becomes equal (up to normalization) to the following average along such a trajectory:

$$\hat{G}_{1}^{cg} \propto \left\langle \sum_j w_h(y(x|j), y(\tilde{x}|j)) \theta_h(x_j - y_g) \theta_h(\tilde{x}_j - \tilde{y}_g) \right\rangle_{M \times N_T},$$

where,

$$w_h(y, \tilde{y}) = \prod_k \theta_h(y_k - \tilde{y}_k)$$

are the coarse grained weights. The sum over the permutations is not required when the random walk continues indefinitely, producing exhaustive sampling (we can take $w_h(y, \tilde{y}) = 1$). However sampling is evidently finite, and not taking the permutations will result in extremely poor statistics because of the small probability to find $y_k$ and $\tilde{y}_k$ in the same bin simultaneously for all $k = 1, \ldots, D$. The sum of products over permutations appearing in Eq. (12) is the formal definition of a permanent of the $(D - 1) \times (D - 1)$ matrix describing the adjacency of particles in the two components of the double walker:

$$\Theta_{kj} = \theta_h(y_k - \tilde{y}_j).$$

Note that the expression of the permanent in Eq. (12) is almost identical to that of the determinant except that in the latter all odd permutations $P$ are multiplied by $-1$. Despite this similarity, the numerical work needed to evaluate the permanent is vastly larger than for the determinant; the former involves exponential complexity, $O(2^{D^2})$ [9], while the latter is polynomial, $O(D^3)$. For this reason, we
use a stochastic method \cite{10} for evaluating the permanent in polynomial time, as discussed in the following algorithm.

\section{Algorithm for calculating the reduced density matrix}

The $M$ DMC double walkers $(\mathbf{x}_m, \mathbf{\tilde{x}}_m)$ ($m = 1, \ldots, M$) are subject to the standard DMC diffusion and birth/death processes in a series of $N_T$ time steps, each of duration $\Delta t$, depending on the Hamiltonian $\tilde{H}(\mathbf{x}) + \tilde{H}(\mathbf{\tilde{x}})$ as follows:

1. **Diffusive step:** the “position” of each walker is changed by $(\Delta \mathbf{x}_m, \Delta \mathbf{\tilde{x}}_m)$, a vector of random numbers, each sampled from the normal distribution with mean $\mu = 0$ and variance $\sigma^2 = \frac{\hbar \Delta t}{m_b}$.

2. **Reproduction/annihilation:** For each walker at time $t$, $(\mathbf{x}_m, \mathbf{\tilde{x}}_m)$, an integer $n = \text{INT} \left[ e^{(E(t) - V(\mathbf{x}_m) + V(\mathbf{\tilde{x}}_m)) \Delta t / (\hbar m - M_0 + r)} \right]$ is computed (where $M_0$ is a preset target number of walkers), $0 \leq r < 1$ is a random fraction and $E(t) = \frac{1}{N} \sum_{k=1}^{M} [V(\mathbf{x}_k) + V(\mathbf{\tilde{x}}_k)]$ is the average potential energy over all walkers at time step $t = 1, \ldots, N_T$.

(a) if $n > 0$ $n$ clones of the walker are generated and $M$ is increased by $n$

(b) if $n = 0$ the walker is eliminated and $M$ is decreased by 1.

3. **Evaluating the energy:** In the appropriate limit ($M \to \infty$, $\Delta t \to 0$ and $N_T \to \infty$) the expected time-step average of $E(t)$ is an unbiased estimate of the ground state energy of the double system:

$$2E_{GS} = \left\langle \frac{1}{N_T} \sum_{n=1}^{N_T} E(n\Delta t) \right\rangle,$$  \hspace{1cm} (14)

and the $M \times N_T$ walker positions $(\mathbf{x}, \mathbf{\tilde{x}})$ are distributed as $\Psi(\mathbf{x}) \Psi(\mathbf{\tilde{x}})$. The numerical procedure uses a finite number $M$ of walkers, a finite time-step $\Delta t$ and a finite number of sampling times $N_T$, leading estimates of $E_{GS}$ having random fluctuations $\Sigma_{E_{GS}} \propto \frac{1}{\sqrt{N_T}}$ as well as a small bias due to the finite time step $\Delta t$.

4. **Estimating the RDM:** Every $N_C$ time steps the DMC double walkers are used update the RDM histogram according to Eq. (11). $N_C$ is taken much larger than the the correlation decay lengths $J_\delta$ of the walk (see Fig. 1). In Eq. (11), the bosonic weight $w_k(y, \mathbf{\bar{y}})$ is equal to the permanent of the $(D - 1) \times (D - 1)$ adjacency matrix $\Theta_{ij}$ of Eq. (13) which is evaluated following these steps:

(a) Preliminary screening: we compute the column sums $c_{ij} = \sum_{i=1}^{D} \Theta_{ij}$ and the row sums $r_i = \sum_{j=1}^{D} \Theta_{ij}$ of the adjacency matrix and if one of these is zero the permanent is immediately set to zero without further computation. The numerical effort in this screening process scales at most as $O(D^2)$ and is effective since typically only a small fraction of the permanents are nonzero (see bottom panel of Fig. 2).

(b) For the adjacency matrices passing step 4a the permanent is estimated as the average $\left\langle |\det \Phi|^2 \right\rangle$ where $\Phi$ is the matrix obtained from $\Theta$ by multiplying each of its elements by $\pm 1$ at random. Mathematically, $\Phi_{ij} = (-1)^{n_{ij}} \Theta_{ij}$ where $n_{ij}$ are random independent integers.\cite{10} The average $\left\langle |\det \Phi|^2 \right\rangle$ is estimated using $K$ samples of the integers $n_{ij}$, where $K$ is on the order of a few hundreds. The relative standard deviation $C_r$, occurring in this stochastic permanent evaluation for a typical DMC trajectory is shown in the top panel of Fig. 2 for $K = 100$.  

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{The application of the stochastic permanent evaluation described in step 4a of the algorithm in section 11.5 to adjacency matrices $\Theta_{ij}$ (Eq. 13) appearing in DMC trajectories corresponding to $D$ interacting bosons inside a Harmonic well ($\alpha_0 = 4, \alpha_1 = 0.1$ in Eqs. (6)-(7)). Top panel: The coefficient of deviation $C_r$ (relative standard deviation) for the stochastic permanent evaluation as a function of $D$. For each adjacency matrix $\Theta$, the permanent is reevaluated stochastically 10 times (every time using $K = 100$ sets of random integers) and $C_r(\Theta)$ is calculated as the ratio of the standard deviation to the average. The results shown in the figure are averages ($C_r(\Theta)$) over 10000 instances of $\Theta$ matrices which arise during the DMC random walk. Bottom panel: The frequency of non-zero permanents as a function of $D$.}
\end{figure}
Figure 3. The deterministic (top panels) and DMC (bottom panels) RDM $\Gamma_1(q, \bar{q})$ for of $D = 4$ unit-mass particles trapped in the potential well $v(x)$ of Eq. [4] and interacting via the potential $u(x_{12})$ of Eq. [5]. The parameters are $k_H = 0.25$, $V_0 = 1.5$, $\sigma_0 = 0.5$ and $\sigma_r = 0.5$ and the values of $c$ are indicated in the figure for each column. A bin-size of $h = 0.375$ atomic units was used for sampling. The DMC calculation used a total of $M = 48000$ walkers ($128000$ for $c = 4$), $N_T = 4000$ time steps ($20000$ for $c = 4$) and $\Delta t = 0.01$ time units ($0.005$ for $c = 4$).

$C_v$ grows roughly in proportion to $D$, for large $D$’s.

(c) Normalize ($\Gamma^{g\bar{g}}_1 \leftarrow \Gamma^{g\bar{g}}_1 \times \frac{P}{tr[\Gamma^{g\bar{g}}_1]}$) and symmetrize ($\Gamma^{g\bar{g}}_1 \leftarrow (\Gamma^{g\bar{g}}_1 + \Gamma^{\bar{g}g}_1)/2$) the completed RDM histogram of Eq. [11].

We found the statistical error $\Sigma_{RDM}$ of any RDM property we looked at (e.g. the expectation value of $P_{(1,2)}$), is proportional to $\frac{1}{\sqrt{N_TMK}}$ where $N_T$ is the number of time steps, $M$ the number of walkers and $K$ the number of determinants used in the permanent evaluation. From this, we conclude that the bias, if it exists, is small and the error is dominated by statistical fluctuations.

The algorithm quickly identifies most of the zero permanents however it is clear that for the sampling to be efficient we cannot afford a situation where the permanents are rarely different than zero. Hence, the bin size $h$ should not be too small, and a general rule of the thumb would be to take $h$ to be of the order of $n^{-1}$ (or a small fraction thereof) where $n$ is the average density. The efficacy of the permanent method is seen in that the fraction of non-zero permanents grows with increasing number of particles for a Harmonic traps (see bottom panel of Fig. [2]). This finding has support of theoretical investigations.[11] Thus, the sampling efficiency is not expected to decrease and perhaps even increases as the number of particles grows.

C. Statistics and validation

In Fig. [3] we show contour plots of a grid-based-deterministic and the DMC-based-stochastic RDM estimates of $\Gamma_1(q, \bar{q})$ for several systems of $D = 4$ particles interacting with increasing repulsion strengths. In each case the DMC-based and grid-based RDMs are indeed nearly identical in appearance, due to extensive sampling, validating in principle, our method.

To show the effect of the stochastic permanent evaluation, we study the three highest-lying RDM eigenvalues for a set of 16 bosons in a Harmonic trap, as shown in Table [1]. The averages and fluctuations using DMC with deterministic permanent evaluation and DMC with stochastic permanent evaluation for $K = 200$ and $400$ stochastic determinants are shown. The expectation values are close and the standard deviations with $K = 400$ are close to the deterministic fluctuations.

$$
\begin{array}{|c|c|c|c|c|}
\hline
K & 0 & 200 & 400 \\
\hline
E(f) & \bar{\sigma}(f) & E(f) & \bar{\sigma}(f) & E(f) & \bar{\sigma}(f) \\
\hline
f_1 & 0.806 & 0.01 & 0.808 & 0.014 & 0.805 & 0.008 \\
\hline
f_2 & 0.853 & 0.006 & 0.850 & 0.009 & 0.855 & 0.007 \\
\hline
f_3 & 0.047 & 0.006 & 0.043 & 0.003 & 0.047 & 0.006 \\
\hline
\end{array}
$$

Table I. The expected value and standard deviation of the 3 largest RDM eigenvalues for a system of 16 bosons in a Harmonic trap, calculated using DMC comparing the deterministic ($K = 0$) and stochastic ($K = 200, 400$) evaluations of permanents. The parameter $K$ is the number of stochastic determinant calculations used for each permanent evaluation. The potential parameters (see Eqs. [6]-[7]) are $\alpha_0 = 4$, $\alpha_1 = 0.1$. The DMC calculation used $M = 64000$ walkers and $N_T = 8000$ time steps with $\Delta t = 0.005\omega^{-1}$ and the RDM bin size was $\Delta x = 0.625l$.

III. APPLICATIONS

In this section we apply the algorithm for two types of trapped boson systems in order to demonstrate the performance and the kind of results that can be obtained. We compare the calculated densities to that of the Thomas-Fermi (TF) approximation,[12,13] given as the positive part of the shifted and negatively-scaled potential well:

$$
n_{TF}(q) = \mathcal{P}\frac{\mu - v(q)}{c}.
$$

Here, the TF chemical potential $\mu$ is determined by the density normalization condition $\int n_{TF}(q) dq = D$.

A. Constant harmonic-well trap

In Fig. [4] we study 16 trapped bosons in a harmonic well as a function of $\alpha_0$, taking the values $4, 8, 16, 32$ with $\alpha_1 = 0.1$ and $V_0 = 0$ (corresponding DMC run parameters given in Table [I]). We choose the regime of small $\alpha_1$ so the interaction is close to “contact”. A useful way to think of this series of systems is to imagine that the repulsion strength $c$ increases (in proportion to $\alpha_0$) while the harmonic trap stays put.
Figure 4. The RDM diagonal, anti-diagonal, condensate \(n_c(q)\) and Thomas-Fermi \(n_{TF}(q)\) densities for \(D = 16\) particles in a Harmonic well interacting via the potential of Eq. (5). The interaction range parameter is \(\alpha_1 = 0.1\) while the interaction strength parameter \(\alpha_0\) is indicated in the panels. The RDM eigenvalues (divided by \(D\)) are the eigenstate fractions \(f_i\) indicated in each panel with \(f_1\) and \(f_2\) having relative errors of 10% and \(f_3\) and \(f_4\) of 20% (largely independent of \(\alpha_0\)). For \(\alpha_0 < 32\) the statistical error bars are not larger than the marker symbols. For \(\alpha_0 = 32\) the statistical error bars are shown explicitly for the diagonal, antidiagonal and condensate densities. The RDM bin size was \(h = 0.625l\).

It is seen that as the repulsion \((\alpha_0)\) grows, the density diminishes and broadens. This happens because at short inter particle distances the repulsion force is stronger than the harmonic force and thus, as repulsion grows the particles can stretch the harmonic spring and spread out.

For \(\alpha_0 = 4\) and 8 the density \(\Gamma_1(q,q)\) in Fig. 4 is similar in shape to the TF density \(n_{TF}(q)\) (Eq. 15). The TF approximation is expected to apply for large numbers of particles, and weak interactions \(\alpha_0 \ll 1\), and is seen here to work surprisingly well beyond this limit. As \(\alpha_0\) increases further, the system gradually assumes a more Fermionic structure, which includes a flattening of the density profile. But the TF density retains the parabolic shape and therefore is not any more a reasonable approximation to the density.

As for the condensate density \(n_c(q)\). For the lowest value \(\alpha_0 = 4\), it is very similar in shape to the total density, just scaled by a factor \(f_1 \approx 0.8\) where \(f_1\) is the condensate fraction. As \(\alpha_0\) increases the condensate is gradually destroyed. This is evidence by the steady decrease of the condensate fraction \(f_1\) and then by the anti-diagonal density \(\Gamma_1(q,-q)\), progressively developing a concave shorter ranged character while deviating in shape from the total density \(\Gamma_1(q,q)\) (see Appendix A for discussion). Finally as interactions grow, the shape of the condensate density \(n_c(q)\), retaining its flexible smoothness, increasingly deviates from that of

| DMC run data | \(\alpha_0\) |
|--------------|-------------|
| \(M \times 10^3\) | 4  | 8  | 16 | 32 |
| \(N_T \times 10^4\) | 96 | 96 | 480 | 640 |
| \(N_l\) | 900 | 900 | 900 | 6000 |
| \(K\) | 250 | 250 | 600 | 500 |
| \(\omega \Delta t \times 10^{-3}\) | 100 | 100 | 100 | 100 |
| Wall time hrs\times CPU | 11 \times 3 | 10 \times 3 | 33 \times 6 | 192 \times 8 |

Table II. The parameters for the DMC runs used to produce the results shown in Fig. 4. The wall time in hours and the number of core-i7 CPU’s used (each CPU running 8 threads).
Figure 5. The RDM diagonal, anti-diagonal, condensate \( n_C(q) \) and Thomas-Fermi \( n_{TF}(q) \) densities for \( D = 32 \) particles with the value of \( c \) indicated in the panels and \( \sigma_x = 0.1, \sigma_y = 0.5 \). The other two potential parameters are taken as \( k_H = 2.86c \) and \( V_0 = 3c \). This forces the TF density to be identical in all four systems. The RDM eigenstate fractions \( f_n, n = 1, \ldots, 4 \) as well as \( f_c = \sum_{n>4} f_n \), are indicated in each panel: \( f_1 \) and \( f_2 \) have relative errors of 10% and \( f_3 \) and \( f_4 \) of 20% (largely independent of \( c \)). The DMC parameters are given in Table III. The bin size was \( \hbar = 0.625 \) length units.

the total density which displays increasing rigidity due to fermionization.

Fig. 5 also displays the statistical error bars for the \( c \). It is seen that the total density is considerably more sensitive to the QMC statistical fluctuations than the condensate density (and the anti-diagonal density). This is reminiscent of the two-fluid model of superfluid He-II [14] according to which the condensate has vanishing viscosity and therefore is immune to fluctuations quite distinct from the behavior of the normal fluid. [14]

B. Constant density in double-well trap

The generality of the DMC-based RDM calculation allows us to study systems beyond the uniform gas and the harmonic trap approximations. One interesting case, is the partially-fragmented trapped gas, which is formed in a double-well potential. When the barrier is extremely wide and tall, the system fragments into two condensates [16, 17] with RDM exhibiting two large and equal eigenvalues. However, if the barrier is only partially separating the condensate the nature of the system is mixed and difficult to describe without detailed calculation.

Here we examined the behavior of the bosons when

| DMC run data | c |
|--------------|---|
| \( M \times 10^4 \) | \( 2 \) | \( 4 \) | \( 8 \) | \( 16 \) |
| \( N_T \times 10^6 \) | 256 | 256 | 256 | 512 |
| \( N_f \) | 75 | 140 | 250 | 350 |
| \( K \) | 50 | 100 | 250 | 500 |
| \( N_{act} = M N_T K / N_f \times 10^{10} \) | 3.8 | 3.6 | 2.6 | 3.6 |
| \( \omega \Delta t \times 10^{-15} \) | 1.25 | 1.25 | 1.25 | 1.25 |
| Wall time hrs/CPUs | 64 x 4 | 64 x 4 | 53 x 4 | 47 x 8 |

Table III. The parameters for the DMC runs \( D = 32 \) bosons in a double well, keeping the density constant as the interaction constant \( c \) grows) used to produce the results shown in Fig. 5. The wall-time in hours and the number of CPU running 8 threads. The DMC correlation time for \( c = 16 \) was large and required large \( N_f \) to reduce fluctuations.
trapped in a double well as the repulsion strength is increased. If we keep the trap constant and just increase the repulsion we find that the effect of the constant barrier becomes negligible and the systems gradually shifts towards that of bosons trapped in a harmonic well. In order to prevent this, we examine systems of increasing repulsion constant $c$ and at the same time but we change the trap (spring constant $k_H$ and barrier height $V_b$ in Eq. (1)) so that the boson density stays (nearly) constant. This is a different limit than that studied in the previous section, where we kept the trap constant as we increased $c$ and the density decreased. We found that with constant $\sigma_\alpha = 0.1$ and $\sigma_\beta = 0.5$, the TF density is unchanged if we preserve the ratios $V_b/c$ and $k_H/c$ (we took these equal to 3 and 2.86 respectively). The RDM properties of 4 such systems with $c = 2$, 4, 8, and 16 are shown in (A5) (corresponding DMC run parameters given in Table III). Since the density is kept constant the main response is expressed as off diagonal changes in the RDM as $c$ grows. What we see is that the anti-diagonal $\Gamma_1 (q, -q)$ gradually diminishes for intermediate values of $q$ and deforms, smearing the double-hump feature. The condensate density, like the total density $\Gamma_1 (q, q)$, seems to preserve it’s shape but reduces as contributions from other eigenfunctions of the RDM grow. Indeed, the strengthening of $c$ reduces the value of the condensate fraction, i.e. the largest RDM eigenvalue fraction, from $f_1 = 0.84$ at $c = 2$ to $f_1 = 0.65$, while compensating by increasing the other eigenvalue fractions $f_2$, $f_3$ and $f_4$. Note that the growing value of the sum of higher state population fractions $f_c = \sum_{k=4}^{\infty} f_k$, reaching 9% at $c = 16$. The second eigenvalue does not grow appreciably larger than the third or fourth eigenvalue fractions, showing that the condensate is not “fragmented” despite the visibly deep cut through the density at $x = 0$.

IV. SUMMARY AND DISCUSSION

In this paper we have developed a new stochastic method for calculating the RDM of trapped Bose particles in the ground state. The method is based on a unguided DMC process in which a double-walker is used to estimate the RDM $\Gamma^{\alpha\beta}$ (where $q$ designate bins on the position axis) as a permanent of the double-walker adjacency matrix. We have used the method to treat systems of up to 32 bosons with usefully converged statistics in harmonic and double-well traps. Based on the tests we ran, we estimate the complexity to scale as $D^6 = D^3 \times D^2 \times D^2$ where the first factor is due to the complexity of a determinant calculation, the second is our estimate of the increase in the number of determinant evaluations needed for each permanent calculation due to the linear increase of the relative statistical fluctuations $C^\nu$ with $D$ (top panel of Fig. 2) and the third is due to the fact that for each double walker we repeat the permanent evaluation $D$ times. In a limited range of $D$, the efficiency of the sampling decreases with increasing $D$ due to the decrease in the number of non-zero permanents (see the bottom panel of the figure). However, when $D$ grows further this effect will diminish since the fraction of non-zero permanents actually grows with $D$. In calculating the RDM of harmonically trapped particles with $\alpha_0 = 4$ and $\alpha_1 = 0.1$, the CPU time increased by a factor $\sim 50$ (keeping the same level of statistical fluctuations) when going from $D = 16$ to $D = 32$, which is consistent with this scaling. Note however, that this estimated complexity is based on experience with the Harmonic-trapped Bosons and short interaction ranges. Its generality needs to be further investigated tested in different settings and applications.

We point out that while in this paper we focused on short ranged repulsive 1D particles, there is no formal reason why the method will not be applicable for higher dimensions and other types of interactions. Indeed the possibility of these issues is left as future directions.

It is important to appreciate, that the present stochastic RDM calculation essentially involves a stochastic post-processing step placed on top of a DMC random walk. As such, the same technique can perhaps be used in conjunction with other types of Monte Carlo methods or even with deterministic approaches that produce a wave function. This too is a possible direction for extending the method.

Appendix A: RDM Diagonal and anti-diagonal for potentials with inversion symmetry

The condensate is associated with the anti-diagonal long range of the density matrix [18] In finite systems it is more difficult to speak of long range yet the relation, e.g. ratio, of the anti-diagonal and diagonal can be considered. We describe this approach here.

For the RDM of the (non-negative) ground-state, as considered here, the RDM $\Gamma_1 (q, \bar{q})$ is also manifestly non-negative. Furthermore, if the trap potential is symmetric $v(q) = v(-q)$, the RDM eigenstates $\psi_n(q) (\Gamma_1 (q, \bar{q}) = \sum_n w_n |\psi_n(q)|^2 \psi_n(q)$ where $1 \geq w_n \geq 0$ are the RDM eigenvalues are either symmetric or antisymmetric to inversion. The diagonal and anti-diagonal densities can thus be written as

$$\Gamma_1 (q, q) = \sum_n w_n |\psi_n(q)|^2$$ \hspace{1cm} (A1)

$$\Gamma_1 (q, -q) = \sum_{\psi \in even} w_n |\psi_n(q)|^2 - \sum_{\psi \in odd} w_n |\psi_n(q)|^2$$ \hspace{1cm} (A2)

Focusing on the sum and difference between the RDM diagonal $\Gamma_1 (q, q)$ and anti-diagonal $\Gamma_1 (q, -q)$, we define two non-negative even (+) and odd (−) state densities

$$n_\pm (q) = \frac{1}{2} (\Gamma_1 (q, q) \pm \Gamma_1 (q, -q)),$$ \hspace{1cm} (A3)

and the corresponding even/odd populations $D_\pm = \int n_\pm (q) dq$. Clearly, the sum $D_+ + D_-$ is the total population $D$, while the difference,

$$D_+ + D_- = \int \Gamma_1 (q, -q) dq$$ \hspace{1cm} (A4)
is the integral of the anti-diagonal (which is thus always positive). Since the the densities $n_+(q)$ and $n_-(q)$ are positive, the RDM diagonal is never smaller than its anti-diagonal and so the ratio $1 \geq \Gamma_1(q,-q) / \Gamma_1(q,q)$ is well-defined. The presence of a condensate can perhaps be associated with a bound of this ratio from below as $q$ grows:

$$a < \Gamma_1(q,-q) / \Gamma_1(q,q) \quad \text{(A5)}$$

Equality of diagonal and anti-diagonal happens when only even states are populated! One such case is for the non-interacting Bose gas in its ground state, where only the (even) ground state is populated, in this case $D = D_{\text{even}}$ and $D_{\text{odd}} = 0$. Once a non-condensate is formed (due to interactions or increase of temperature, for example) some of population is transferred into odd states and therefore $D_{\text{even}} - D_{\text{odd}}$ diminishes. From Eq. (A4) this latter effect causes the reduction of the RDM anti-diagonal integral $\int \Gamma_1(q,-q) \, dq$. All the while, the diagonal integral $\int \Gamma_1(q,q) \, dq$, remains equal to $D$. For this reason, a small anti-diagonal population is indicative of a large non-condensate being formed.

[1] MD Girardeau, EM Wright, and JM Triscari. Ground-state properties of a one-dimensional system of hard-core bosons in a harmonic trap. Phys. Rev. A, 63(3):033601, 2001.
[2] T Papenbrock. Ground-state properties of hard-core bosons in one-dimensional harmonic traps. Phys. Rev. A, 67(4):041601, 2003.
[3] Kaspar Sakmann, Alexej I Streletsov, Ofir E Alon, and Lorenz S Cederbaum. Reduced density matrices and coherence of trapped interacting bosons. Phys. Rev. A, 78(2):023615, 2008.
[4] Jonathan L DuBois and Henry R Glyde. Natural orbitals and bose-einstein condensates in traps: A diffusion monte carlo analysis. Phys. Rev. A, 68(3):033602, 2003.
[5] GE Astrakharchik, D Blume, S Giorgini, and BE Granger. Quantum monte carlo study of quasi-one-dimensional bose gases. Journal of Physics B: Atomic, Molecular and Optical Physics, 37(7):S205, 2004.
[6] Jonathan L. DuBois. Bose-Einstein condensation in traps: a quantum Monte Carlo study. PhD thesis, University of Delaware, 2002.
[7] DS Petrov, GV Shlyapnikov, and JTM Walraven. Regimes of quantum degeneracy in trapped 1d gases. Phys. Rev. Lett., 85(18):3745, 2000.
[8] MA Cazalilla, Roberta Citro, Thierry Giamarchi, Edmond Orignac, and Marcos Rigol. One dimensional bosons: From condensed matter systems to ultracold gases. Rev. Mod. Phys., 83(4):1405, 2011.
[9] Herbert John Ryser. Combinatorial mathematics, volume 14. JSTOR, 1963.
[10] Christopher David Godsil. Matchings and walks in graphs. Journal of Graph Theory, 5(3):285–297, 1981.
[11] Terence Tao and Van Vu. On the permanent of random bernoulli matrices. Advances in Mathematics, 220(3):657–669, 2009.
[12] L H Thomas. The calculation of atomic fields. Proceedings of the Cambridge Philosophical Society, 23:542, 1927.
[13] E. Fermi. Un metodo statistico per la determinazione di alcune priorietà dell’atomo. Rend. Accad. Naz., 6:602, 1927.
[14] Laszlo Tisza. Transport phenomena in helium ii. Nature, 141(3577):913, 1938.
[15] The viscosity of a fluid is related momentum fluctuations by the Green-Kubo formula.
[16] P. Nozières. Some comments on bose-einstein condensation. In Allan Griffin, David W Snoke, and Sandro Stringari, editors, Bose-Einstein Condensation, chapter 2, pages 15–30. Cambridge University Press, 1995.
[17] Erich J Mueller, Tin-Lun Ho, Masahito Ueda, and Gordon Baym. Fragmentation of bose-einstein condensates. Phys. Rev. A, 74(3):033612, 2006.
[18] L Landau. Theory of the superfluidity of helium ii. Phys. Rev., 60(4):356, 1941.
[19] Oliver Penrose and Lars Onsager. Bose-einstein condensation and liquid helium. Phys. Rev., 104(3):576, 1956.