Squeezed and fragmented states of strongly interacting bosons in a double well. Part II: Quantum Monte Carlo simulations

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We present path integral ground state (PIGS) quantum Monte Carlo calculations for the ground state \((T = 0)\) properties of repulsively interacting bosons in a three-dimensional external double well potential over a range of interaction strengths and potential parameters. We focus our calculations on ground state number statistics and the one-body density matrix in order to understand the level of squeezing and fragmentation that the system exhibits as a function of interaction strength. We compare our PIGS results to both a two-mode model and a recently-proposed eight-mode model. For weak interactions, the various models agree with the numerically exact PIGS simulations. However, the models fail to correctly predict the amount of squeezing and fragmentation exhibited by the PIGS simulations for strong interactions. One novel and somewhat surprising result from our simulations involves the relationship between squeezing and interaction strength: rather than a monotonic relationship between these quantities, we find that for certain barrier heights the squeezing increases as a function of interaction strength until it reaches a maximum, after which it decreases again. We also see a similar relationship between fragmentation and interaction strength. We discuss the physical mechanisms that account for this behavior and the implications for the design of atom interferometers, which can use squeezed states to reduce measurement uncertainty.

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I. INTRODUCTION

The ground state properties of interacting bosons in a double well potential are of great fundamental and practical interest, with broad implications for a variety of open questions in many-body condensed matter physics and applications in quantum computation. One potentially powerful application of the double well system involves the development of methods for reducing the lower bound on the uncertainty of interferometric measurements from the standard quantum limit of \(N^{-1/2}\) to the Heisenberg limit of \(N^{-1}\) (where \(N\) is the total number of particles involved in the measurement) \[1\, 3\]. Initial proposals to reduce this uncertainty called for using superpositions of macroscopic quantum states (Schrödinger cat states), but sensitivity to dissipation was found to limit the benefits of this strategy \[4\]. This problem may be avoided by using squeezed states, which are many-body states that have a distribution of particles with respect to some variable of interest that is narrower than a binomial distribution \[5\, 6\].

In the context of the double well, the differential number distribution (the difference in the number of particles on the two sides of the barrier) is the distribution that can be squeezed. Broadly speaking, one can increase squeezing (narrow the differential number distribution) for atomic systems either by increasing the strength of the repulsive interparticle interaction (e.g., via a Feshbach resonance \[7\]) or by decreasing the tunneling strength between the wells (e.g., by increasing the barrier height). Beginning in 2001, experimental efforts have succeeded in realizing number squeezed states with cold atoms in the laboratory \[8\, 12\].

For a system with symmetry like the double well, the strength of interparticle interactions also impacts the degree of fragmentation and depletion exhibited by the system. For an atomic system undergoing Bose-Einstein condensation, some fraction of the system’s atoms will generically not be in the condensed state; this fraction is known as the depletion. Additionally, if all of the atoms in the condensate occupy the same single-body state, the condensate is unfragmented. However, if the condensed atoms occupy two or more different single-body states, then the condensate is fragmented. Roughly speaking, both fragmentation and depletion increase with increasingly repulsive interactions. Experimental studies have confirmed the presence of depletion in an atomic BEC in an optical lattice \[13\] as well as fragmentation in a quasi-1D atomic BEC in a magnetic waveguide \[14\].

This paper is the second in a series of two papers in which we study both squeezing and fragmentation for a Bose-Einstein condensate in a three dimensional double well potential over a range of interaction strengths and barrier heights. In this second paper, we employ the full many-body formalism of quantum Monte Carlo (QMC)
by evaluating the ground state properties of the BEC using the path integral ground state (PIGS) method. The numerically exact PIGS method allows us to move beyond the range of validity of standard mean-field methods and into the regime of strongly interacting systems. We determine the amount of squeezing and fragmentation present in the BEC as a function of interaction strength and compare with the predictions of the two- and eight-mode models that we presented in the first paper of this series to understand when, how, and why these approximate models break down.

II. THE DOUBLE WELL SYSTEM, SQUEEZING, FRAGMENTATION, AND TRUNCATED BASIS MODELS

We provide here a brief summary of the Hamiltonian for $N$ bosons in a three-dimensional double well potential, our definitions of the squeezing and fragmentation parameters for this system, and two reference models in which the Hamiltonian is expressed in a truncated basis of single-particle states. The latter are the two- and eight-mode models that are analyzed in detail in [19]. We refer the reader to that paper for a more detailed description of the Hamiltonian, the squeezing and fragmentation parameters, and the truncated basis models.

A. The Many-Body Double Well Hamiltonian

We employ the many-body Hamiltonian for $N$ bosons of mass $m$ interacting pairwise in an external potential:

$$\hat{H} = \sum_{j=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_j^2 + V_{\text{ext}}(r_j) \right) + \sum_{j<k}^{N} V_{\text{int}}(r_j, r_k). \quad (1)$$

We use a three-dimensional double well potential for the external potential:

$$V_{\text{ext}}(r) = \frac{1}{2} m \omega_{ho}^2 \left( x^2 + y^2 + \alpha \left( z^2 - L^2 \right)^2 \right), \quad (2)$$

where $\omega_{ho}$ is the characteristic harmonic trap frequency in the $xy$ plane, $\alpha$ characterizes the height of the barrier between wells at $z = 0$, and $2L$ is the distance between the minima of the wells (see Fig. 1).

As in the first paper in this series, our external potential parameters are motivated by the experiment described in [20], which employed $^{23}$Na atoms and a trap with $L = 65 \mu m$, $\omega_{ho}/2\pi = 615$ Hz, and $\frac{1}{2} m \omega_{ho}^2 \alpha L^4 = \hbar \times 4.7$ kHz (equivalently, $\alpha = 6.1 \times 10^{-9} \text{nm}^{-2}$). Our analysis and results are presented in terms of the characteristic length $a_{ho} = (\hbar/m \omega_{ho})^{1/2}$ and energy $\hbar \omega_{ho}$ of the system. In [20], the trap length and frequency parameters were $a_{ho} = 845 \text{ nm}$ and $\hbar \omega_{ho} = 2.54 \text{ peV}$, corresponding to scaled parameters $L = 7.7 a_{ho}$ and $\alpha = 0.26 a_{ho}^{-2}$. These are comparable to the values in the systems we study here.

To compute ground state (i.e., low energy) properties, we use a hard sphere interaction potential (i.e., we assume $s$-wave scattering):

$$V_{\text{int}}(r_{jk}) = \begin{cases} \infty & r_{jk} \leq a \\ 0 & r_{jk} > a \end{cases}, \quad (3)$$

where $r_{jk} = |r_j - r_k|$ and $a$ is the (positive) $s$-wave scattering length, which is proportional to interaction strength. Substantial tunability of $a$ has been demonstrated in the laboratory using Feshbach resonances. A particularly impressive example is [21], in which $a$ for $^7\text{Li}$ was tuned between 0.53 pm and 10.6 pm (between $3.5 \times 10^{-7} a_{ho}$ and $7 a_{ho}$, given the value of $\omega_{ho}$ above). Our calculations employ values of $a$ up to $0.5 a_{ho}$ (about 420 nm), and are thus well within the range of experimental accessibility.

B. Squeezing and Fragmentation

The degree of squeezing exhibited by a state is related to the operator $\hat{n} = \frac{1}{2}(\hat{L} - \hat{R})$, where $\hat{L}$ and $\hat{R}$ measure the fraction of the probability density of the many-body state that exists in the left and right wells, respectively. Because the many-body ground state of the double well potential is symmetric no matter the interaction strength, $\langle \hat{L} | \hat{L} \rangle = \langle R | R \rangle = N/4$ in all cases. The interaction strength does affect the width of the distribution, which can be characterized by its standard deviation $\sigma_n = \sqrt{\langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2}$: $\sigma_n = \sqrt{N}/2$ when $a = 0$, whereas $\sigma_n < \sqrt{N}/2$ when $a > 0$ (i.e., the width of the distribution narrows for nonzero $a$). This narrowing is what is meant by number squeezing, and we characterize it by defining a squeezing parameter $S$:

$$S = 1 - \frac{\sigma_n^2}{N/4}, \quad (4)$$

which varies from 0 (no squeezing) to 1 maximal squeezing.

Figure 1. (Color online) The $z$ part of the external potential for $\alpha = 4/81 a_{ho}^{-2}$. The height of the barrier, $V_{\text{ext}}(0) = m \omega_{ho}^2 \alpha L^4/2$, is $2/81 \hbar \omega_{ho}$, $32/81 \hbar \omega_{ho}$, and $2 \hbar \omega_{ho}$ for $L = a_{ho}$, $2 a_{ho}$, and $3 a_{ho}$, respectively.
The degrees of fragmentation and depletion exhibited by a state are related to the one-body density matrix (OBDM), which is given by [22]

$$\rho(r, r') = \langle \Psi'(r) \Psi(r') \rangle,$$  \hspace{1cm} (5)

where $\Psi(r)$ is the field operator that annihilates a single particle at the position $r$. One can diagonalize the OBDM, producing a set of eigenfunctions $\phi_i(r)$ and eigenvalues $N_i$ that are known as the natural orbitals and occupation numbers, respectively. In certain cases, one can think of the many-body ground state as being equivalent to a state with $N_i$ atoms occupying the single-body state $\phi_i(r)$. The signature of condensation is for one or more of the occupation numbers to be close to $N$. If this is true for only one occupation number, the condensate is unfragmented; if it is true for more than one, the condensate is fragmented. In either case, the small amount of occupation in the non-condensed states constitutes the depletion. One way to understand this distinction is that in the thermodynamic limit ($N \rightarrow \infty$), the occupation fraction $n_i = N_i/N$ remains finite for orbitals in the condensate and goes to zero for orbitals in the depletion.

Because of the near-degeneracy in the ground state of the double well, we expect at most two natural orbitals to have significant occupation [23]. Hence, $n_0 + n_1 \approx 1$. This motivates us to define a fragmentation parameter $F$ and a depletion parameter $D$ [19]:

$$F = 1 - |n_0 - n_1|$$ \hspace{1cm} (6)

$$D = 1 - (n_0 + n_1).$$ \hspace{1cm} (7)

With these definitions, a single condensate is represented by $F \approx D \approx 0$ and a doubly fragmented condensate is represented by $F \approx 1$ and $D \approx 0$.

C. The Two- and Eight-Mode Models

The models used to describe the double well system involve writing the Hamiltonian in second quantized form and expanding the field operator $\Psi(r)$ in terms of a truncated basis of single particle states. In the two-mode model, the basis consists of linear combinations of the single particle ground and first excited states of the double well; the linear combinations are chosen to localize the modes in the left and right sides of the potential. We can think of these modes as being the $n = 1$ energy level of the system. In the eight-mode model, one adds linear combinations of the next six single particle excited states to the basis; again, these are chosen to localize the modes on the two sides of the potential, and we can think of these as constituting the $n = 2$ energy level of the system. The $n = 2$ modes are localized less well than the $n = 1$ modes (i.e., a larger fraction of the probability density of one of “left” $n = 2$ modes can be found in the region $z > 0$ compared to the “left” $n = 1$ mode, and vice versa).

Once the Hamiltonian is constructed in this way, it can be numerically diagonalized to compute the ground state in a Fock basis $|n\rangle$ with a definite number of atoms in each mode (i.e., for the two-mode model, $|n\rangle = |n\rangle_l |N - n\rangle_r$, where $l$ and $r$ denote the left- and right-localized modes). Because the size of the Hilbert space of the system grows rapidly with the number of modes, this explicit diagonalization procedure becomes intractable for more than about 10 atoms in the eight-mode model.

As we reported in [19], for the two-mode model:

- squeezing is not necessarily monotonic with $a$, especially for weak barriers,
- for a given $N$, squeezing tends to increase with barrier strength,
- for a given barrier strength, squeezing tends to decrease with $N$ for large $a$, and
- for fixed $a$, fragmentation tends to increase with $N$ for weak barriers, whereas fragmentation tends to decrease with $N$ for strong barriers.

These trends can be explained by understanding how $a$, $N$, and the double well geometry parameters influence the relative importance of the terms in the two-mode Hamiltonian, and therefore change the nature of the ground state. The terms in the Hamiltonian come in three types:

1. Terms that involve a single Fock state. The ground state of these terms considered alone is $|N/2\rangle$, which exhibits high squeezing and high fragmentation.

2. Terms that involve transitions between Fock states that involve a single atom. The ground state of these terms considered alone is a mix of states binomially distributed around $|N/2\rangle$, which exhibits low squeezing and low fragmentation.

3. Terms that involve transitions between Fock states that involve two atoms. The ground state of these terms considered alone is a mix of alternating states distributed around $|N/2\rangle$ (i.e., it includes $|N/2\rangle$, $|N/2 \pm 2\rangle$, $|N/2 \pm 4\rangle$, etc.), which exhibits high squeezing and low fragmentation.

When interactions are weak, type 2 terms dominate regardless of the strength of the barrier. When interactions are strong, the strength of the barrier matters: for low barriers, type 3 terms dominate, while for high barriers, type 1 terms dominate.

Additionally, when comparing the eight-mode ground state to the two-mode ground state, we found that the eight mode ground state

- exhibits less squeezing, especially for high barriers,
- exhibits a maximum in $S$ vs. $a$ for high barriers, and
exhibits less fragmentation and more depletion.

These differences are a consequence of two main factors. First, the addition of extra modes leads to a much larger variety of type 3 terms in the Hamiltonian. Because of this, all Fock states are connected by type 3 terms, so the alternating pattern exhibited in the corresponding two-mode ground state vanishes. Instead, the eight-mode types 2 and 3 ground states look similar and share similar properties. Second, the occupation of the eight-mode ground state vanishes. Instead, there are two-mode ground states that accompany an increase in interaction strength to (sometimes) produce a maximum in $S$ and $F$ as a function of $a$.

III. THE PATH INTEGRAL GROUND STATE METHOD

In order to calculate the ground state properties of our system, we use the path integral ground state (PIGS) quantum Monte Carlo method. PIGS is an exact, many-body, ground state ($T = 0$) method that uses imaginary time propagation and path sampling techniques to calculate the ground state expectation value for observables in a quantum system.

Conceptually, PIGS starts with a trial wave function that may be written as a sum over the energy eigenstates of the system: $|\psi_T\rangle = \sum_{n=0}^{\infty} c_n |\psi_n\rangle$. After applying the operator $e^{-\tau \hat{H}}$, normalizing, and taking the $\tau \to \infty$ limit, the trial wave function decays into the ground state wave function:

$$\lim_{\tau \to \infty} \frac{e^{-\tau \hat{H}} |\psi_T\rangle}{\sqrt{\langle \psi_T | e^{-2\tau \hat{H}} |\psi_T\rangle}} = |\psi_0\rangle. \quad (8)$$

We will ignore the normalization factor for the rest of this discussion.

We denote the configuration of the system with a 3N-dimensional vector $R$ that encodes the coordinates of the system’s $N$ particles: $R \equiv \{r_1, r_2, \ldots, r_N\}$. In the position representation, it is generally not possible to express $\langle R | e^{-\tau \hat{H}} | R' \rangle$ analytically unless $\tau$ is small. Therefore, we define $\tau \equiv \beta M$, with $\beta \ll 1$. We can then write the expectation value for an observable of interest $A$ (assumed to be diagonal in the position basis) as

$$\langle A \rangle = \langle \psi_T | e^{-\beta \hat{H}} M A e^{-\beta \hat{H}} M |\psi_T\rangle \quad \text{(9)}$$

where we have inserted $2M + 1$ complete sets of position eigenstates. Here $G(R_i, R_{i+1}, \beta)$ is the short time propagator $\langle R_i | e^{-\beta \hat{H}} | R_{i+1} \rangle$, which can be approximated for sufficiently small $\beta$. Note that this procedure allows for the calculation of expectation values of observables in the ground state, but not the ground state wave function itself.

Given an analytical form for $G(R_i, R_{i+1}, \beta)$, our problem has been transformed into that of solving an integral of very high dimension, which can be done with standard Monte Carlo sampling techniques. The paths $X \equiv \{R_0, R_1, \ldots, R_{2M}\}$ are statistically sampled from the probability density

$$\pi(X) = \psi_T^*(R_0) \psi_T(R_{2M}) \prod_{i=0}^{2M-1} G(R_i, R_{i+1}, \beta), \quad (10)$$

using the Metropolis algorithm [24], which ensures that the sampling is ergodic (i.e., that the set of accepted paths samples the set of all paths with probabilities given by $\pi(X)$). If this condition is met, then the average value of $A(R_M)$ for the set of accepted paths can be used to estimate the value of $\langle A \rangle$. In general, one wants long paths (large $M$) so that $R_M$ is sampled from a probability density as close to the square of the exact ground state wave function as possible.

The main computational difficulty that one faces in simulating interacting bosons in double well potentials is properly estimating the squeezing $S$ for high barriers, because in this situation it is difficult to achieve ergodicity with respect to moving particles across the barrier. Below we describe computational details regarding the trial function, the propagator, methods for path sampling, and the computation of off-diagonal observables, with explicit consideration of this issue.

A. Trial function

We use a trial wave function which is a product of single-particle ground state wave functions and pair correlation (Jastrow) terms:

$$\psi_T(R) = \prod_{i=1}^{N} \psi_0(r_i) \prod_{j<k}^{N} \left(1 - \frac{a}{r_{jk}}\right), \quad (11)$$

where $\psi_0(r_i) = \psi_{HO}^x(x_i)\psi_{HO}^y(y_i)\psi_{DW}^z(z_i)$, a product of the analytical harmonic oscillator ground state wave function in the $x$ and $y$ directions and a numerically calculated one-dimensional double well ground state wave function in the $z$ direction. The pair correlation term is the exact zero-energy $s$-wave scattering solution for two hard spheres [25].
B. Propagator

For our short-time propagator, we use both a fourth-order propagator decomposition and a modification of the free particle propagator that exactly incorporates the hard sphere interaction.

1. External potential decomposition

First, we use a fourth-order factorization to approximate $G(R_i, R_{i+1}, \beta)$ [26]:

\[
G(R_i, R_{i+1}, \beta) = \int dR_j \ e^{-\frac{3}{8}V(R_i)} \langle R_i | e^{-\frac{3}{8}(T+V_{hs})} | R_j \rangle \\
\times e^{-\frac{23}{8}V(R_j)} \langle R_j | e^{-\frac{3}{8}(T+V_{hs})} | R_{i+1} \rangle \\
\times e^{-\frac{2}{8}V(R_{i+1})},
\]

(12)

where $T$ is the kinetic energy, $V$ is the external potential, $V_{hs}$ is the hard-sphere potential,

\[
\tilde{V} = V + \frac{\pi^2}{48} [V, [(T + V_{hs}), V]] \\
= V + \frac{\lambda \pi^2}{24} |\nabla V|^2,
\]

(13)

and $\lambda = \frac{h^2}{2m}$. It is essential to group $V_{hs}$ with $T$ rather than $V$ in the computation of $\tilde{V}$ to take advantage of the fact that $[V, V_{hs}] = 0$, which allows us to avoid taking the gradient of the (singular) hard sphere potential.

By using this factorization, we have introduced a new configuration $R_j$ between each pair of original configurations $R_i$ and $R_{i+1}$, so that there are now $4M+1$ configurations instead of $2M+1$. Treating all of these on equal footing, we can rewrite [10] as

\[
\pi(X) = \psi_T^2(R_0)\psi_T(R_{4M})e^{\frac{3}{8}(V(R_0) - V(R_{4M}))} \\
\times \prod_{i=0}^{4M-1} f(R_i) \ G_{hs}(R_i, R_{i+1}, \beta/2),
\]

(14)

where

\[
f(R_i) = \begin{cases} 
  e^{-\frac{1}{2}\beta V(R_i)} & i = 0, 2, \ldots \\
  e^{-\frac{1}{2}\beta V(R_i) - \frac{1}{4}\lambda \beta |\nabla V(R_i)|^2} & i = 1, 3, \ldots
\end{cases}
\]

and \(G_{hs}(R_i, R_{i+1}, \beta/2) = \langle R_i | e^{-\frac{3}{8}(T+V_{hs})} | R_{i+1} \rangle\) is the hard sphere propagator.

2. Hard sphere propagator

In order to compute the hard sphere propagator, we use the pair product approximation [27]:

\[
G_{hs}^m(R_i, R_{i+1}, \beta) = G_{free}^m(R_i, R_{i+1}, \beta) \\
\times \prod_{j<k} G_{hs}^{m/2}(r_{jk}^{i}, r_{jk}^{i+1}, \beta),
\]

(16)

Here $G_{free}^{m/2}$ is the free/hard sphere propagator for the relative motion between two particles (so it involves the relative coordinate $r_{ij}$ and the reduced mass $m/2$).

Several methods have been proposed in the literature for approximating $G_{hs}$, including the image approximation [27, 28] and the propagator of Cao and Berne [29]. One critical consideration for choosing a propagator for the double well system is that we need long paths to assure that the system has decayed to the ground state because the decay goes as $\exp(-\tau \Delta E)$, where $\Delta E$ (the energy gap between the ground and first excited state) is small. Hence, we must use as large a time step as possible. We chose to implement the exact hard sphere propagator because it allows larger time steps than the Cao and Berne propagator (e.g., $10^{-2} (\hbar \omega_h)^{-1}$ compared to $10^{-4} (\hbar \omega_h)^{-1}$ for equivalent results).

The exact expression for $G_{hs}^{m/2}$ is [30]:

\[
G_{hs}^{m/2} = \frac{1}{2\pi^2} \sum_{l=0}^{\infty} P_l(\cos \gamma)(2l + 1) \\
\times \int_0^{\infty} k^2 e^{-2\beta \lambda k^2} R_l(r_{jk}^i, k) R_l(r_{jk}^{i+1}, k) \frac{D_l(k)}{D_l(ka)} \,dk,
\]

(17)

where

\[
R_l(r, k) = j_l(kr)y_l(ka) - y_l(kr)j_l(ka),
\]

(18)

\[
D_l(k) = j_l^2(ka) + y_l^2(ka),
\]

(19)

\(j_l(x)\) and \(y_l(x)\) are spherical Bessel functions, and $\gamma$ is the angle between $r_{jk}^i$ and $r_{jk}^{i+1}$. This expression cannot be rewritten in a convenient analytical form. To use it, we must terminate the sum at some appropriate $l_{max}$ and tabulate it as a function of $r_{jk}^i$, $r_{jk}^{i+1}$, and $\gamma$.

In addition to writing $G_{hs}^{m/2}$ in its "traditional" form,

\[
G_{free}^{m/2} = \frac{1}{(8\pi \beta \lambda)^{3/2}} e^{-\frac{(r_{jk}^i - r_{jk}^{i+1})^2}{28}}.
\]

(20)

one can also write it in a form similar to Eq. (17):

\[
G_{free}^{m/2} = \frac{1}{2\pi^2} \sum_{l=0}^{\infty} P_l(\cos \gamma)(2l + 1) \\
\times \int_0^{\infty} k^2 e^{-2\beta \lambda k^2} j_l(kr_{jk}^i)j_l(kr_{jk}^{i+1}) \,dk.
\]

(21)

This observation is useful because the difference between $G_{hs}^{m/2}$ and $G_{free}^{m/2}$ converges with respect to $l_{max}$ much faster than $G_{hs}^{m/2}$ alone (see Fig. 2). We can use this fact to reexpress the quotient in the pair product approxima-
Figure 2. (Color online) The ratio of the hard sphere propagator to the free propagator for \( r_{jk}^i = r_{jk}^{i+1} \), \( \gamma = 0 \), and \( a^2 = 2/\lambda \). The blue curves are computed as in Eq. (17) for various \( l_{\text{max}} \): the lowest blue curve has \( l_{\text{max}} = 0 \) and the highest \( l_{\text{max}} = 8 \). The red curves are computed as in Eq. (22) for various \( l_{\text{max}} \): the highest red curve has \( l_{\text{max}} = 0 \) and the lowest \( l_{\text{max}} = 8 \) (although the curves from \( l_{\text{max}} = 2 \) through \( l_{\text{max}} = 8 \) are visually indistinguishable). The rapid convergence of Eq. (22) compared with Eq. (17) is a general feature of these functions.

The main “workhorse” update method we use is the Brownian bridge move, which is a specific realization of the more general Lévy construction [31, 32]. In the Brownian bridge move, a portion of the path of a single particle is updated. The particle is chosen randomly, as is the section of its path that is updated; the length of this section is a fixed parameter \( K \), defined such that the section consists of \( K + 1 \) time slices including the endpoints.

The move proceeds as follows. The endpoints of the section to be updated are chosen and held fixed; call these \( \mathbf{r}_0 \) and \( \mathbf{r}_K \). Next, the coordinate of the particle at the first time slice, \( \mathbf{r}_1 \), is replaced with one drawn from the probability distribution

\[
P(\mathbf{r}_1) \propto e^{-\frac{n(\mathbf{r}_1 - \mathbf{r}_0)^2}{4a^2}},
\]

where

\[
\mathbf{r}^* = \frac{\tau_1 \mathbf{r}_0 + \tau_2 \mathbf{r}_K}{\tau_1 + \tau_2}.
\]
for determining $r_1$, but with the updated left endpoint. This process continues until the entire section of path is reconstructed.

In general, the Brownian bridge move is an efficient way of sampling new paths, although it is susceptible to the ergodicity problem described above if the barrier is too strong and enough of the new path ends up in the barrier region. For the vast majority of our simulations, however, it was the only update method that was necessary.

2. Swap moves

One potential way to address the ergodicity issue is to implement an additional type of move that explicitly transfers a particle from one well to the other \[33\]. In our implementation of this “swap move”, the $z$-coordinate is negated for the entire path of a random particle. If this leads to an overlap between the swapped path and another path (i.e., two particles at the same time slice with a separation less than $a$), then the other path is also swapped. This “cascade” continues until no overlaps remain.

Unfortunately, swap moves do not work as well as intended. As the simulation progresses, Brownian bridge moves tend to nudge the particle paths into tight clusters near the well minima, as noted above. Once the system is in that sort of configuration, a swap move has a high probability of leading to a cascade that swaps every particle. Because of the symmetry of the double well, this is equivalent to not swapping any particle. This effect is worse for longer paths and larger $N$, and in practice, the swap move was found to be mostly ineffective for the double well simulations made here.

3. Potential moves

Our “potential moves” were inspired by the parallel tempering technique \[34\]. In parallel tempering, one runs multiple copies of a simulation at different temperatures simultaneously, and exchanges configurations between two different simulations based on the Metropolis criterion. This allows a simulation at a given temperature to sample a wider variety of configurations, potentially avoiding an ergodicity problem.

In our potential moves, we run only one simulation, but we implement a move that changes the shape of the external potential, specifically by changing $L$ from among a set of pre-defined values. Given the current value of $L$, the potential move attempts to change $L$ to the next highest or lowest value in the pre-defined set and uses the Metropolis criterion to accept or reject the move. The motivation here is to allow for a way to more easily change $(n_i - n_e)^2$ for a high-barrier potential than would be possible with only Brownian bridge moves. Lowering the potential barrier and then raising it again provides one convenient way to facilitate this.

One challenge with this method is that certain potentials are more probable (i.e., have higher average values of $\pi(X)$, with the average taken over all configurations) than others, so a simulation with potential moves as described above would eventually end up only sampling the most probable potential. To avoid this problem, we introduce a set of weights, one per potential, that we multiply by $\pi(x)$ before applying the Metropolis algorithm. We choose these weights so that the average probability of transitioning from one potential to another is the same as the probability of the reverse, which ensures that all of the potentials will be visited with equal probability in the long run. One can choose these weights using a version of the Wang and Landau algorithm \[35\].

In practice, these moves often work quite well once the correct weights are chosen. However, there is still a problem: while weights can be chosen to equalize the back-and-forth transition probabilities between two potentials, the actual value of that probability cannot be tuned at will and can be quite small. If that is the case, then even though in principle all potentials will be visited with equal frequency, that will only happen in practice in the limit of a very long simulation. This situation arises for high-barrier potentials, and worsens for larger $N$ and longer paths; see Table I for an example.

| Number of slices | 100 | 200 | 800 |
|------------------|-----|-----|-----|
| 8                | $4.8 \times 10^{-1}$ | $3.9 \times 10^{-1}$ | $6.1 \times 10^{-2}$ |
| 16               | $3.0 \times 10^{-1}$ | $1.5 \times 10^{-1}$ | $1.8 \times 10^{-2}$ |
| 32               | $1.2 \times 10^{-1}$ | $4.6 \times 10^{-2}$ | $1.0 \times 10^{-5}$ |
| 64               | $4.8 \times 10^{-2}$ | $1.1 \times 10^{-2}$ | $3.1 \times 10^{-12}$ |

Table I. Probability of making a potential move that transitions between two potentials of different shape, characterized by $L = 2.875 \, a_{ho}$ and $3 \, a_{ho}$, for various numbers of particles $N$ and path lengths (number of slices). In all cases, $a = 0.1 \, a_{ho}$.

D. Off-diagonal observables

The discussion of PIGS above describes the calculation of observables diagonal in the position basis. To compute an off-diagonal observable, such as the OBDM, we must insert an extra set of position eigenstates into Eq. \[9\]:

$$\langle \hat{A} \rangle = \int dR_0 \cdots dR_{2M+1} A(R_M, R_{M+1}) \psi_T^*(R_0) \psi_T(R_{2M}) \times \prod_{i=0}^{M-1} G(R_i, \gamma_i, \beta) \prod_{i=M+1}^{2M} G(R_i, \gamma_i, \beta).$$

There is no propagator connecting the configurations $M$ and $M + 1$; the path is said to be “broken.” The paths
are sampled in the same way as for diagonal observables, and the value of \( \langle A \rangle \) is estimated by averaging over \( A(R_M, R_{M+1}) \) for the accepted paths, just as before.

To compute the OBDM \( \rho \), the path of only one of the \( N \) particles is broken (i.e., \( r_M \) is allowed to differ from \( r_{M+1} \) for the broken path) while \( r_M \) is set equal to \( r_{M+1} \) for the others. One then samples paths as usual and uses the set of accepted configurations to make a histogram of the occurrences of particular pairs of \( z_M, z_{M+1} \) on the broken path; this histogram is \( \rho(z, z') \). In order to normalize the OBDM, we multiply it by a factor such that the sum of its eigenvalues (i.e., the total occupation of the natural orbitals) is 1. This method can generate non-physical negative eigenvalues, but these vanish given long enough simulations.

IV. RESULTS & DISCUSSION

We now present numerically exact PIGS results for the squeezing and fragmentation of a BEC in a three-dimensional double well potential, and compare them to the corresponding results from the two- and eight-mode approximations \[16\]. The PIGS results presented here are calculated for double well potentials with \( \alpha = 4/81 a_{ho}^{-2} \) and \( L = a_{ho}, 2a_{ho}, \) and \( 3a_{ho} \). The reader is encouraged to refer to \[19\] for full details of the calculations and results within the two- and eight-mode models.

A. Squeezing

In Fig. 3 we plot the squeezing parameter \( S \) as a function of \( a \) for the PIGS simulations, together with comparisons to the corresponding two-mode and eight-mode model results from \[19\]. Following Eq. (12) in \[36\], we estimate that the two-mode model should be valid as long as

\[
a \ll \frac{1}{N} \sqrt{\frac{9\pi}{8L}}.
\]

These values of \( a \) are indicated in Fig. 3. In general, we see that the models and the PIGS results agree well when this condition is met but deviate as \( a \) increases. As one would expect, the two-mode model deviates from PIGS first, followed by the eight-mode model (for the cases where data is available).

Whether the models tend to over- or underestimate the PIGS results for large \( a \) depends on the strength of the double well barrier (i.e., the value of \( L \)): for strong barriers \((L = 3a_{ho})\), we find less squeezing the more accurate the model (i.e., when going from two-mode to eight-mode to PIGS), whereas for weak barriers \((L = a_{ho})\), we find the opposite. The intermediate-strength case \((L = 2a_{ho})\) is a “crossover” between the other two cases, where the models and PIGS more closely agree. We propose two mechanisms to account for the discrepancies between the two-mode model and the PIGS data.

a. Occupation of higher modes The first mechanism has to do with the idea that the ground state should, in general, have as low an interaction energy as possible. reduction of the interaction energy of the ground state. As the strength of repulsive interactions increases, the ground state has to change to minimize its energy given the value of \( a \), and this of course causes \( S \) to change with \( a \). One can argue that strong repulsive interactions should suppress number fluctuations (and hence increase squeezing) because configurations with many particles on one side of the double well are disfavored due to their large interaction energy. This argument assumes that equalizing the difference in atoms between the two wells is the dominant mechanism that the system uses to reduce its interaction energy (we will refer to this as the “traditional mechanism”).

However, the behavior of the eight-mode ground state suggests another possible way in which the ground state interaction energy is reduced. As alluded to in Sec. IIC, the eight-mode ground state contains increasingly large occupation of modes in the \( n = 2 \) energy level as \( a \) increases. It is reasonable to suspect that this pattern would also hold true were we to study models that included \( n = 3 \) modes, \( n = 4 \) modes, and so on. Hence, if we think of PIGS conceptually as an “infinite-mode” model, then we would expect similar behavior in our simulations.

How does this impact squeezing? As discussed above, the more that a set of modes encroach into the “wrong” side of the double well, the less squeezing that set can support. Certain modes with higher \( n \) tend to have more such encroachment than the \( n = 1 \) modes, which implies that they can support less squeezing. Hence, when strong repulsion drives particles into modes of higher \( n \), it is driving some of them into modes that support less squeezing. Therefore, this will reduce squeezing compared with the two-mode model, in which all particles have \( n = 1 \). We note that this mechanism has nothing to do with the strength of the double well barrier.

b. Additional two-body tunneling terms The second mechanism has to do with the types of two-body tunneling terms present in the Hamiltonian due to the presence of higher modes. As described in Sec. IIC, two-particle tunneling terms dominate the dynamics of the system for large \( a \) and small \( L \). In the two-mode model, these tunneling terms force the ground state to occupy even-numbered Fock states only, which causes large number fluctuations and hence little squeezing. The availability of higher modes changes this situation by dramatically increasing the variety of two-particle tunneling terms in the Hamiltonian; in principle, two particles can tunnel from any two modes to any other two modes as long as the total value of the \( z \)-component of their angular momentum is conserved. Hence, the alternating Fock state restriction is lifted, and the ground state can have contributions from Fock states with any value of the difference in the number of particles occupying left and right modes. This will lead to a reduction in the occupation of modes with
Figure 3. (Color online) Squeezing $S$ vs. scattering length $a$ for four different particle numbers ($N = 8$, 16, 32, and 64, from top to bottom) and three different potentials ($L = a_{ho}$, $2a_{ho}$, and $3a_{ho}$, from left to right). The plots include results from the two-mode model, the eight-mode model, and the PIGS simulations. Vertical lines indicate the values of $a$ below which we expect the two-mode models to be valid. See [19] for details of the two- and eight-mode calculations.
large values of that difference, and hence squeezing will be greater than predicted by the two-mode model. Again thinking of the PIGS simulations as “infinite-mode”, this effect will be more pronounced in the simulation results than in the eight-mode model results.

This second mechanism varies in importance depending on the value of $L$. For small $L$, it operates as described above. However, for large $L$, tunneling between the wells is highly suppressed for all modes. In the two-mode case, this drives the ground state towards $|N/2\rangle$, an equal splitting of particles. The presence of higher modes has little effect on this distribution, again because all tunneling between the wells is suppressed. Therefore, the amount of squeezing will not be affected for large $L$. This is in contrast to the first mechanism, where modes with more “spillover” are occupied in about the same amount regardless of the value of $L$.

**B. Validity of the Two-Body Interaction Approximation**

In Fig. 4 we plot the same PIGS squeezing data as in Fig. 3 except that we plot it as a function of $Na$ for each value of $L$. The most striking feature of this plot is that the data for the various values of $N$ overlap each other (except that the $N = 8$ data for the strongest barrier ($L = 3a_{ho}$) shows slightly more squeezing than the data for the other values of $N$ for large $Na$). In other words, we have found that $S$ is a function of the product $Na$ to good approximation for the potentials and ranges of $N$ and $a$ presented here.

This is an interesting result because one can show that the only situation in which the interaction Hamiltonian depends on the product $Na$ is when only two-body interactions are relevant to the physics. If higher-body interactions play a significant role, then the interaction Hamiltonian depends in a more complicated way on $N$ and $a$ [27]. Hence, only two-body interactions are relevant for the squeezing of the double well system in the parameter regime presented here. This is a non-trivial observation because the form of the hard sphere propagator used in the PIGS simulations, Eq. (22), can take into account interactions among an arbitrary number of particles.

**C. Fragmentation and Depletion**

We now move on to our fragmentation and depletion results. In Fig. 5 we plot the fragmentation parameter $F$ as a function of $a$ for PIGS simulations with the usual values of $N$, $L$, and $a$ (except that we do not have $N = 64$ data), along with comparisons to the equivalent two-mode and eight-mode models. For weak barriers ($L = 2a_{ho}$ and $3a_{ho}$), there is a relatively modest amount of fragmentation at large $a$. For $L = 3a_{ho}$ and small $N$, there is a relatively large amount of fragmentation for large $a$. The amount of fragmentation decreases with increasing $N$. Additionally, as in the squeezing plots, the amount of fragmentation present does not vary monotonically with $a$.

In Fig. 6 we plot the depletion parameter $D$ as a function of $a$ in the same way as we plotted $F$ vs. $a$ in Fig. 5. We see a modest increase in depletion of comparable size across all plots for large values of $a$.

In both the fragmentation and depletion plots, we indicate by vertical lines the values of $a$ below which the two-mode model should be sufficient to describe the physics of the system. As with the squeezing data, the models and the PIGS results agree well when this condition is satisfied but deviate as $a$ increases. This deviation takes the form of less fragmentation than predicted in the multimode models. In terms of depletion, we see less than in the eight-mode model but more than zero, which is all that is possible for the two-mode model. We also see roughly the same amount of depletion in the system regardless of $N$ and $L$.

The reduction in fragmentation can be accounted for via both of the mechanisms described in Section IV A. Fragmentation in the double well system increases the more “isolated” the wells are, that is, the less likely it is for a particle to tunnel from one well to the other. This is the reason why potentials with larger $L$ experience more fragmentation. The first mechanism entails the occupation of modes with higher values of $n$, some of which have more spillover into the “wrong” side of the double well than the $n = 1$ modes. Hence, the occupation of these modes will lessen the isolation of the wells by putting atoms in states that span both sides of the double well barrier. This will reduce fragmentation.

Additionally, we found that $F$ is large in the two-mode case when every other Fock state is occupied. This is only possible for small $L$. The second mechanism involves the presence of many two-body tunneling terms in the double well Hamiltonian due to the addition of modes beyond $n = 1$, and these terms prevent the system from forming a state that occupies every other Fock state. Hence, this effect causes a dramatic reduction in fragmentation.
Figure 4. (Color online) Monte Carlo results for the squeezing parameter $S$ vs. $Na$ (the product of the number of atoms and the scattering length) for three different potentials ($L = a_{ho}$, $2a_{ho}$, and $3a_{ho}$, from left to right). The plots include all of the PIGS results from Fig. 3.

Figure 5. (Color online) Monte Carlo results for the fragmentation parameter $F$ vs. scattering length $a$ for four different particle numbers ($N = 8$, $16$, $32$, and $64$, from top to bottom) and three different potentials ($L = a_{ho}$, $2a_{ho}$, and $3a_{ho}$, from left to right). The plots include results from the exact two-mode model, the eight-mode model, and the PIGS simulations. Vertical lines indicate the values of $a$ below which we expect the two-mode model to be valid.
Figure 6. (Color online) Monte Carlo results for the depletion parameter $D$ vs. scattering length $a$ for four different particle numbers ($N = 8, 16, 32$, and $64$, from top to bottom) and three different potentials ($L = a_{ho}$, $2a_{ho}$, and $3a_{ho}$, from left to right). The plots include results from the exact two-mode model, the eight-mode model, and the PIGS simulations. Vertical lines indicate the values of $a$ below which we expect the two-mode model to be valid. See [19] for details of the two- and eight-mode calculations.

V. CONCLUSION

In this work, we have made a detailed numerical study of the squeezing and fragmentation exhibited by the ground state of an ultracold, bosonic atomic gas in a three-dimensional double well trap for a variety of particle number, interaction strengths, and double well trap geometries using numerically exact quantum Monte Carlo methods to simulate the system. These results were compared with the predictions obtained for two- and eight-mode models of the same systems in [19].

The quantitative understanding of the double well system gained from this study allows for a more sophisticated qualitative picture of the way in which squeezing and fragmentation come about in this system than was previously possible. Recall that the suppression of number fluctuations corresponds to increased squeezing and the suppression of tunneling corresponds to increased fragmentation. Both the old and the new qualitative pic-
Figure 7. (Color online) Monte Carlo results for the dimensionless quantity $an^{1/3}$ vs. scattering length $a$ for four different particle numbers ($N = 8, 16, 32,$ and $64$) and three different potentials ($L = a_h$, $2a_h$, and $3a_h$, from left to right). The condition $an^{1/3} \ll 1$ specifies the condition under which depletion should be negligible in a homogeneous BEC. Notice that the relationship between $an^{1/3}$ and $a$ is essentially unaffected by changes in $N$ or $L$. 

Tones start the same way:

The ground state of the noninteracting double well is a product of the single-body ground state of each particle, and these single-body states each occupy both wells equally. Hence, if one were to measure the number of atoms in the left well minus the number in the right well, one could get any value from $N$ to $-N$. Therefore, number fluctuations are large and squeezing is small. An equivalent way to think of this situation is that the structure of the noninteracting ground state is such that tunneling is strong, and therefore fragmentation is small. In fact, both $S$ and $F$ are defined to be 0 in the noninteracting case.

In the old picture, the introduction of repulsive interactions proceeds like this:

The introduction of repulsive interactions causes the system to minimize its interacting energy by suppressing configurations in which many particles are in one well and few are on the other. This reduces number fluctuations and increases squeezing. Additionally, moving towards a configuration in which $N/2$ particles are locked into each side of the double well suppresses tunneling and increases fragmentation. These effects increase with increasing interacting strength.

Whereas in the new picture, it proceeds like this:

The introduction of repulsive interactions causes the system to minimize its interacting energy, but it can do this in several ways. One way is to suppress configurations in which many particles are in one well and few are on the other. This increases squeezing and fragmentation as in the old picture. Additionally, the system can also reduce its interaction energy by promoting atoms to modes in higher energy levels ($n > 1$). One can approximate these modes as each being localized in one of the two wells, although they will extend into the "wrong" well based on the strength of the double well barrier. There are some modes in each energy band $n > 1$ that extend into the wrong well much further than the $n = 1$ modes. Hence, a ground state dominated by modes with larger values of $n$ naturally have larger number fluctuations and tunneling than ground states dominated by $n = 1$ modes, and therefore they exhibit less squeezing and fragmentation. These two effects compete with each other to determine the overall amount of squeezing and fragmentation, which is not monotonic in many cases.

Thus, for sufficiently large values of $a$, one cannot appeal to either mean-field or multi-mode modes to correctly predict the amount of squeezing and fragmentation exhibited by the system. Instead, one must deploy the full machinery of a numerically-exact method like quantum Monte Carlo, which allows for full three-dimensional calculations without restriction to a truncated basis set representation.

Finally, we would like to connect back with one of the main motivations of this project discussed in the introduction, namely the application of squeezed states to reduce the measurement uncertainty of atom interferometers. In general, the more squeezed the states used in the interferometers, the smaller the uncertainty. One way to generate a highly squeezed state is to use a Feshbach resonance to tune the interaction strength of the atoms in a BEC, thereby changing the amount of squeezing exhibit-
ited by the system. However, what interaction strength is the one that maximizes squeezing? In the context of the old qualitative picture described above, the answer is simple: stronger repulsive interactions mean more squeezing, so one should tune $a$ to as large a value as one can. However, we have shown that the real picture is far more complicated: squeezing does not increase monotonically with interaction strength in many situations, and there is often some optimal value of $a$ that maximizes squeezing that one cannot predict through the use of multimode models but must instead calculate using an exact method like PIGS. With the increasingly rapid advances of experimental methods for the study Bose-Einstein condensates, we look forward to laboratory confirmation of the results of this study in the near future.

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