Bose-Einstein condensates in $^{85}$Rb gases at higher densities

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The Bose-Einstein condensation in trapped gases of $^{85}$Rb at densities beyond the dilute regime can now be realized taking advantage of Feshbach resonances. The gas density may be characterized by the parameter $n a^3$, where $n=N/V$ is the number density and $a$ is the scattering length which is tuned using Feshbach resonance. We explore the properties of interacting trapped bosons in the density range $5 \times 10^{-3} \leq n a^3 \leq 5 \times 10^{-2}$ using Monte Carlo methods to compare with experiments. We find that there is a significant depletion of the condensate at $T=0$ K, for example, $25\%$ at $n a^3=10^{-2}$. The condensate is not concentrated at the center of the trap but is spread out over four or five trap lengths. The condensate density distributions and the total density distributions within the trap are similar and the condensate fraction is $100\%$ at the edges of the trap.

I. INTRODUCTION

The observation of the Bose Einstein condensation (BEC) in dilute gases confined in magnetic traps [1–5] has opened an exciting new field of physics. To date, chiefly dilute gases, in which almost $100\%$ of the atoms can be in the condensate have been explored. In this case, a description of the condensate alone provides an excellent description of the whole gas. The Gross-Pitaevskii (GP) theory, a mean-field theory, of this condensate has been enormously successful in describing the extraordinary properties of the condensate [6]. The GP theory is successful because short-range correlations between the bosons induced by the interatomic potential are relatively unimportant. The strength of the interatomic interactions can be characterized by the atomic, $s$-wave scattering length $a$. The importance of the interactions is determined by the parameter $n a^3=N a^3/V$, the ratio of the volume of the atoms ($Na^3$) to that occupied by the gas ($V$). In the dilute limit, $n a^3 \leq 10^{-5}$.

Denser Bose gases are now being explored [7–10]. For example, the scattering length of $^{85}$Rb can be increased using Feshbach resonances so that densities in the range $na^3 \approx 10^{-2}$ are reached. In this density region, the interatomic interaction will deplete the condensate and new phenomena involving the interplay between atoms in the condensate and those above the condensate will emerge. The sign of the scattering length can also be changed, from positive to negative values, leading to collapse of the condensate and ejection of atoms from the condensate. Bose condensates of He$^4$, $^4$He in an excited electronic state, have been created, for which $a$ is large and not independently known but is inferred from the density distribution of the condensate itself.

In this context, our goal is to explore the general properties of Bose gases at higher densities, $5 \times 10^{-3} \leq n a^3 \leq 5 \times 10^{-2}$. What is the condensate fraction and how much of the condensate is depleted by interaction as a function of $n a^3$? Where is the condensate in the trap and how does this change with $n a^3$? What is the total density distribution $n(r)$ of atoms in the trap compared to the condensate distribution $n_0(r)$? And how well does the Gross-Pitaevskii equation for the condensate describe the Bose gas properties at higher densities? Particularly, our goal is to reveal the important role that the atoms above the condensate play in determining the location of the condensate in the trap.

We consider hard spheres in a spherical, harmonic trap at $T=0$ K using Monte Carlo (MC) methods, where no assumption of weak interaction is made. At $n a^3 \approx 10^{-2}$, we find $\approx 25\%$ of the condensate is depleted, that the condensate and total density distributions in the trap are similar and are not well described by a Thomas-Fermi (TF) approximation to the GP equation. The total energy, which includes atoms above the condensate lies 20–35% above the condensate energy.

II. METHOD

The Hamiltonian for $N$ trapped, interacting particles is

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N} V_{\text{trap}}(r_i) + \sum_{i<j}^{N} V_{\text{int}}(|r_i-r_j|),$$

where $V_{\text{trap}}(r_i)=\frac{1}{2}m\omega_{ho}^2r_i^2$ is the spherically symmetric trap potential and $r_i$ is the position vector of particle $i$, $m$ is the mass of a $^{85}$Rb atom, and $\omega_{ho}$ is the trap frequency. The pair interaction $V_{\text{int}}(|r_i-r_j|)$ is represented by a hard-core (HC) potential of diameter $a$. The scattering length of two particles interacting in the low-energy, long-wavelength limit via a hard-core potential is purely $s$-wave with scattering length $a$. Similarly, the scattering length of two particles interacting in this limit via a contact potential $V(r) = (4\pi\hbar^2/ma)\delta(r)$ is also purely $s$-wave with scattering length $a$. For this reason, MC results using a hard-core potential may be compared directly with GP theory that uses a contact potential in the low-energy limit.

We use chiefly variational Monte Carlo (VMC) techniques, which treat the gas exactly within the limits of a trial variational wave function. We also use diffusion Monte Carlo (DMC) [11] to check the dependence of the VMC technique on the variational wave function.

The trial variational wave function we use is

$$\psi_{T}(r_1, \ldots, r_N; \alpha) = \prod_i \phi(r_i)\Pi_{i<j} \delta(\alpha \cdot |r_i-r_j|),$$

where $\phi(r) = e^{-a r^2}$ is a Gaussian with one variational parameter $\alpha$ and
The density was tuned by adjusting the HC diameter \( a \) from 35 to 70 times \( a_{Rb} \), where \( a_{Rb} = 4.333 \times 10^{-3} a_{ho} \). We express lengths in units of the trap length \( a_{ho} = (\hbar m \omega_{ho})^{1/2} \), the density distribution as \( n(r)a_{ho}^3 \) and energies \( E \) in units of \( \hbar \omega_{ho} \).

We define and calculate the condensate fraction from the one-body density matrix (OBDM) \( \rho(\mathbf{r}, \mathbf{r'}) = \langle \psi(\mathbf{r'}) \psi(\mathbf{r}) \rangle \). The \( \rho(\mathbf{r}, \mathbf{r'}) \) is calculated using \( |\psi(i)|^2 \) as discussed in Ref. [12] and the natural orbitals (NO) [13], \( \phi_i(\mathbf{r}) \) and their occupation \( N_i \), are obtained by diagonalizing the OBDM using \( \int d^2 r \psi_i^*(\mathbf{r}) \rho(\mathbf{r}, \mathbf{r'}) \psi_j(\mathbf{r'}) = N_i \delta_{ij} \). The NO with the highest occupation number corresponds to the condensate orbital \( \phi_0(\mathbf{r}) \), and \( N_0 \) is the number of atoms in the condensate.

### III. RESULTS

Figure 1 shows the calculated density distributions: the VMC total density \( n(r)a_{ho}^3 \), the VMC condensate density \( n_0(r) = N_0 |\phi_0(r)|^2 a_{ho}^3 \), and the TF \( n_{TF}(r)a_{ho}^3 \), for two HC diameters \( a = 35a_{Rb} \) and \( 70a_{Rb} \), and for \( N = 128 \) and \( N = 1000 \). The equation for \( n_{TF}(r) \) can be found in the excellent review of Dalfovo et al. [6]. The VMC \( n(r) \) is considerably flatter than \( n_{TF}(r) \) and does not have the TF parabolic shape. Further, the VMC \( n(r) \) is broader than \( n_{TF}(r) \). The condensate is not concentrated at the center of the trap, but rather is spread out to 4–6 trap lengths. Qualitatively, the VMC \( n(r) \) and \( n_0(r) \) are similar in shape. Quantitatively \( n(r) \) is larger than \( n_0(r) \) in the bulk of the system, except near the edges of the trap, where the condensate fraction approaches 100%. The radius of the condensate depends on \( N \) and increases with it.

To investigate how well the approximate TF density could be adjusted to fit the VMC density \( n(r) \), we treated the HC diameter in \( n_{TF}(r) \) as a fitting parameter. Figure 2 shows the best fit of \( n_{TF}(r) \) to \( n(r) \) with \( a_{TF} \) in \( n_{TF}(r) \) adjusted. The best fit itself is not very good and the value of \( a_{TF} \) needed in \( n_{TF}(r) \) to get this fit is 2–4 times larger than the actual HC diameter in \( n(r) \). A larger \( a_{TF} \) is needed in \( n_{TF}(r) \) because \( n(r) \) is broader than \( n_{TF}(r) \) for a given \( a \) (see Fig. 1). This means that values of \( a \) determined from the observed density distribution by fitting \( n_{TF}(r) \) to it will be overestimated. Also, the shape of \( n(r) \) is more like that found in liquid \(^4\)He droplets than that found in dilute gases in traps.

Figure 3 shows comparisons between the VMC and DMC total densities \( n(r)a_{ho}^3 \). Our goal is to check the dependence of the VMC density on the trial wave function.

The VMC and DMC \( n(r) \) have the same shape for \( r > 2.5 \) but for \( r \leq 2.5 \), the DMC \( n(r) \) is larger than the VMC \( n(r) \). Essentially, we have found that the pair Jastrow function \( f(a,r) \) in Eq. (2) does not go rapidly enough to unity. This keeps pairs of particles from getting closer together. As a result, the VMC density is somewhat low at the center of the trap since getting a high density requires getting the bosons close together. The DMC and VMC densities are qualitatively the same.

Table I summarizes our results numerically. From left to right, we list the input HC diameter \( a \), the density at the center of the trap \( n(r=0)a_{ho}^3 \), \( n_a^2 = Na^3/V \), the VMC energy per particle \( E_{VMC}/N \), the TF condensate energy per particle \( E_{TF}/N \), the fractional difference \( \Delta E/E_{TF} \), where

\[
f(a,r) = \begin{cases} \frac{1 - \frac{a}{r}}{a}, & r > a \\ 0, & r \leq a \end{cases}
\]
N out Fermi result for the density throughout a spherical trap of the trap, \( n/\text{boson} \), E VMC E TF, we see that the energy and depletion increases with the in-

N out in Table I, gives a good indication of \( D_{a} \) to the actual VMC diameter, \( a_{TF} \) as adapted to a spherical trap [12]. There is some apparent dependence of \( N_{out}/N \) and \( \Delta E/N \) on \( N \), the total number of atoms in the trap, as well as on \( na^{3} \). When \( N \) is larger (e.g., \( N = 1000 \)), the density distribution is flatter (see Fig. 1). Thus, the larger density at the center covers a larger fraction of the trap. This increases both \( N_{out}/N \) and \( \Delta E/N \). The condensate energy also increases with \( N \) because the gas expands to higher potential regions at larger \( N \).

IV. DISCUSSION AND SUMMARY

Fabrocini and Polls [17] used a local-density approximation (LDA) to calculate the total density in traps and investigate the accuracy of the GP equation. Our VMC and DMC density distributions, as shown in Figs. 1–3, are flatter than their total LDA density distributions. A direct comparison is not possible because Fabrocini and Polls calculate a somewhat different density in a nonspherical trap.

Dalfovo and Stringari [18] have proposed that the density distribution of bosons in traps is parabolic because of the confining potential. In contrast, the distribution is flat in the center of self-bound systems such as liquid \(^4\)He droplets [19]. We find that the distribution of HC bosons in traps at higher densities is also quite flat as in \(^4\)He droplets (see Fig. 2). The density distribution appears to depend more on the density of the bosons than on whether they are confined in a trap or bound by attractive interactions as in the \(^4\)He droplet case. At higher densities than those considered here, the distribution also develops peaks and valleys related to correlations induced by the HC [12].

Cornish et al. [5] have extracted the scattering lengths of \(^85\)Rb atoms in a Feshbach resonance by fitting a Thomas-Fermi model width to their observed \(^85\)Rb distributions. We find that this procedure overestimates the scattering length by a factor of 3 or 4 in the current-density range (see the ratios of \( a_{TF}/a \) in Table I). Subsequently, Roberts et al. [8] determined the scattering lengths independently.

To summarize, the present Monte Carlo results show that be well described by the energy associated with the atoms above the condensate given by the Lee, Huang, and Yang expression [15], both in the bulk [16] and as adapted to a spherical trap [12]. There is some apparent dependence of \( N_{out}/N \) and \( \Delta E/N \) on \( N \), the total number of atoms in the trap, as well as on \( na^{3} \). When \( N \) is larger (e.g., \( N = 1000 \)), the density distribution is flatter (see Fig. 1). Thus, the larger density at the center covers a larger fraction of the trap. This increases both \( N_{out}/N \) and \( \Delta E/N \). The condensate energy also increases with \( N \) because the gas expands to higher potential regions at larger \( N \).
there is substantial depletion of the condensate at higher densities, for example, 40% at \( na^3 = 5 \times 10^{-2} \). The atoms above the condensate play a critical role in determining the condensate density \( n_0(r) \) in the trap. The condensate is not at the center but is spread out in the trap and the condensate fraction is 100% at the edges of the trap. The condensate fraction is 100% at the edges of the trap because the condensate "seeks" the lower-density regions at the edges of the trap. The condensate and total densities have similar shapes within the trap, they are "flat" (nearly) in the center of the trap as in liquid \(^4\)He droplets and not parabolic as predicted by Gross-Pitaevskii theory. The total energy lies above the condensate (Gross-Pitaevskii) energy. This difference is remarkably well described by the energy attributed to atoms above the condensate within the Lee-Yang-Huang perturbation expression [12]. The condensate fraction is reasonably well predicted by the Bogoliubov perturbation expression. Currently, interesting investigations on the growth and collapse of a BEC with changing interactions are in progress [10,20]. In future work, we plan to explore Bose systems with both attractive and repulsive interactions.

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