

Ground-State Properties of Magnetically Trapped Bose-Condensed Rubidium Gas

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In light of the recent experimental observation of Bose-Einstein condensation in dilute ⁸⁷Rb gas cooled to nanokelvin-scale temperatures, we give a quantitative account of the ground-state properties of magnetically trapped Bose gases. Using simple scaling arguments, we show that at large particle number the kinetic energy is a small perturbation, and find a spatial structure of the cloud of atoms and its momentum distribution dependent in an essential way on particle interactions. We also estimate the superfluid coherence length and the critical angular velocity at which vortex lines become energetically favorable.

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In a remarkable experiment, Anderson *et al.* [1] have cooled magnetically trapped ⁸⁷Rb gas to nanokelvin-range temperatures, and observed a rapid narrowing of the velocity distribution and density profile, which is interpreted as the onset of Bose-Einstein condensation. Trapped atom clouds are new systems, beyond liquid ⁴He [2] and excitons in semiconductors [3], in which particles obeying Bose-Einstein statistics condense at low temperatures [4,5]; indeed, the condensation of trapped atoms has been a "Holy Grail" of atomic physics [6]. In this paper we give simple quantitative arguments, taking into account the effects of the repulsive interatomic interactions, to determine the properties of the quantum ground state of the trapped ⁸⁷Rb system, including its geometry, momentum distribution, coherence length, and critical angular velocity for vortex formation. Our aim here is to provide a general framework for discussing phenomena, rather than to explain in detail particular experimental results. We defer consideration of the dynamics of the system to later publications.

In such an experiment, the gas is magnetically trapped in an effective three-dimensional harmonic well (TOP trap) cylindrically symmetric about the z axis, with tunable angular frequencies ω_z^0 in the axial (z) direction and $\omega_\perp^0 = \omega_z^0/\sqrt{8}$ in the transverse (x - y) plane. The oscillators are characterized by lengths $a_\perp = (\hbar/m\omega_\perp^0)^{1/2}$ and $a_z = (\hbar/m\omega_z^0)^{1/2}$, where m is the atomic mass. In the "strong trap," $\omega_z^0/2\pi = 211$ Hz nominally and $a_\perp \approx 1.25 \times 10^{-4}$ cm, while in the "weak trap," $\omega_z^0/2\pi = 23$ Hz and $a_\perp \approx 3.8 \times 10^{-4}$ cm. During condensation the distribution rapidly sharpens with falling temperature, as a macroscopic number of the Rb atoms begins to occupy the lowest mode of the well. In the absence of interparticle interactions the lowest single-particle state has the familiar wave function

$$\phi_0(\vec{r}) = \frac{1}{\pi^{3/4} a_\perp a_z^{1/2}} e^{-m(\omega_\perp^0 r_\perp^2 + \omega_z^0 z^2)/2\hbar}, \quad (1)$$

where \vec{r}_\perp is the component of \vec{r} in the x - y plane; the density distribution at zero temperature, $\rho_0(\vec{r}) =$

$N\phi_0(\vec{r})^2$, is Gaussian, with central density $\rho_0(0) = 1.57 \times 10^{11} N[(\omega_z^0/2\pi)/(211 \text{ Hz})]^{3/2} \text{ cm}^{-3}$. However, interatomic interactions strongly modify the particle structure in the well.

The low-energy interactions between polarized ⁸⁷Rb atoms are repulsive, and are described by an s -wave triplet-spin scattering length, a , determined to be in the range $99a_0 < a < 119a_0$, where a_0 is the Bohr radius [7]. (In numerical estimates we take $a = 100a_0$, unless otherwise stated.) In the limit in which the density varies slowly on a scale a , the interaction energy of the gas per unit volume is given by $E_{\text{int}} = (2\pi\hbar^2 a/m)|\rho(\vec{r})|^2$. The repulsive interactions favor a reduction of the density from the free particle situation. As the number of particles increases, the first effect of interactions is to cause the cloud of particles to expand in the transverse direction, where the restoring forces are weaker. With further increase in the number, the cloud expands in the z direction. The eventual size of the cloud is determined, in the limit in which the interparticle interactions dominate, by a balance between the harmonic oscillator and interaction energies.

To see the physics of this balance, let us neglect the anisotropy of the oscillator potential and assume that the cloud occupies a region of radius $\sim R$, so that $\rho \sim N/R^3$; then the scale of the harmonic oscillator energy per particle is $\sim m\omega_\perp^2 R^2/2$, while each particle experiences an interaction energy with the other particles $\sim (4\pi\hbar^2 a/m)N/R^3$. The characteristic length scale is thus $\sim a_\perp \zeta$, where the dimensionless parameter characterizing the system is

$$\zeta \equiv (8\pi Na/a_\perp)^{1/5} \approx 4.21[(a/100a_0)(N/10^4)(10^{-4} \text{ cm})/a_\perp]^{1/5}; \quad (2)$$

under the conditions of the experimental trap with large N , $\zeta \gg 1$. The kinetic energy per particle, on the other hand, is of order $\hbar^2/2mR^2$, so that the ratio of the kinetic to interaction or oscillator energies is of order $\zeta^{-4} \sim N^{-4/5}$.

To estimate the interaction effects more quantitatively we examine the ground state of the system in terms of its order parameter $\psi(\vec{r})$, where $\int d^3r |\psi(\vec{r})|^2 = N$. (We do not distinguish N and N_0 , the number of particles in the condensate, in the weakly interacting system at zero temperature.) In the Hartree approximation, in which $\psi(\vec{r})/N^{1/2}$ is the lowest single particle mode, the ground state energy of the system is given by a Ginzburg-Pitaevskii-Gross energy functional [8],

$$E(\psi) = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla\psi(\vec{r})|^2 + \frac{m}{2} [(\omega_\perp^0)^2 r_\perp^2 + (\omega_z^0)^2 z^2] |\psi(\vec{r})|^2 + \frac{2\pi\hbar^2 a}{m} |\psi(\vec{r})|^4 \right]. \quad (3)$$

This approach is familiar in prior studies of Bose-condensed polarized atomic hydrogen [9,10]; see also Refs. [11–13]. The Rb experiments with lower density, larger atomic mass, and stronger interactions fall, however, in a rather different parameter range.

For a first solution we take ψ in the form of the ground-state wave function, Eq. (1):

$$\psi(\vec{r}) = N^{1/2} \omega_\perp^{1/2} \omega_z^{1/4} \left(\frac{m}{\pi\hbar} \right)^{3/4} e^{-m(\omega_\perp r_\perp^2 + \omega_z z^2)/2\hbar}, \quad (4)$$

with effective frequencies, ω_\perp and ω_z , treated as variational parameters. Substitution of (4) into (3) yields the ground state energy

$$E(\omega_\perp, \omega_z) = N\hbar \left(\frac{\omega_\perp}{2} + \frac{(\omega_\perp^0)^2}{2\omega_\perp} + \frac{\omega_z}{4} + \frac{(\omega_z^0)^2}{4\omega_z} + \frac{Nam^{1/2}}{(2\pi\hbar)^{1/2}} \omega_\perp \omega_z^{1/2} \right); \quad (5)$$

minimizing E with respect to ω_\perp we derive $\omega_\perp = \omega_\perp^0/\Delta$, where

$$\Delta = \left(1 + \frac{\zeta^5}{(32\pi^3)^{1/2}} \left(\frac{\omega_z}{\omega_\perp^0} \right)^{1/2} \right)^{1/2}. \quad (6)$$

Interactions, by reducing the effective transverse oscillator frequency by Δ , spread out the distribution in the transverse direction by a factor $\Delta^{1/2}$; when N is sufficiently large that $\zeta \gg 1$, $\Delta^{1/2} \approx 2.55[(N/10^4)(a/100a_0)(10^{-4} \text{ cm})/a_\perp]^{1/4} (\omega_z/\omega_\perp^0)^{1/8}$.

Spreading in the z direction begins to become significant when the interaction energy per particle becomes comparable with $\hbar\omega_z^0$; using (6) and minimizing the resultant ground state energy, $E(\omega_z) = N\hbar[\omega_\perp^0/\Delta + \omega_z/4 + (\omega_z^0)^2/4\omega_z]$, with respect to ω_z , we see that this condition is $Na/a_\perp \gtrsim (\omega_z^0/\omega_\perp^0)^{1/2}$, which is realized under the experimental conditions. Solving for the minimum numerically we find, representatively, that in the strong (or weak) trap for $N = 10^4$, $\omega_z/\omega_z^0 = 0.40$ (0.55), and $\omega_\perp/\omega_\perp^0 = 0.16$ (0.26), while for $N = 900$, $\omega_z/\omega_z^0 = 0.72$ (0.84), and $\omega_\perp/\omega_\perp^0 = 0.43$ (0.63). In the limit $\zeta \gg 1$, the kinetic energy terms in (5) are negligible, and the shifts in the frequency are given by $\omega_z/\omega_z^0 = \lambda\omega_\perp/\omega_\perp^0 = 2(\pi\lambda)^{3/5}/\zeta^2$, where $\lambda \equiv \omega_z^0/\omega_\perp^0$. The leading contribu-

tion to the energy per particle is

$$\frac{E}{N} = \frac{5\zeta^2}{8\pi^{3/5}} \lambda^{2/5} \hbar\omega_\perp^0 \propto N^{2/5}. \quad (7)$$

To obtain the ground-state wave function more precisely, we minimize the total energy (3) with respect to ψ , keeping the total number of particles fixed, and thus derive the nonlinear Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m(\omega_\perp^0)^2 (r_\perp^2 + \lambda^2 z^2) + \frac{4\pi\hbar^2 a}{m} |\psi(\vec{r})|^2 \right] \psi(\vec{r}) = \mu\psi(\vec{r}), \quad (8)$$

where μ is the chemical potential. The physical scales are conveniently brought out by rescaling the lengths, letting $\vec{r} = a_\perp \zeta \vec{r}_1$, and writing $\psi(\vec{r}) = (N/\zeta^3 a_\perp^3)^{1/2} f(\vec{r}_1)$, where $\int d^3r_1 |f|^2 = 1$; then (8) becomes the dimensionless equation

$$\left[-\frac{1}{\zeta^4} \nabla_1^2 + r_{1\perp}^2 + \lambda^2 z_1^2 + |f(\vec{r}_1)|^2 \right] f(\vec{r}_1) = \nu^2 f(\vec{r}_1), \quad (9)$$

where $\nu^2 \equiv 2\mu/\zeta^2 \hbar\omega_\perp^0$.

In the limit of large N , we can obtain an essentially exact expression for the ground-state wave function, corresponding to the Thomas-Fermi approximation, by neglecting the kinetic energy term, which falls as ζ^{-4} ; then

$$f(\vec{r}_1)^2 = \nu^2 - r_{1\perp}^2 - (\lambda z_1)^2 \quad (10)$$

in the region where the right side is positive, and $f = 0$ outside this region. This form for the wave function is good, except where the density is small, in which case the kinetic energy causes the wave function to vanish smoothly [14]. The normalization condition on f implies that $\nu = (15\lambda/8\pi)^{1/5} = 1.11$, which translates into the relation between μ and N ,

$$\mu = \frac{\hbar\omega_\perp^0}{2} (\nu\zeta)^2 = \frac{\hbar\omega_\perp^0}{2} \left(\frac{15\lambda Na}{a_\perp} \right)^{2/5}. \quad (11)$$

Since $\mu = dE/dN$, the energy per particle is simply $E/N = (5/7)\mu$, a result smaller than the effective oscillator frequency calculation (7) by a factor $(3600\pi)^{1/5}/7 \approx 0.92$. The central density of the blob is $\rho(0) = m\mu/4\pi\hbar^2 a = \nu^2 N/(a_\perp \zeta)^3 = (4.08/\zeta^3) \rho_0(0) \approx (9.7 \times 10^{13} \text{ cm}) (N/10^4)^{2/5} [(\omega_z^0/2\pi)/(211 \text{ Hz})]^{6/5}$. Inclusion of kinetic energy corrections spreads the distribution and decreases the central density [14].

In the limit of large N , the transverse radius of the cloud is given by $R/a_\perp = \nu\zeta$, and the half height in the z direction is $Z = R/\lambda$. In the strong (weak) trap, for $N = 10000$, $R/a_\perp \approx 4.5$ (3.6), while for $N = 900$, $R/a_\perp \approx 2.8$ (2.2). For large N the aspect ratio R/Z equals λ , whereas in the absence of interactions it is $\lambda^{1/2}$; thus for the experimental conditions, one would expect the aspect ratio to be $\sqrt{8}$.

The momentum distribution of particles in the trap is given by $f(\vec{p}) = |\int d^3r e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi(\vec{r})|^2$, where \vec{p} is the particle momentum. For the Thomas-Fermi wave function, $f(\vec{p}) \sim |J_2(\kappa)/\kappa^2|^2$, where J_2 is the Bessel function of order 2, $\kappa^2 = (\nu\zeta\hbar a_\perp)^2 [p_\perp^2 + (p_z/\lambda)^2]$. When $Na/a_\perp \gg 1$, the width of the momentum distribution is $\sim 1/\nu\zeta$ times that for a single particle in the oscillator potential, while the axial/transverse aspect ratio of the momentum distribution is larger by a factor $\lambda^{1/2}$ than the free particle distribution. For the Thomas-Fermi wave function, the rms velocity diverges because of the square-root behavior at the outer edge. If one improves the wave function by allowing for the rounding at the outer edge [14], one finds to logarithmic accuracy that $\langle p^2 \rangle \approx 5(\hbar/R)^2 \ln \zeta$, of order $(\ln \zeta)/\zeta^2$ compared with $\langle p^2 \rangle$ in the noninteracting system.

The asymptotic result for the mean square velocity given above becomes quantitatively accurate only for very large N . Consequently, it is useful to consider the effective oscillator trial wave function, (4), which leads to a Gaussian momentum distribution, $f(\vec{p}) \sim e^{-[p_\perp^2/\omega_\perp + p_z^2/\omega_z]/m\hbar}$, with $\langle p^2 \rangle = m\hbar(\omega_z + 2\omega_\perp)/2$. The values of ω_z and ω_\perp computed above for the strong trap with $N = 10^4$ (or 900) imply an rms velocity $v_{\text{rms}} \approx 0.49$ (0.70) mm/sec, and an axial/transverse aspect ratio is a factor ≈ 2.5 (1.7) larger than the free particle case. In the weak trap with $N = 10^4$ (or 900), $v_{\text{rms}} \approx 0.19$ (0.26) mm/sec, and the aspect ratio is a factor ≈ 2.1 (1.3) larger than for free particles.

The estimates of mean square velocities and aspect ratios are comparable to those deduced experimentally from measurements made when the cloud is released from the TOP trap [1]. However to compare quantitatively with experiment it is necessary to take into account the fact that the mutual repulsion between particles accelerates them as they leave the trap [15]. From energy conservation the observed kinetic energy is given by $\langle p^2/2m \rangle_{\text{obs}} = \langle p^2/2m \rangle + E_{\text{int}}$, where the quantities on the right refer to matter in the equilibrium in the trap; note that since the oscillator is switched off rapidly, the oscillator energy does not enter this conservation law. Evaluating the initial energy from the Thomas-Fermi wave function, we find an rms final velocity $v_{\text{rms}} = (2/7)^{1/2} \zeta \nu \hbar / ma_\perp$, which for 900 particles released from the weak trap is ≈ 0.23 mm/sec, consistent with the 0.5 mm/sec quoted in Ref. [1]. We note that in making the theoretical estimate we have neglected the zero-point energy, which while negligible for large N , will make a significant contribution for such a small number of atoms.

The sound velocity, c_s , in the interior of the cloud is given by $c_s^2 = (\rho/m)\partial\mu/\partial\rho = \mu/m$, which in the large N limit equals $(\hbar\omega_\perp^0/2m)(\nu\zeta)^2$. In this limit, the lowest mode of excitation in the transverse direction of the system has frequency of order $c_s/R \sim \omega_\perp^0$.

The superfluid coherence length [8,16] ξ , which determines the distance over which the condensate wave func-

tion can heal, can be estimated by equating the kinetic energy term in Eq. (8), $\sim \hbar^2/2m\xi^2$, to the interaction energy which yields

$$\xi^2 = (8\pi\rho a)^{-1}, \quad (12)$$

where ρ is the local density. With the central density of the cloud computed in the Thomas-Fermi approximation, $\rho(0) = m\mu/4\pi\hbar^2 a$, we have $\xi = a_\perp/\nu\zeta$, and so

$$\frac{\xi}{R} = \left(\frac{a_\perp}{R}\right)^2 = \frac{1}{(\nu\zeta)^2}. \quad (13)$$

Thus when the number of particles is sufficiently large that the Thomas-Fermi approximation is valid, the coherence length is small compared with the size of the blob, and the system should exhibit superfluid properties more like those of a bulk superfluid than an atomic nucleus, where $\xi \gg R$.

An experimentally important confirmation of Bose-Einstein condensation would be the observation of formation of a vortex line in a rotating system. The critical angular frequency Ω_{c1} , at which it becomes energetically favorable for a vortex line to be created under rotation about the z axis [16], is

$$\Omega_{c1} \sim \frac{\hbar}{mR^2} \ln(R/\xi). \quad (14)$$

For cloud radii $\sim 5 \times 10^{-4}$ cm, this value corresponds to a rotation frequency of order 10 Hz.

Finally, we consider the case of atoms, such as spin-polarized ^{85}Rb [7] or ^7Li [11] with a negative scattering length, corresponding to a low energy attractive interaction. A uniform state of such atoms at low density would be unstable to formation of long-wavelength density waves, signaling a gas-liquid phase transition. However, as discussed theoretically in [12,13], and seen experimentally in [5], the physics in a trap is different; this can be understood in the present context by considering the variational calculation above. With increasing N , the spatial extent of the wave function is reduced. Provided $\Delta^2 = 1 - (2/\pi)^{1/2}(N|a|/a_\perp)(\omega_z/\omega_\perp^0)^{1/2}$ [cf. (6)] remains positive, the kinetic energy term is able to stabilize the system. However, if Δ^2 becomes negative, the attractive forces overwhelm the kinetic energy, and the cloud becomes unstable to collapse. The critical number of particles for collapse is $\sim (\pi/2\lambda)^{1/2} a_\perp/|a|$. In ^{85}Rb , for which $-1000a_0 < a < -120a_0$ [7], under the experimental conditions in Ref. [1] with $\omega_z^0/2\pi = 211$ Hz, this number is $\sim 20 - 150$; in the ^7Li trap of Ref. [11] it is ~ 3000 . The final state of the collapsed cloud is determined by the shorter-range repulsive components of the interatomic potential.

To summarize, our calculations provide quantitative results that confirm and extend the qualitative considerations in Ref. [1] on the effect of particle interactions on the properties of a cloud of bosons. Experimental confirmation of the dependence on trap parameters, particle

number and atomic properties of the size of the cloud, and the momentum distribution would give one increased confidence in the interpretation of the data.

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