Bose-Einstein Condensation in a Dilute Gas: Measurement of Energy and Ground-State Occupation

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We measure the ground-state occupation and energy of a dilute Bose gas of ^{87}Rb atoms as a function of temperature. The ground-state fraction shows good agreement with the predictions for an ideal Bose gas in a 3D harmonic potential. The measured transition temperature is $0.94(5)T_o$, where T_o is the value for a noninteracting gas in the thermodynamic limit. We determine the energy from a model-independent analysis of the velocity distribution, after ballistic expansion, of the atom cloud. We observe a distinct change in slope of the energy-temperature curve near the transition, which indicates a sharp feature in the specific heat. [S0031-9007(96)01891-1]

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The ability to create Bose-Einstein condensation (BEC) in magnetically trapped alkali gases [1–4] provides an opportunity to experimentally study the thermodynamics of bosonic systems in which the interactions are (i) weak, (ii) binary, and (iii) experimentally adjustable [5–7]. One goal of experimental and theoretical work in this field is to understand a variety of low-temperature phenomena from both macroscopic and microscopic points of view, with a quantitative reconciliation of these two approaches. The recent experimental studies of collective excitations of zero-temperature condensates [5,8] were a step in this direction. The purpose of the present effort is to explore the nature of the BEC phase transition by performing quantitative measurements of BEC in a different regime—near the critical temperature.

In this paper we analyze a series of images of ultracold clouds of rubidium gas to determine the critical temperature and to extract ground-state occupation and mean energy as a function of temperature. Mean energy (or its derivative, specific heat) has a certain historical significance because it was London's comparison [9] of the specific heats of liquid helium and an ideal Bose gas that began the rehabilitation of BEC as a useful physical concept. Moreover, measurements of thermodynamic quantities such as specific heat are essential in studying any phase transition. Ground-state occupation and critical temperature of a Bose gas are interesting because in liquid helium the former is very difficult to measure, while the latter is almost impossible to calculate accurately.

The apparatus and procedures we use for creating an ultracold Bose gas and BEC are described elsewhere [1,10,11]. In summary, we optically trap [12] and precool [13] ^{87}Rb atoms, then load [14] them into a purely magnetic trap. We use a time-averaged orbiting potential (TOP) trap consisting of a static quadrupole field plus a small rotating transverse bias field [11]. The effective potential is axially symmetric and harmonic, with a ratio of axial to radial trapping frequencies of $\sqrt{8}$. We further cool the atoms in the TOP trap with forced evaporation [15] by applying a radio frequency (rf) magnetic field which induces Zeeman transitions of the most energetic atoms to untrapped spin states [16]. By ramping down the frequency of the rf field we control the cloud temperature. The final stages of evaporative cooling are performed in a $\nu_z = 373$ Hz trap.

We observe the atom cloud, after a period of free expansion, with resonant absorption imaging [5]. The confining TOP potential is turned off suddenly, and the cloud of atoms is allowed to expand freely for 10 ms. The cloud is then probed by a 26 μs pulse of light resonant with the $5S_{1/2}$, $F = 2$ to $5P_{3/2}$, $F = 3$ transition. The atoms scatter photons, impressing a shadow onto the probe beam. The shadow is imaged onto a CCD array, and the data are digitally processed to extract the optical depth of the cloud at each point. After point-by-point corrections for imperfect polarization and saturation effects, the result is a 2D projection of the velocity distribution in the expanded cloud.

These distributions contain a wealth of thermodynamic information. For instance, the integrated area under the distribution is proportional to the total number N of atoms in the sample. The condensate appears as a narrow feature centered on zero velocity [1]; the number of atoms in the ground state, N_o, is then proportional to the integrated area under this feature. From the mean square radius of the expanded cloud and the expansion time, we get the mean square velocity, or average energy, of the cloud. Finally, as discussed below, the temperature T is extracted from the images, even though the temperature is not merely proportional to mean energy in a degenerate Bose cloud.

We have gone to some lengths to extract these thermodynamic quantities in a model-independent way. For instance, if we were to fit the observed velocity distributions to a Bose-Einstein distribution, we could hardly avoid coming to the conclusion that the specific heat is discontinuous—the singular behavior is built-in to the assumed functional form. Moreover, such a fit would preclude our being able to observe effects due to interactions, finite N, critical fluctuations, etc. Fortunately, useful thermodynamic information about the sample can be extracted from direct calculation of various moments of the velocity distribution, without specific reference to the nature of the distribution. The total number and energy of the atoms, as mentioned above, are simply proportional to the zeroth and second moments, respectively, calculated directly by summing over the velocity distribution images [17].

We define the number of atoms in the ground state to be the number of atoms contributing to the narrow, central feature in the optical depth images [1]. To avoid biased and noisy results we provide the least-squares fitting routine with a tightly constrained template to use in its search for a condensate. With an independent set of measurements on condensates near zero temperature, we have found that the condensate shapes are well-fit with 2D Gaussians whose widths, aspect ratios, and peak-heights, for a given trap frequency and expansion time, are functions only of the total number of atoms in the feature [7,18]. The width, for instance, is parametrized by $\sigma = \sigma_o(1 + \alpha N_o)^{1/5}$, where σ_o is the predicted noninteracting condensate width and α is extracted empirically. The procedure yields robust values of N_o, as long as the temperature is high enough that the noncondensate atoms form a distribution that is significantly broader than the sharp condensate feature. At temperatures below $T/T_o = 0.5$, both T and N_o measurements become suspect, as it is no longer possible to cleanly separate the condensate and the noncondensate components without recourse to a detailed model, which is contrary to the spirit of this treatment.

Our thermometry differs from previously reported methods for ultracold trapped gases [1–3,5–8]. For an ideal gas far from quantum degeneracy the velocity distribution is a Gaussian whose width is proportional to $T^{1/2}$. As the cloud is cooled closer to the BEC phase transition, higher densities and lower temperatures cause a rapid increase in the significance of quantum statistics and of residual atom-atom interactions. Rather than attempt to model these effects, we assume that the high-energy tail of the velocity distribution (i) remains in thermal equilibrium with the rest of the cloud and (ii) can be characterized by a purely ideal Maxwell-Boltzmann (MB) distribution. The latter is plausible because these highest-energy atoms spend most of their trajectories in the low-density, and therefore weakly interacting, outer part of the trapped cloud. Furthermore the occupation numbers of the corresponding energy states are much less than one. Finally, during the free expansion the high-energy atoms undergo on average much less than one collision. Guided by these assumptions, we determine the temperature by fitting a 2D Gaussian to only the wings of our velocity-distribution images, excluding the central part of the cloud, where degeneracy, interactions, fluctuations, etc. may be significant. To test the assumption of thermal equilibrium we have checked that the measured temperature of clouds is independent of the size of the exclusion region, outside of the degenerate regime [19].

The first quantity we examine is the ground-state fraction N_o/N as a function of scaled temperature T/T_o (Fig. 1). The temperature scaling removes the trivial shift in the transition temperature which occurs because as we evaporatively cool through the transition we also reduce the total number of atoms N (Fig. 1, inset). We choose our scaling temperature to be $T_o(N) = \hbar\overline{\omega}/k_B[N/\zeta(3)]^{1/3}$ where $\overline{\omega}$ is the geometric mean of the trap frequencies and ζ is the Riemann Zeta function. $T_o(N)$ is also the critical temperature, in the thermodynamic limit, for noninteracting bosons in an anisotropic harmonic potential [20,21]. For this case the temperature dependence of the ground-state fraction is $N_o/N = 1 - (T/T_o)^3$ below T_o (solid line, Fig. 1). We emphasize that, in contrast with the recent work of Mewes *et al.* [6], this line contains no free parameters and is not fit to the data, and so comparing this line to our data provides a detailed test of theory. From our data we find a critical temperature of $T_c = 0.94(5)T_o$. The uncertainty is dominated by the systematic uncertainty in our measurement of the scaled temperature stemming mostly from a 2% uncertainty in the magnification of our imaging system. Our measurements are thus only marginally different from the theory for noninteracting bosons in the thermodynamic limit. Finite number corrections [22] will shift the transition temperature $T_c(N)$ down about 3%

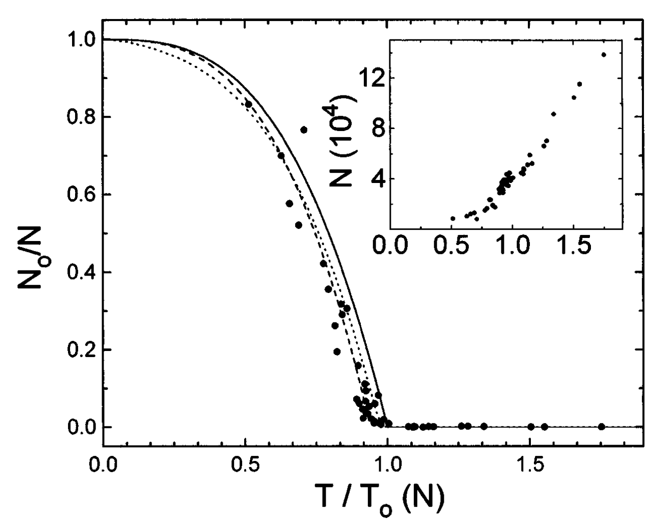

FIG. 1. Total number N (inset) and ground-state fraction N_o/N as a function of scaled temperature T/T_o. The scale temperature $T_o(N)$ is the predicted critical temperature, in the thermodynamic (infinite N) limit, for an ideal gas in a harmonic potential. The solid (dotted) line shows the infinite (finite) N theory curves. At the transition, the cloud consists of 40 000 atoms at 280 nK. The dashed line is a least-squares fit to the form $N_o/N = 1 - (T/T_c)^3$ which gives $T_c = 0.94(5)T_o$. Each point represents the average of three separate images.

(dotted line, Fig. 1). Mean-field [21,23] and many-body [24] interaction effects may also shift $T_c(N)$ a few percent.

The second result we present is a measurement of the energy and specific heat. Ballistic expansion, which facilitates quantitative imaging, also provides a way to measure the energy of a Bose gas [6,7,18]. The total energy of the trapped cloud consists of harmonic potential, kinetic, and interaction potential energy contributions, or E_{pot}, E_{kin}, and E_{int}, respectively. As the trapping field is nonadiabatically turned-off to initiate the expansion, E_{pot} suddenly vanishes. During the ensuing expansion, the remaining components of the energy, E_{kin} and E_{int}, are then transformed into purely kinetic energy E of the expanding cloud: $E_{\mathrm{kin}} + E_{\mathrm{int}} \rightarrow E$, where E is the quantity we actually measure. According to the virial theorem, if the particles are ideal ($E_{\mathrm{int}} = 0$), E will equal half the total energy, i.e., $E = \frac{1}{2}E_{\mathrm{tot}}^{\mathrm{ideal}}$. However, for a system with interparticle interactions the energy per particle due to E_{int} can be non-negligible and then $E = \alpha E_{\mathrm{tot}}$, where α is not necessarily $\frac{1}{2}$.

The scaled energy per particle, E/Nk_BT_o, is plotted versus the scaled temperature T/T_o in Fig. 2. E/N is normalized by the characteristic energy of the transition $k_BT_o(N)$ just as the temperature is normalized by T_o. The data shown are extracted from the same cloud images as those analyzed for the ground-state fraction. Above T_o, the data tend to the straight solid line which corresponds to the classical MB limit for the kinetic energy. Most interesting is the behavior of the gas at the transition. By examining the deviation Δ of the data from the classical line we see (Fig. 2, inset) that the energy curve clearly changes slope near the empirical transition temperature $0.94T_o$ obtained from the ground-state fraction analysis discussed above.

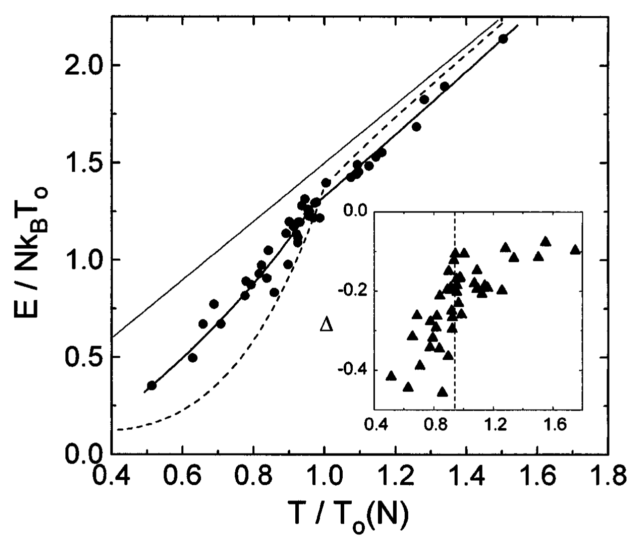

FIG. 2. The scaled energy per particle E/Nk_BT_o of the Bose gas is plotted vs scaled temperature T/T_o. The straight, solid line is the energy for a classical, ideal gas, and the dashed line is the predicted energy for a finite number of noninteracting bosons [22]. The solid, curved lines are separate polynomial fits to the data above and below the empirical transition temperature of $0.94T_o$. (inset) The difference Δ between the data and the classical energy emphasizes the change in slope of the measured energy-temperature curve near $0.94T_o$ (vertical dashed line).

The specific heat is usually defined as the temperature derivative of the energy per particle, taken with either pressure or volume held constant. In our case the derivative is the slope of the scaled energy vs temperature plot (Fig. 2), with neither pressure nor volume, but rather confining potential held constant. To place our measurement in context, it is instructive to look at the expected behavior of related specific heat vs temperature plots (Fig. 3). The specific heat of an ideal classical gas (MB statistics), displayed as a dashed line, is independent of temperature all the way to zero temperature. Ideal bosons confined in a 3D box have a cusp in their specific heat at the critical temperature (dotted line) [9]. Liquid ^{4}He can be modeled as bosons in a 3D box, but the true behavior is quite different from an ideal gas, as illustrated by the specific heat data [25] (dot-dashed line): The critical (or lambda) temperature is too low, and the gentle ideal gas cusp is replaced by a logarithmic divergence. We can compare our data with the calculated specific heat of ideal bosons in a 3D anisotropic simple harmonic oscillator (SHO) potential [20] (solid line). Note that because we do not measure E_{pot}, we must divide the SHO theory values by two to compare with our measured expansion energies. The specific heat of the ideal gas is discontinuous and finite at the transition.

In order to extract a specific heat from our noisy data, we assume that, as predicted, there is a discontinuity in the

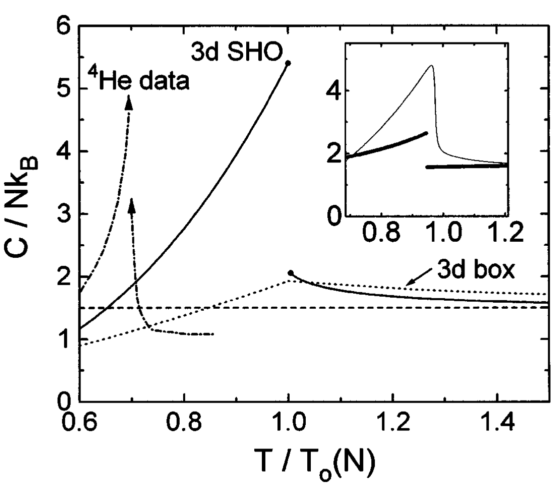

FIG. 3. Specific heat, at constant external potential, vs scaled temperature T/T_o is plotted for various theories and experiment: theoretical curves for bosons in a anisotropic 3D harmonic oscillator and a 3D square well potential, and the data curve for liquid ^{4}He [25]. The flat dashed line is the specific heat for a classical ideal gas. (inset) The derivative (bold line) of the polynomial fits to our energy data is compared to the predicted specific heat (fine line) for a finite number of ideal bosons in a harmonic potential.

slope at the empirically determined transition temperature and fit the data to separate polynomials on either side of T_c (curved, solid lines in Fig. 2). We extract the specific heat curve shown in Fig. 3 (bold line in inset). The observed step in the specific heat at the critical temperature is considerably smaller than predicted by a finite number, ideal gas theory [22] (Fig. 3, inset, thin line). A more sensible comparison is to avoid taking the model-dependent derivative and instead to compare theory and experiment directly in the energy-temperature plot (Fig. 2). The major deviation between the data and the SHO ideal gas theory (dotted line) occurs at scaled temperatures of 0.85 and below. The difference is probably due in part to the effects of interactions. Mean-field repulsion will tend to increase the energy at a given temperature.

We have measured the critical temperature, ground-state occupation, and energy of a dilute Bose gas of ^{87}Rb atoms. Our analysis is unique in that it does not rely on detailed models of the quantum degenerate cloud shape. We are thus able to examine the thermodynamics of the Bose gas in an unbiased and quantitative way. The measured ground-state fraction and transition temperature agree well with the theory for noninteracting bosons. However, the qualitative features of the energy data are significantly different from the noninteracting theory. In future work we will attempt to elucidate the role interactions play in the phase transition and the specific heat. For example, we can control the interactions by adjusting the magnetic trap spring constants and changing the number of trapped atoms [5]. In addition, with larger clouds [4] we can reduce our uncertainty in T_c, allowing us to investigate finite number and mean-field effects at the 1% level.

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