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Atomic hydrogen in an inhomogeneous magnetic field: Density profile and Bose-Einstein condensation

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The density profiles for an interacting gas of atomic hydrogen in an inhomogeneous axial magnetic field are determined by extending the Gross-Pitaevskii theory to finite temperature. The profiles can be used as an identifying feature of Bose-Einstein condensation for all T. Radial inhomogeneities in the field are also treated.

The recent success at stabilizing atomic hydrogen[1,2] ($H\downarrow$) to moderate densities (10^{16}–10^{17} atoms/cm^3) has provided a new opportunity to further understand Bose systems. Achievement of densities sufficiently high for Bose-Einstein condensation (BEC) and its detection is presently an area of intense research activity. It has been suggested by Walraven and Silvera[3] that an inhomogeneous magnetic field may be exploited to study BEC in this system. The idea is that the ground-state atoms will be localized in the region of highest magnetic field, and BEC into this state will result in a density profile which will be a characteristic distinguishing feature of the condensate. Walraven and Silvera illustrate this by considering a noninteracting gas of $H\downarrow$ atoms in a parabolic axial magnetic field which has an exact solution in terms of harmonic oscillator wave functions for the axial translational states. They also treated interactions at $T=0$ K and showed that the condensate can be broadened by orders of magnitude; however, they did not address themselves to finite temperatures. This left open the question of whether the condensate could at all be distinguished from the normal component under realistic experimental conditions (in particular near T_c where first experimental observation would be made) and thus left some serious doubt as to the usefulness of their method. In this Communication we extend the $T=0$ theory for an interacting Boson gas in an inhomogeneous field to finite temperature to determine the density profile. We find that, indeed, this suggestion for studying BEC remains valid for all T. Finally, we give some consideration of the effect of a radial field gradient which must be present in a real magnetic field.

We begin by formulating a microscopic Gross-Ginzburg-Pitaevskii[4] theory for a weakly interacting Bose gas in an external field at finite temperatures. Let the external field be denoted by $u_{\text{ext}}(r)$ and $v(\vec{r})$ be the ${}^3\Sigma_u^+$ interaction[5] between the $H\downarrow$ atoms. [We shall assume that this interaction can be described by a scattering length a so that $v(\vec{r}) = v_0\delta(\vec{r}) = (\hbar^2/m)4\pi a\,\delta(\vec{r})$; we obtain[6] $a=0.74$ Å and $v_0 = 0.447\times10^{-18}$ mK cm^3.] The second quantized Hamiltonian H takes the form:

$$H=\sum_{pq} w(p;q)a_p^\dagger a_q+\frac{1}{2}\sum_{pqrs} v(pq;rs)a_p^\dagger a_q^\dagger a_s a_r \ ,$$

where $w=p^2/2m+u_{\text{ext}}(\vec{r})$ and the matrix elements of the operators are taken with respect to an *as yet undetermined* single-particle basis $\{\phi_p(\vec{r})\}$. Constructing a free-energy functional in the manner of Bogolyubov[7] and minimizing with respect to occupation numbers, we obtain Hartree-Fock (mean-field) equations for bosons[8]:

$$-(\hbar^2/2m)\nabla^2\phi_k(\vec{r})+2[\rho_n(\vec{r})+\rho_0(\vec{r})]v_0\phi_k(\vec{r}) + u_{\text{ext}}(\vec{r})\phi_k(\vec{r})=\epsilon_k\phi_k(\vec{r}) \ , \quad k\neq 0 \qquad (1)$$

$$-(\hbar^2/2m)\nabla^2\psi_0(\vec{r})+2\rho_n(\vec{r})v_0\psi_0(\vec{r}) + \rho_0(\vec{r})v_0\psi_0(\vec{r})+u_{\text{ext}}(\vec{r})\psi_0(\vec{r})=\epsilon_0\psi_0(\vec{r}) \ , \qquad (2)$$

where

$$\rho_n(\vec{r})=\sum_{k\neq0} n_k|\phi_k(\vec{r})|^2$$

is the density of uncondensed particles [hereafter referred to as the "normal component," without any implication that $\rho_n(r)$ is necessarily identical to the "normal density" defined in two-fluid hydrodynamics]. $\rho_0(\vec{r})=N_0|\psi_0(\vec{r})|^2$ is the condensate density, $n_k=\{\exp[(\epsilon_k-\mu)/kT]-1\}^{-1}$ and $N_0=\{\exp[(\epsilon_0-\mu)/kT]-1\}^{-1}$ are the occupation numbers, and μ is the chemical potential. Above the transition temperature T_c, $N_0 \sim O(1)$, $\rho_0(\vec{r})=0$, and we only need consider Eq. (1). Below T_c, $N_0 \simeq O(N)$, $\mu=\epsilon_0+O(N^{-1})$, $\rho_0(r)>0$, and both Eqs. (1) and (2) must be considered simultaneously.

We shall now solve these equations for the density under conditions similar to those which may be experimentally accessible for H↓.[9] Assume that N atoms are confined in a tube in a magnetic field configuration, $\vec{B}(\vec{r})$, identical to that of Ref. 3:

$$B_x(\vec{r})=B_0\left(1-\frac{x^2}{x_m^2}+\frac{1}{2}\frac{r_\perp^2}{x_m^2}\right) ,$$
$$B_\perp=\frac{xr_\perp B_0}{x_m^2},\quad B_\phi=0,\quad x_m=51\text{ mm} . \tag{3a}$$

Neglect for the moment the radial dependence of $\vec{B}(\vec{r})$, then

$$u_{\text{ext}}(\vec{r})=\tfrac{1}{2}m\,\omega_0^2x^2 ,$$

where

$$\omega_0^2=2\mu_BB_0/mx_m^2 . \tag{3b}$$

Furthermore, assume that $B_0=10$ T ($\omega_0=6.5\times10^3$ rad sec^{-1}), and that the central densities involved are of the order of 10^{18} atoms/cm^3. It is useful to first take note of the relative magnitude of the energies which are involved: the zero-point energy, $\epsilon_{\text{zp}}\sim\hbar\omega_0\simeq5\times10^{-5}$ mK; the interaction energy, $\epsilon_{\text{int}}\sim\rho v_0\simeq0.4$ mK$(\rho/10^{18})$; and the thermal energy, $\epsilon_{\text{th}}\sim kT_c=16$ mK$(\rho/10^{18})^{2/3}$. Associated with these are the following lengths:

$$x_{\text{zp}}=(\hbar/2m\,\omega_0)^{1/2}\simeq2\times10^{-4}\text{ cm} ,$$

$$x_{\text{int}}=(2\rho v_0/m\,\omega_0^2)^{1/2}\simeq0.04\text{ cm}(\rho/10^{18})^{1/2} ,$$

and

$$x_{\text{th}}=(2kT_c/m\,\omega_0^2)^{1/2}\simeq0.2\text{ cm }(\rho/10^{18})^{1/3} .$$

x_{int} and x_{th} give the approximate half-widths of the condensate and normal components, respectively. Noting the thermal de Broglie wavelength

$$\lambda(T_c)=(2\pi\hbar^2/mkT_c)^{1/2}\simeq140\text{ Å}(10^{18}/\rho)^{1/3} ,$$

we observe that the inequality:

$$\lambda(T)\ll x_{\text{zp}}\ll x_{\text{int}}\lesssim x_{\text{th}}$$

holds in a broad range of densities and temperatures. One additional length of interest is the healing length[4,10]

$$\xi\equiv(8\pi a\rho)^{-1/2}\ (=2x_{\text{zp}}^2/x_{\text{int}})=230\text{ Å}(10^{18}/\rho)^{1/2} .$$

This is the characteristic length required for the condensate to spatially adjust to a nonuniformity imposed by a boundary condition or a rapidly varying potential. The fact that $\lambda(T)$ is much smaller than x_{int} and x_{th} allows one to use the WKB solutions[11] for Eq. (1) and to write

$$\rho_n(x)=\lambda^{-3}g_{3/2}(\exp\{[\mu-2\rho_n(x)v_0-2\rho_0(x)v_0-u_{\text{ext}}(x)]/kT\}) , \tag{4}$$

where $g_{3/2}(z)=\sum_{l=1}^{\infty}z^l/l^{3/2}$ is a so-called Bose integral.[12] Furthermore, because $\xi\ll x_{\text{int}}$ (except just below T_c, as discussed later), the kinetic energy term in Eq. (2) can be neglected and one can express the condensate density as

$$\rho_0(x)=[\mu/v_0-2\rho_n(x)-u_{\text{ext}}(x)/v_0]\times\Theta(\mu-2\rho_n(x)v_0-u_{\text{ext}}(x)) , \tag{5}$$

where $\Theta(x)$ is the Heaviside unit-step function. Equation (5), which generalizes the work of Ref. 3 to finite temperatures, expresses the fact that the condensate density will adjust itself so that the interaction energy balances the energy of the external field. Note that $\rho_0(x)$ vanishes at and beyond the classical turning points of Eq. (2). Neglecting the kinetic energy terms means that Eq. (5) is valid everywhere except in a small neighborhood

$$|\delta x/x_{\text{int}}|\simeq\tfrac{1}{2}(\xi/x_{\text{int}})^{2/3}\simeq7\times10^{-4}(10^{18}/\rho)^{2/3}$$

about the turning points, where $\rho_0(x)$ must go to zero smoothly. By substituting Eq. (5) into (4) one can obtain a more symmetric form for $\rho_n(x)$ which does not explicitly depend on ρ_0:

$$\rho_n(x)=\lambda^{-3}g_{3/2}\{\exp[-|\mu-2\rho_n(x)v_0-u_{\text{ext}}(x)|/kT]\} . \tag{6}$$

If the number of particles, N, is kept constant, as it is in the present case, μ must satisfy the additional constraint $N=\int d^3r\,[\rho_n(r;\mu T)+\rho_0(r;\mu,T)]$ for all temperatures.

As an illustration consider the temperature dependence of the density profiles of 10^{16} H↓ atoms which are confined by a tube having a cross-sectional area $A=0.01$ cm^2, in an axial parabolic field described by Eq. (3). For a given temperature T, Eqs. (6) and (5) can be solved simultaneously for $\rho_n(r)$ and $\rho_0(r)$. Below some critical temperature T_c, the condensate begins to be occupied ($\rho_0\neq0$). For $B_0=10$ T, T_c was calculated to be 29.34 mK, while the result for the noninteracting simple harmonic oscillator (SHO) is 30.2 mK [$T_c^{\text{SHO}}=\hbar^2(6N/\pi A)^{1/2}/mk_Bx_{\text{zp}}$]. Figure 1 shows density profiles for three temperatures in the neighborhood of T_c. As the transition temperature is crossed the condensate grows as a clearly discernable peak above the normal component. At 26 mK $N_0=21.6\%$ and the width of the condensate is ~0.1 cm. The results indicate that in this model the onset of BEC can be easily detectable by observing the density profiles. For the simple harmonic oscillator (noninteracting) problem one would expect the following behavior for the condensate fraction:

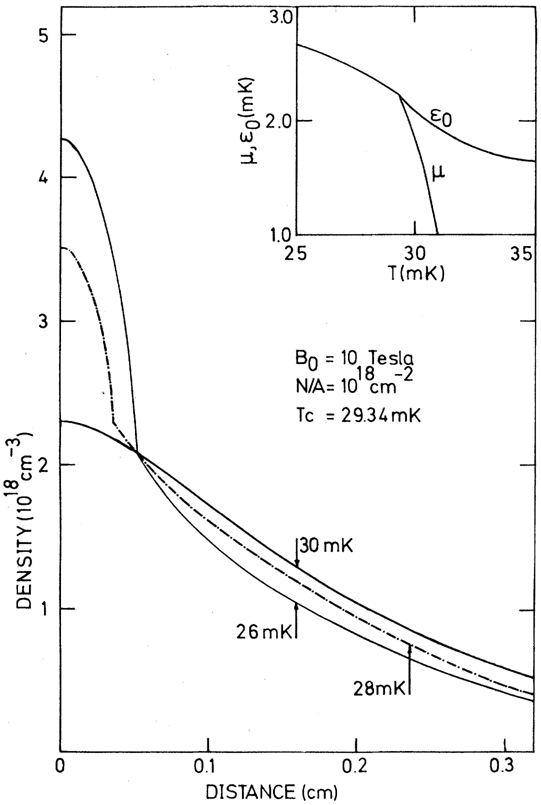

FIG. 1. Axial density profiles of atomic H↓ for various temperatures in the neighborhood of T_c. The inset shows the behavior of the chemical potential μ and single-particle ground-state energy ϵ_0 in the neighborhood of T_c. Below T_c, $\epsilon_0 = \mu$.

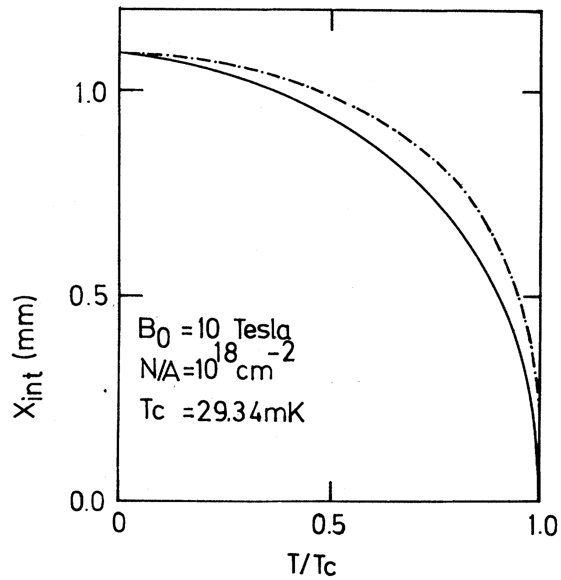

FIG. 2. Temperature dependence of the condensate half-width, x_{int}. Dashed line: Eq. (8).

$N_0/N = 1-(T/T_c)^2$. Numerical evaluations show that for the interacting gas this behavior is very closely displayed.

The temperature dependence of the condensate half-width, x_{int}, is plotted in Fig. 2. Neglecting the effect of the normal component interaction, one would expect

$$\rho_0(0) \simeq \left[\frac{3N}{4A}\right]^{2/3}\left[\frac{m\omega_0^2}{2v_0}\right]^{1/3}\left[1-\left[\frac{T}{T_c}\right]^2\right]^{2/3}, \quad T<T_c\ , \tag{7}$$

$$x_{\text{int}} \simeq \left[\frac{3N}{4A}\right]^{1/3}\left[\frac{m\omega_0^2}{2v_0}\right]^{-1/3}\left[1-\left[\frac{T}{T_c}\right]^2\right]^{1/3} . \tag{8}$$

As can be seen from Fig. 2, Eq. (8) gives a good estimate for the temperature dependence of x_{int}. A similarly good agreement for the condensate density at the center, $\rho_0(0)$, is obtained with Eq. (7).

For temperatures arbitrarily close to T_c, both x_{int} and $\rho_0(0)$ tend to zero, and the assumption $x_{\text{int}} >> \xi$ will fail. Using Eqs. (7) and (8) one finds the regime of validity of the inequality to be $(T_c-T)/T_c << A/(N6\pi a x_{zp}) \simeq 10^{-8}$, which amply justifies our assumption for all practical purposes (cf. Ref. 8).

A realistic external field must be divergenceless as in Eq. (3a). In this case the absolute maximum field is in the central plane ($x=0$) at the wall of the confining tube. In the radial direction atoms will experience a magnetic potential that decreases, up to an infinite barrier at the wall. For small N, BEC will first occur in an annulus at the wall of the tube. This results in enormous density gradients[3] or values of $\rho_0(\text{wall})/\rho_0(\text{center})$. However, as more particles are introduced there will be a point where ρ_0 is finite at the center of the magnet ($x=0$, $r_\perp=0$). This condition is reached when the number of particles is greater than

$$\nu = (\sqrt{2}\pi/15)\, m\omega_0^2 r_0^5/v_0 \simeq 34\times 10^{18}(B_0 r_0^5)\ ,$$

where B_0 is in T and r_0 (the tube radius) in cm. This implies that in present-day geometries ($2r_0 \simeq 1$ cm) and densities, the condensate will be confined to the surface of the container. However, by reducing the cross section to $A \simeq 0.01\ \text{cm}^2$ ($r_0 \simeq 0.1$ cm) at $B=10$ T, then $\nu \simeq 2\times 10^{14}$ atoms which is much smaller than the 10^{16} atoms used in the example. In this case

$$\rho_0(\text{wall})/\rho_0(\text{center}) \simeq 1 + r_0^2/(2x_{\text{int}}^2) \simeq 1.13\ ,$$

implying that the cross-sectional density is essentially uniform.

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[8] Obviously we do not expect Eq. (1) to give a correct description of the normal spectrum in the low-energy limit, when it will presumably have phononlike behavior as in the homogeneous case. However, it follows from the order of magnitude estimates given below for the case of practical interest [or for $T \geq \rho_0 v_0 \simeq 0.4$ mK $(\rho/10^{18})$] most of the normally excited particles have energies such that the true Bogolyubov-like spectrum is well approximated by the solution of Eq. (1). The scattering-length approximation should be valid for thermal wavelengths greater than atomic dimensions, or $T \lesssim 2 \times 10^4$ mK. Furthermore, we have neglected in Eqs. (1) and (2) mixing terms which preserve the orthogonality of the condensate and the excitations. Here this only affects states with zero-transverse momentum and, of these, only low-lying states (spacing $\lesssim 10^{-3}$ mK) which are confined to the vicinity of the classical turning points of the condensate. This does not measurably affect the obtained results. We note also that the Hartree-Fock approach is likely to fail in the critical region very close to T_c, which, however, for the case considered is $\Delta T/T_c \sim 10^{-2}$. [T. J. Greytak (private communication).]

[9] In a gas of H$\downarrow$ there are two hyperfine states, a and b, with a splitting of 55 mK in a field of 10 T. We shall assume that only the lowest is populated at T_c, although in the example below, T_c is 30 mK and 14% of the atoms will be in state b.

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