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Bose Condensation of Idealized Spin-Polarized Atomic Hydrogen in Equilibrium

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A model of spin-polarized hydrogen (H↑) is treated in which interactions between atoms are neglected while the single-atom Zeeman and hyperfine interactions are treated exactly. These magnetic terms in the Hamiltonian are found to affect substantially the Bose-Einstein condensation and the various thermodynamic variables. Computations are discussed of the condensation temperature, condensate density, and specific heat in order to indicate how changes in magnetic field strength might be expected to affect future measurements on this quantum system.

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Spin-polarized hydrogen (H↑) was recently stabilized in very dilute amounts[1]; if it can be produced in bulk amounts, it will be an extremely interesting quantum system. Hydrogen atoms, kept from recombining into the molecular state by a strong external magnetic field, interact via the very weak $^3\Sigma_u{}^+$ pair potential. The parameter $\eta=\hbar^2/m\sigma^2\epsilon$, which measures the "quantumness" of a Lennard-Jones system (with σ and ϵ the potential parameters), is 0.55 for H↑ whereas for ^{3}He it is 0.24. The high interest in this substance has resulted in numerous theoretical treatments[2-10] and some preliminary experimental studies.[11] The recent report[1] that small amounts of H↑ have been maintained without decay for long periods of time gives one strong reason to believe that bulk amounts will soon be available. H↑ is expected[4,7] to remain a Bose gas all the way to absolute zero, undergo a Bose-Einstein condensation (BEC), and presumably exhibit superfluid properties.

A BEC might be expected to manifest itself in a specific-heat peak, however, that in itself might not be enough to identify it unambiguously. Walraven and Silvera[10] have suggested that, in the nonuniform magnetic field configuration used by their group, a BEC will result in a characteristic density profile. The purpose of this paper is to identify other signatures of the BEC, which are dependent on the presence of the external field.

The present approach to the study of the H↑ BEC involves several simplifications. First, since an anlaysis involving the fully interacting Bose system is difficult, a more preliminary approach which neglects interatomic interactions is used here. However, the spin states of a single hydrogen atom in an external field are treated exactly. That is, the Zeeman and hyperfine interactions are included. Second, the external field used in the Silvera-Walraven experiment on H↑ was nonuniform so that down electron-spin states would be drawn in but up spins would be repelled. The field used in the present study is uniform but a portion of its effect is simulated in most of our calculations by simply eliminating the "wrong" electron-spin states from the energy spectrum used. Differences, of course, remain from the real situation. The condensation in a nonuniform field is a *spatial* BEC[10,12] while the one considered here is in momentum space. Thus it is expected that the present analysis will yield only a qualitative view of real H↑ which, however, may be useful in guiding experimenters in their search for effects characteristic of the BEC.

The computations reported below give results for the critical temperature T_c, the condensate fraction n_0/N, and the heat capacity at constant volume. Perhaps the most interesting results are those concerning T_c and n_0/N as a function of external field B. T_c is found to increase with in-

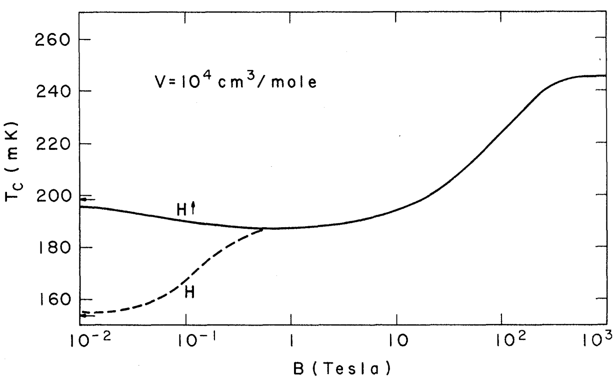

FIG. 1. Condensation temperature T_c vs magnetic field B for H↑ ($\nu = 0$ and $\nu = 1$ states only) and H (all four spin states). The arrows indicate the $B = 0$ values of T_c.

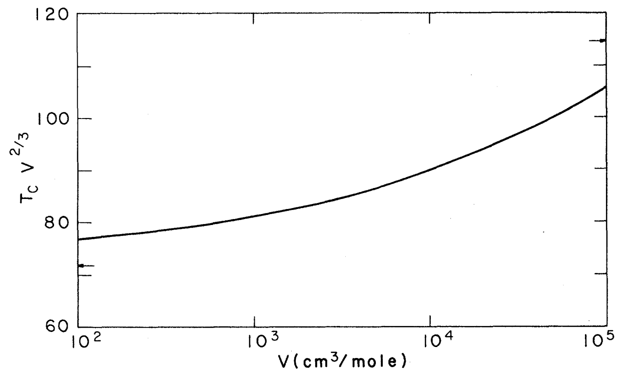

FIG. 2. $T_c V^{2/3}$ vs V for H↑ at $B = 10$ T. A spinless ideal gas would have constant $T_c V^{2/3}$. The arrows indicate the $V = 0$ and $V = \infty$ limits.

creasing B, a result which has a simple physical interpretation given below. Further, starting at a given field for which $T > T_c$ and $n_0/N = 0$, one can raise B at constant T until $T_c(B) \geq T$, i.e., a condensation may be precipated by altering the field. Such field dependence could be a useful clue to the nature of any experimental transition found in H↑ gas.

The Hamiltonian for each H atom is taken as

$$H = (p^2/2m) - \vec{\mu}_e \cdot \vec{B} - \vec{\mu}_p \cdot \vec{B} + \alpha \vec{\sigma} \cdot \vec{I} \qquad (1)$$

in which $\vec{p}$ is the momentum of the center of mass having total mass m, $\vec{\mu}_e$ and $\vec{\mu}_p$ are the electron and proton magnetic moments, respectively, and $\vec{\sigma}$ and $\vec{I}$ are the electron and proton spins, respectively, appearing in the hyperfine interaction of strength α. The single-particle energy levels of (1) are

$$\epsilon_{\vec{k}\nu} = \hbar^2 k^2/2m + \lambda_\nu , \qquad (2)$$

$$\lambda_0 = -\alpha - \gamma \quad (\downarrow ⇞), \qquad (2a)$$

$$\lambda_1 = +\alpha - b_e + b_p \quad (\downarrow ⇟), \qquad (2b)$$

$$\lambda_2 = \alpha + b_e - b_p \quad (\uparrow ⇞), \qquad (2c)$$

$$\lambda_3 = -\alpha + \gamma \quad (\uparrow ⇟), \qquad (2d)$$

in which $b_e = \frac{1}{2} g_e \mu_B B$ and $b_p = \frac{1}{2} g_p \mu_B B$ and μ_B is the Bohr magneton. Also $\gamma = [(b_e + b_p)^2 + 4\alpha^2]^{1/2}$. The plain arrow stands for electron spin and the crossed arrow for proton spin. The spin symbols associated with each state in Eqs. (2a)–(2d) are the high-field Zeeman states if one neglects the small admixtures of "wrong" spins due to the hyperfine interaction. In units of temperature one has $\alpha = 0.017$ K, $b_e/B = 6.7 \times 10^{-5}$ K and b_e/B

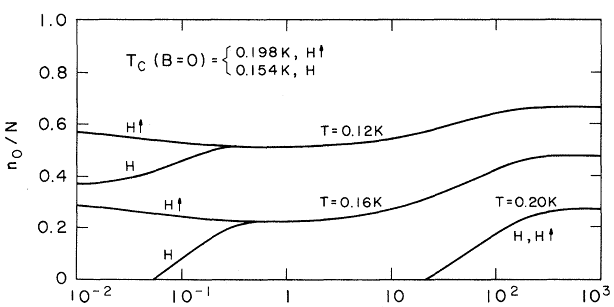

FIG. 3. Condensate fraction n_0/N vs B. For $T < T_c$ ($B = 0$) the condensate is nonzero for any B, but for $T > T_c$ ($B = 0$), a condensate may be induced by an increase in field. Curves for both H↑ and H are shown.

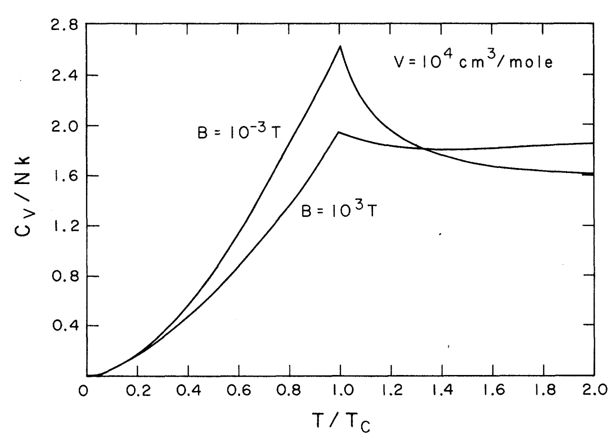

FIG. 4. Specific heat at constant valume vs T for very small and very large magnetic field.

$=1.0\times10^{-7}$ K. In this work described below the H↑ system is treated by considering only the spin-down electron states ϵ_{k0} and ϵ_{k1}. When unpolarized atomic hydrogen is considered all four states are used.

The usual procedure of the grand canonical ensemble gives, for the average number of particles in the H↑ system,

$$N=V(2\pi mkT/h^2)^{3/2}\{F_{3/2}(\beta(\lambda_0-\mu))+F_{3/2}(\beta(\lambda_1-\mu))\},\quad T>T_c, \tag{3}$$

where V is the volume of the system, μ the chemical potential, and $F_\sigma(x)$ are the Bose integrals.[12] Note that $\lambda_\nu-\mu$ is always positive. For high temperatures one can always find a μ that satisfies Eq. (3) for fixed N. This fails when $\lambda_0-\mu$ vanishes, which is the signal for the onset of the BEC. T_c is thus given by the transcendental equation

$$N=V(2\pi mkT_c/h^2)^{3/2}\{F_{3/2}(0)+F_{3/2}((\lambda_1-\lambda_0)/kT_c)\}. \tag{4}$$

T_c depends on density explicitly through Eq. (4) and on magnetic field through the level difference $\lambda_1-\lambda_0$. Figure 1 is a plot of T_c versus field for a fixed density. Increasing the field above 10 T causes the Zeeman-hyperfine (ZH) bands ϵ_{k0} and ϵ_{k1} to separate sufficiently that particles are dumped from the ϵ_{k1} states into the ϵ_{k0} states. The increase in density of the particles associated with these states caused an increase in the BEC critical temperature. Only those particles in a given spin state are indistinguishable and those in the lowest act collectively to precipitate the BEC. At low field T_c has a shallow minimum as a function of field because $\lambda_1-\lambda_0$ has such a minimum at $B=0.6$ T. If one extends the sum of Eq. (4) over all four ZH states in order to consider unpolarized atomic hydrogen (ignoring its inherent instability), the resulting T_c drops even lower at the lowest fields because all four states become populated and the density in the lowest condensing state is smaller by a factor of almost 4. Note that the values of T_c quoted in Ref. 4 apply only to $B=\infty$ because the authors chose to neglect the spin states in their analysis.

Even if variations in magnetic field are not feasible for a particular experiment, the results of Eq. (4) can easily be tested by variations in density. A plot of $T_cV^{2/3}$ vs V would be a straight line for a spinless ideal gas. However, Fig. 2 shows the variation of T_c with V given by Eq. (4) for fixed field. For very small V, T_c is quite large and the second $F_{3/2}$ in Eq. (4) contributes little; for large V, T_c is small and both $F_{3/2}$ give similar values. The resulting variation in $T_cV^{2/3}$ from $V=0$ to $V=\infty$ is then $2^{2/3}$.

For $T<T_c$, the average particle number is given by

$$N=n_0+V(2\pi mkT/h^2)^{3/2}\{F_{3/2}(0)+F_{3/2}(\beta(\lambda_1-\lambda_0))\}, \tag{5}$$

where n_0 is the number of particles in the $k=0$, $\nu=0$ state. One may solve for n_0 to find the condensate fraction

$$\frac{n_0}{N}=1-\left(\frac{T}{T_c}\right)^{3/2}\frac{F_{3/2}(0)+F_{3/2}((\lambda_1-\lambda_0)/kT)}{F_{3/2}(0)+F_{3/2}((\lambda_1-\lambda_0)/kT_c)}. \tag{6}$$

A plot of n_0/N as a function of T appears much like the nonmagnetic case. The behavior of n_0/N vs B for fixed temperature is more interesting as shown in Fig. 3. The rise in the curves for $B>10$ T again shows the effect of the splitting ϵ_{k1} states from the ϵ_{k0}. For temperature less than the zero-field critical temperature there is an $n_0/N>0$ for any field. However, for $T<T_c(B=0)$, there is no condensate for sufficiently small field; increasing the field can induce a condensate because it increases the density of particles in the $\nu=0$ states to above criticality. Results are shown for the four-spin-state atomic hydrogen case as well in Fig. 3. $T_C(B=0)$ is lower for this system than for H↑ so that n_0/N is smaller for this system and for a small enough field can even be zero when H↑ has a condensate.

The energy and specific heat at constant volume have also been computed. Figure 4 shows how c_v varies with T and how it changes over a very wide range of magnetic field. The change in c_v at the peak occurs mainly because Δ_{10}, the average splitting between the $\nu=0$ and $\nu=1$ bands, moves from $\Delta_{10}\lesssim kT_c$ to $\Delta_{10}>kT_c$. Indeed c_v has a weak maximum for $T/T_c\gtrsim2$ for the larger field shown because Δ_{10} has been shifted to comparable energies. The largest peak value of c_v comes for $\Delta_{10}\approx kT_c$. This occurs for $B\approx10^2$ T. However, the peak is only slightly larger than that shown for $B=10^{-3}$ T. The peak value drops off quickly over the range 10^2–10^3 T.

In the present model, the BEC is a first-order transition just as is the spinless case considered by London.[13]

The work reported here ought to be generalized to include interatomic interactions and the nonuniformity of the magnetic field. One might expect, however, that the basic qualitative results of the present paper would be unchanged.

A basic assumption of this work is that the system is in thermal equilibrium. The following Letter[14] suggests that the relaxation time for the $\nu=1$ to $\nu=2$ transition may be long enough that some interesting nonequilibrium effects, involving condensation into the lowest state of each band, may be observable.

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Bose Condensation in Spin-Polarized Atomic Hydrogen

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A phenomenological description of spin-polarized hydrogen is proposed in terms of two Bose fields which correspond in the low-density limit to the two lowest atomic hyperfine states. Experiments should initially populate both states and the equilibration time of the relative population will be long. When Bose condensation occurs in both states, a spontaneous coherent magnetization perpendicular to the stabilizing field will appear that may be observable in a magnetic resonance experiment.

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A number of authors have suggested that atomic hydrogen would be an interesting bosonlike quantum fluid at low densities and temperatures.[1] It became obvious that to stabilize the atoms against recombination into molecules, an external magnetic field was needed although for any field attainable in the laboratory the atomic state will still be only metastable.[2] The calculation of precise recombination rates is a difficult problem in chemical physics that has not been quantitatively settled.[3,4] Recent experiments have provided some hope that long-term stabilization may be possible,[5] so that it seems worthwhile to inquire how the Bose condensed states might be observed.

Here a number of seemingly awkward aspects of spin-polarized hydrogen, (H↑), as contrasted with ^{4}He, work to our advantage. We shall see that H↑ is expected to act in many ways like a spin-$\frac{1}{2}$ Bose fluid with a magnetic moment several times the proton's. The stabilizing field is ready made for a magnetic resonance experiment[6] that is noninvasive and can be done on a much shorter time scale than the traditional su-

