Bose-Einstein condensation in an external potential

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We present theoretical results for the critical temperature for Bose-Einstein condensation, condensate fraction, and heat capacity of a gas of Bose particles that are confined by a generic power-law potential trap. All three of these quantities are found to vary markedly with the shape of the potential. Both the ideal and the weakly interacting Bose gas are considered.

I. INTRODUCTION

For almost a decade there has been sustained experimental interest in observing Bose-Einstein condensation (BEC) in an atomic gas. Until recently the only candidate was spin-polarized atomic hydrogen. (A general review of spin-polarized hydrogen research is presented in Ref. 1.) However, with the development of techniques to trap atoms and cool them to the submillikelvin regime by laser light,²⁻⁴ other systems such as lithium and sodium have become possible candidates for study.⁵

For an ideal Bose gas of N particles, with mass M confined in a rigid container of volume V, BEC occurs at the temperature⁶

$$T_{c} = \frac{h^{2}}{2\pi kM} \left[\frac{1}{2.612} \frac{N}{V} \right]^{2/3}.$$
 (1)

However, if the atoms are confined by a spatially varying potential rather than rigid walls, T_c can be significantly altered. In general, as the mean energy decreases, the effective volume available to the system also decreases, increasing T_c . The coupling between energy and space fundamentally alters the nature of the Bose-Einstein condensation.^{7,8} These effects must be understood in order to interpret proposed experiments on atoms in traps. Furthermore, they offer the possibility of new strategies for achieving BEC.

To understand BEC in the proposed atom-trapping experiments, and to evaluate the merits of proposed trap geometries, a general treatment is needed for BEC in an arbitrary potential. That is the goal of this paper. Section II presents the general formalism for describing BEC in an arbitrary potential including expressions for the critical temperature, condensate fraction, and specific heat. Section III applies the procedure to a generic power-law potential and gives results for a number of potential configurations. The weakly interacting Bose gas in an external potential is analyzed in Sec. IV. Application and discussion of the results are presented in Sec. V.

II. IDEAL BOSE GAS IN AN EXTERNAL POTENTIAL

We consider N particles of an ideal Bose gas distributed over various quantum states of arbitrary potential. The occupation number n_{ε} of particles in an energy level ε with degeneracy g_{ε} is

$$n_{\varepsilon} = g_{\varepsilon} \left[\exp\left[\frac{\varepsilon - \mu}{kT} \right] - 1 \right]^{-1}, \qquad (2)$$

where μ is the chemical potential, k is Boltmann's constant, and T the temperature. The ground-state energy is taken to be zero.

For the potentials to be considered here, the energy level spacing is such that $kT \gg \varepsilon_{i+1} - \varepsilon_i$. Consequently, the system can be described by a continuum of states plus the discrete ground state, which must be explicitly retained. Multiplying Eq. (2) by the density of states $\rho(\varepsilon)$ and integrating over ε , one obtains the relation between μ and N.

The density of states can be found by a generalization of the familiar calculation for the free gas.⁶ The volume in phase space between the surfaces of energy ε and $\varepsilon + d\varepsilon$ is proportional to the number of states in that energy interval. However, the external potential $U(\mathbf{r})$ constrains the space available to the gas. The density of states is

$$\rho(\varepsilon) = \frac{2\pi (2M)^{3/2}}{h^3} \int_{V^*(\varepsilon)} \sqrt{\varepsilon - U(\mathbf{r})} d^3 r , \qquad (3)$$

where $V^*(\varepsilon)$ is the available space for particles with energy ε .

The total number of particles of a boson gas is implicitly related to the chemical potential μ by

$$N = N_0 + \int_0^\infty n_\varepsilon \rho(\varepsilon) d\varepsilon .$$
 (4)

 N_0 , the number of particles in the ground state, is explicitly retained because $\rho(0)=0$. The integral in Eq. (4) has a maximum value for $\mu=0$. (The integral diverges for $\mu>0$.) The critical temperature T_c can be found from Eq. (4) by taking $N_0=0$ and $\mu=0$. The total energy of the system is

$$E(T) = \int_0^\infty \varepsilon n_\varepsilon \rho(\varepsilon) d\varepsilon .$$
 (5)

The heat capacity $C(T) = \partial E(T) / \partial T$ can be shown to be

35

4354

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$$C(T) = \frac{1}{kT} \int_0^\infty \frac{\varepsilon \rho(\varepsilon)}{g_\varepsilon} (n_\varepsilon)^2 \left[\mu'(T) + \frac{\varepsilon - \mu}{T} \right] \\ \times \exp\left[\frac{\varepsilon - \mu}{kT} \right] d\varepsilon , \qquad (6)$$

where $\mu'(T) = \frac{\partial \mu}{\partial T}$. C(T) is analogous to C_p in that it includes work done against the potential as the energy of the gas is increased. However, for obvious reasons the volume and pressure are not useful thermodynamic variables.

To evaluate E(T) an explicit expression for $\mu(T)$ is needed. This can be obtained by writing Eq. (4) as

$$N = N_0 + \sum_{j=1}^{\infty} \exp(j\mu/kT) \int_0^{\infty} \rho(\varepsilon) \exp(-j\varepsilon/kT) d\varepsilon , \qquad (7)$$

and considering the leading terms of the series. $(g_{\varepsilon}$ has been taken as unity.) However, if we are interested in values of C(T) close to T_c where $\mu \approx 0$, only $\mu'(T_c^+)$

needs to be evaluated. $[\mu'(T_c^-)=0]$. From Eq. (6) it is evident that if $\mu'(T_c^+) \neq 0$ the heat capacity will exhibit a discontinuity at T_c . Appendix A presents more details on the calculation of $\mu'(T)$ and $\mu''(T) = \frac{\partial^2 \mu}{\partial T^2}$.

III. BOSE-EINSTEIN CONDENSATION IN A POWER-LAW POTENTIAL

We shall apply the results of Sec. II to a generic power-law potential

$$U(\mathbf{r}) = \varepsilon_1 \left| \frac{x}{a} \right|^p + \varepsilon_2 \left| \frac{y}{b} \right|^l + \varepsilon_3 \left| \frac{z}{c} \right|^q.$$
(8)

After some manipulation, the density of states, Eq. (3), can be shown to be given by

$$\rho(\varepsilon) = \left[\frac{2\pi (2M)^{3/2}}{h^3} \right] \frac{abc}{\varepsilon_1^{1/p} \varepsilon_2^{1/l} \varepsilon_3^{1/q}} \varepsilon^{\eta} F(p,l,q) , \qquad (9)$$

where $\eta = 1/p + 1/l + 1/q + \frac{1}{2}$ and F(p, l, q) is defined by

$$F(p,l,q) = \left[\int_{-1}^{1} (1-X^p)^{1/2+1/q+1/l} dX\right] \left[\int_{-1}^{1} (1-X^l)^{1/q+1/2} dX\right] \left[\int_{-1}^{1} (1-X^q)^{1/2} dX\right].$$
(10)

The critical temperature is obtained by incorporating this result in Eq. (4). The result is

$$T_{c} = \left[\frac{h^{3}}{2\pi (2M)^{3/2}} \frac{N}{abc} \frac{\varepsilon_{1}^{1/p} \varepsilon_{2}^{1/l} \varepsilon_{3}^{1/q}}{k^{\eta+1} F(p,l,q) Q(\eta)}\right]^{1/(\eta+1)}, \quad (11)$$

where $Q(\eta) = \int_0^\infty \{\theta^{\eta} / [\exp(\theta) - 1]\} d\theta$. This result can be applied to a rigid box by letting $(p,l,q) \rightarrow \infty$. In this case $F(\infty,\infty,\infty) = 8$ and $Q(\eta)$ becomes the well-known $g_{3/2}(0)$ Bose function⁶ that has the value $(\sqrt{\pi}/2)2.612$. The quantity abc = V/8, where V is the volume of the system. The expression for the critical temperature becomes identical to Eq. (1), as expected.

Equation (11) describes how the critical temperature depends on the potential's strength and the power law, providing a criterion for optimizing the potential within the constraint of the cooling process. By combining Eqs. (4) and (11) the ground-state population fraction for $T < T_c$ can be obtained. The result is

$$\frac{N_0}{N} = 1 - (T/T_c)^{\eta+1} .$$
(12)

Values for $T_c, N_0/N$ and heat capacity for a number of potential configurations are shown in Table I.

TABLE I. Critical temperature, ground-state population, heat capacity, and discontinuity in C(T) for several cases of threedimensional 3(D) confinement. (V represents volume and S, area). In the first two cases where the potential is one dimensional, rigid walls are assumed in the other direction. For the harmonic oscillator, the result agrees with previous calculation (Ref. 7).

T _c	$N_0/N \ (T < T_c)$	$C(T_c^-)/Nk$	$\Delta C(T_c)/Nk$
$\left(\frac{h^3N}{1.4Sk^{5/2}(2\pi M)^{3/2}}\right)^{2/5} \left(\frac{\varepsilon_3}{a}\right)^{2/5}$	$1 - \left[\frac{T}{T_c}\right]^{5/2}$	6.88	3.35
$\left[\frac{3h^3N}{\sqrt{2}Sk^2\pi^4M^{3/2}}\right]^{1/2}\left[\frac{\varepsilon_3}{a^2}\right]^{1/4}$	$1 - \left[\frac{T}{T_c}\right]^2$	4.38	0
$\left(\frac{h^3N}{2.612k^{3/2}(2M\pi)^{3/2}V}\right)^{2/3}$	$1 - \left[\frac{T}{T_c}\right]^{3/2}$	1.92	0
$\left[\frac{Nh^3}{1.202\pi^3k^{3}(2M)^{3/2}}\right]^{1/3}\left(\frac{\varepsilon_1}{a^2}\right)^{1/2}$	$1 - \left(\frac{T}{T_c}\right)^3$	10.82	6.57
$\left(\frac{Nh^3}{1.202\pi^3k^{3}(2M)^{3/2}}\right)^{1/3} \left(\frac{\varepsilon_1}{a^2}\right)^{1/6} \left(\frac{\varepsilon_2}{b^2}\right)^{1/3}$	$1 - \left[\frac{T}{T_c}\right]^3$	10.82	6.57
	$\frac{T_{c}}{\left[\frac{h^{3}N}{1.4Sk^{5/2}(2\pi M)^{3/2}}\right]^{2/5} \left[\frac{\varepsilon_{3}}{a}\right]^{2/5}} \left[\frac{\frac{h^{3}N}{\sqrt{2}Sk^{2}\pi^{4}M^{3/2}}}{\sqrt{2}Sk^{2}\pi^{4}M^{3/2}}\right]^{1/2} \left[\frac{\varepsilon_{3}}{a^{2}}\right]^{1/4}} \left[\frac{h^{3}N}{2.612k^{3/2}(2M\pi)^{3/2}V}\right]^{2/3}} \left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/2}} \left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/6} \left[\frac{\varepsilon_{2}}{b^{2}}\right]^{1/3}}$	$\frac{T_{c}}{\left[\frac{h^{3}N}{1.4Sk^{5/2}(2\pi M)^{3/2}}\right]^{2/5} \left[\frac{\varepsilon_{3}}{a}\right]^{2/5}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{5/2}}{\left[\frac{3h^{3}N}{\sqrt{2}Sk^{2}\pi^{4}M^{3/2}}\right]^{1/2} \left[\frac{\varepsilon_{3}}{a^{2}}\right]^{1/4}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{2}}{\left[\frac{h^{3}N}{2.612k^{3/2}(2M\pi)^{3/2}V}\right]^{2/3}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{2}}{\left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/2}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3}}{\left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/6}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3}}{\left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/6}} \left[\frac{\varepsilon_{2}}{b^{2}}\right]^{1/3}} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3}}$	$\frac{T_{c}}{\left[\frac{h^{3}N}{1.4Sk^{5/2}(2\pi M)^{3/2}}\right]^{2/5} \left[\frac{\varepsilon_{3}}{a}\right]^{2/5}} \qquad N_{0}/N (T < T_{c}) \qquad C(T_{c}^{-})/Nk}$ $\left[\frac{h^{3}N}{1.4Sk^{5/2}(2\pi M)^{3/2}}\right]^{1/2} \left[\frac{\varepsilon_{3}}{a^{2}}\right]^{1/4} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{5/2} \qquad 6.88$ $\left[\frac{3h^{3}N}{\sqrt{2}Sk^{2}\pi^{4}M^{3/2}}\right]^{1/2} \left[\frac{\varepsilon_{3}}{a^{2}}\right]^{1/4} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{2} \qquad 4.38$ $\left[\frac{h^{3}N}{2.612k^{3/2}(2M\pi)^{3/2}}\right]^{2/3} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3/2} \qquad 1.92$ $\left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/2} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3} \qquad 10.82$ $\left[\frac{Nh^{3}}{1.202\pi^{3}k^{3}(2M)^{3/2}}\right]^{1/3} \left[\frac{\varepsilon_{1}}{a^{2}}\right]^{1/6} \left[\frac{\varepsilon_{2}}{b^{2}}\right]^{1/3} \qquad 1 - \left[\frac{T}{T_{c}}\right]^{3} \qquad 10.82$

As Table I illustrates, the deeper the potential well (i.e., the larger the value of the strength ε), the higher the value of T_c . The "confinement power" of the potential, defined as $\eta + 1 = -N^{-1}T_c(dN_0/dT)_{T=T_c}$, can be seen to depend on the shape of the potential well but not on its strength.

The heat capacity can be calculated from Eq. (5). Results are given in Table I. Depending on the exponents p,l,q of the potential, the system may or may not display a discontinuity in C(T) or its derivatives. If $\eta > 1$, C(T)is discontinuous at T_c . If $\eta \le 1$, C(T) is continuous at T_c , but $\partial C(T)/\partial T$ is discontinuous. Note that in general C(T) is larger for a power-law potential than for a rigid wall container. This is because increasing the energy of the gas requires work against the confining potential.

IV. WEAKLY INTERACTING BOSE GAS IN AN EXTERNAL POTENTIAL

Because the noninteracting Bose gas can lead to unphysical results, we now consider the effect of twoparticle interactions using the mean-field approximation.¹ Representing the interaction energy per particle by a term proportional to the local density $n(\mathbf{r})$, the Hamiltonian for a particle in this gas becomes

$$H(\mathbf{p},\mathbf{r}) = \frac{p^2}{2M} + U(\mathbf{r}) + \gamma n(\mathbf{r}) , \qquad (13)$$

where γ is the interaction constant. At low temperatures, where only s-wave scattering is important, γ depends on a single parameter, the scattering length α . For the oneparameter interparticle potential $V(\mathbf{r}_1 - \mathbf{r}_2) = V_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$, it can be shown that $V_0 = 4\pi\hbar^2 \alpha/M$. In the selfconsistent field approximation⁹ $E(0)/N = \frac{1}{2}V_0 n(r)$, so that $\gamma = 2\pi\hbar^2 \alpha/M$.

In a semiclassical approximation the density of the gas is given by (see Appendix B)

$$n(\mathbf{r}) = \frac{1}{\Lambda^3} \sum_{j=1}^{\infty} \exp\{j [\mu - U(\mathbf{r})] / kT\} / j^{3/2}, \qquad (14)$$

where $\Lambda = \hbar/\sqrt{2\pi MkT}$ is the thermal de Broglie wavelength. At very low temperatures where $\mu \sim 0$ the major contribution to $n(\mathbf{r})$ comes from the term j = 1. In this case $n(\mathbf{r}) \sim \exp[-U(\mathbf{r})/kT]/\Lambda^3$, and Eq. (13) becomes

$$H(\mathbf{r},\mathbf{p}) = p^2/2M + U(\mathbf{r}) + \frac{\gamma}{\Lambda^3} \exp[-U(\mathbf{r})/kT] . \qquad (15)$$

The particle moves in an effective potential

 $U_{\rm eff}(\mathbf{r}) = U(\mathbf{r}) + (\gamma/\Lambda^3) \exp[-U(\mathbf{r})/kT]$.

The density of states is given by Eq. (3) with $U(\mathbf{r})$ replaced by $U_{\rm eff}(\mathbf{r})$. Because the gas is weakly interacting, $\rho(\varepsilon)$ can be expanded in powers of γ . Retaining the first term yields

$$\rho(\varepsilon) = \frac{2\pi (2M)^{3/2}}{h^3} \int_{V^*(\varepsilon)} \left[\sqrt{\varepsilon - U(\mathbf{r})} + \frac{\gamma}{2\Lambda^3} \frac{\exp[-U(\mathbf{r})/kT]}{\sqrt{\varepsilon - U(\mathbf{r})}} \right] d^3r .$$
(16)

To estimate the effect of the atomic interactions, we shall consider the case of a cylindrical potential,

$$U(\mathbf{r}) = \varepsilon_1 (\rho/b)^m + \varepsilon_3 (z/a)^q , \qquad (17)$$

where $r^2 = \rho^2 + z^2$. However, the following results can be easily extended to a general power-law potential. After some straightforward algebra, the density of states is found to be

$$\rho(\varepsilon) = \frac{4\pi^2 (2M)^{3/2}}{h^3} \frac{b^2 a}{\varepsilon_1^{2/m} \varepsilon_3^{1/q}} \times \left[F_1(q,m) \varepsilon^{\eta} + \frac{\gamma G_1(q,m) \varepsilon^{\eta-1} \exp(-\varepsilon/kT)}{2\Lambda^3} \right],$$
(18)

where $\eta = 1/q + 2/m + \frac{1}{2}$, and G_1 and F_1 are defined by

$$F_{1}(q,m) = \left[\int_{0}^{1} x (1-x^{m})^{1/2} dx \right] \\ \times \left[\int_{-1}^{1} (1-y^{q})^{2/m+1/2} dy \right],$$
(19)

$$G_{1}(q,m) = \left[\int_{0}^{1} \theta / (1 - \theta^{m})^{1/2} d\theta \right] \times \left[\int_{-1}^{1} (1 - x^{q})^{2/m - 1/2} dx \right].$$
(20)

Incorporating this result in Eq. (4) eventually gives

$$N = N_0 + D_1(T)^{\eta+1} + D_2 \gamma(T)^{\eta+3/2} , \qquad (21)$$

where

$$D_1 = \frac{4\pi^2 (2M)^{3/2}}{h^3} F_1(q,m) k^{\eta+1} \frac{b^2 a}{\varepsilon_1^{2/m} \varepsilon_3^{1/q}}$$
(22)

and

$$D_2 = G_1(q,m)k^{1/2}(2\pi M)^{3/2} \frac{D_1}{F_1(q,m)h^3} .$$
 (23)

The condensate fraction is

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c^0}\right)^{\eta+1} - \gamma A \left(\frac{T}{T_c^0}\right)^{\eta+3/2},$$
 (24)

where in the present case,

$$T_{c}^{0} = \{ [h^{3}/4\pi^{2}(2M)^{3/2}](N/ab^{2}) \\ \times [\varepsilon_{1}^{2/m}\varepsilon_{3}^{1/q}/k^{\eta+1}F_{1}(q,m)Q(\eta)] \}^{1/(\eta+1)} .$$
(25)

 T_c^0 is the critical temperature for $\gamma = 0$; $A = (D_2/D_1)(T_c^0)^{1/2}$. The critical temperature T_c is found from Eq. (24) with $N_0 = 0$. T_c is larger or smaller than T_c^0 , according to whether the scattering length is negative or positive. As a numerical example, consider $N = 2.0 \times 10^{18}$ polarized hydrogen atoms in a rigid container of about 1 cm³. Taking $q, m \to \infty$, a = b = 0.5 cm, $\alpha = 0.72$ Å,¹⁰ then from Eq. (24), $\Delta T_c = T_c^0 - T_c$ $=1.5\times10^{-3}$ K. This corresponds to a correction of 5% in the value of T_c^0 . (This result agrees with previous calculations for a rigid box.⁹) For a potential that has larger confinement power than a rigid container, the coefficient A in Eq. (24) and η assume larger values.

The heat capacity is also sensitive to the interaction term in $\rho(\varepsilon)$ [Eq. (18)]. Evaluating Eq. (6) in the vicinity of T_c reveals that for $\eta > 2$ there is a discontinuity in C(T), and that for $\eta \le 2$, C(T) is continuous but $\partial C(T)/\partial T$ is discontinuous.

V. DISCUSSION

Intuitively one expects Bose condensation to begin when the density of particles is approximately Λ^{-3} , i.e., one particle per cubic de Broglie wavelength. In fact, Eq. (14) reveals that the density at the onset of BEC is $n_c = 2.612\Lambda^{-3}$, irrespective of the nature of the trapping potential. [This follows from evaluating Eq. (14) with U(0)=0, $\mu=0$). This critical density is well known for the particle in a box; we point out that it is universal. Note, however, that this density occurs only at the minimum of the potential: The chief effect of the trap is merely to concentrate the particles to the density at which BEC commences.

In spite of the universal onset density of BEC in different traps, there are significant differences in the behavior of the condensate fraction at temperatures below T_c , and in the possible discontinuity in the heat capacity. In addition, a strongly confining potential can greatly facilitate experimental efforts to achieve BEC. If the number of trapped particles is limited, such a potential can allow BEC to occur at a much higher critical temperature. If the minimum temperature is limited, a strongly confining potential reduces the number of trapped particles required for BEC. If collisional mechanisms are important, it may be easier to reach BEC in a stronger confining potential, simply because the fraction of the volume of the system that is at the critical density is small.

To illustrate these results, we shall apply them to an isotropic harmonic¹¹ potential given by $U(\mathbf{r}) = \frac{1}{2}M\omega^2 r^2$. The critical temperature, Eq. (11), can be written as $kT_c = 0.941\hbar\omega N^{1/3}$. If the atoms in this trap have an average energy of 3kT/2, then the effective volume they occupy is $\overline{V} = (4\pi/3)r^3$, where r is found from $U(\mathbf{r}) = 3kT/2$. To compare the transition temperature in the trap with that for a rigid box of the same volume, we can rewrite the expression for T_c as $(kT_c)^{3/2} = 0.175(h^3/M^{3/2})(N/V) = 2.1(kT_c)_{\text{box}}$. Thus, the critical temperature is approximately two times larger than for a rigid container of the same effective volume.

The effect of interparticle interactions in the harmonic trap can be evaluated using the method of Sec. IV, Eqs. (19) and (20) yield $F_1 = \pi/8$ and $G_1 = \pi/2$. Equation (24) can then be written in the form

$$\frac{N_0}{N} = 1 - \left[\frac{T}{T_c^0}\right]^2 - 4\frac{\alpha}{\Lambda_c} \left[\frac{T}{T_c^0}\right]^{7/2},$$
(26)

where $\Lambda_c = h / (2\pi M k T_c^0)^{1/2}$ is the thermal wavelength at T_c^0 . As expected, the correction is proportional to the ra-

tio α/Λ_c . The critical temperature is decreased, or increased according to whether $\alpha > 0$ or $\alpha < 0$, respectively. If the potential becomes more shallow, the numerical factor of the correction term decreases. In the limit of a rigid box, the numerical factor is unity.

A cylindrical magnetic quadrupole trap, with dipole axial confining magnets, has been proposed for spinpolarized hydrogen by Hess¹². In the configuration designed for use at lower temperature, the trap is described by $U(\mathbf{r}) = \varepsilon_1(z/a)^2 + \varepsilon_2(\rho/b)$ with $\varepsilon_1 = \varepsilon_2$ $= 2 \times 10^{-20}$ erg and a = 5 cm, b = 1.3 cm. Following the procedure of Sec. III, we obtain for $N = 10^{12}$ atoms, $T_c = 7.5 \times 10^{-6}$ K. The heat capacity has the value $C(T_c^-) = 18.48Nk$ and it has a discontinuity $\Delta C(T_c) = 13.53Nk$. The ground-state population varies as $1 - (T/T_c)^4$. The interaction correction to T_c is negligible.

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APPENDIX A: EVALUATION OF μ' AND μ'' NEAR T_c

For a closed system, the total number of particles given in Eq. (4) is constant. Therefore $\partial N / \partial T = 0$. For $T > T_c$, $N_0 = 0$ so from Eqs. (2)-(4) considering $g_{\varepsilon} = 1$, we obtain

$$\int_{0}^{\infty} \frac{\exp[(\varepsilon - \mu)/kT] \left[\frac{(\varepsilon - \mu)}{kT^{2}} + \frac{\mu'}{kT} \right]}{\{\exp[(\varepsilon - \mu)/kT] - 1\}^{2}} \rho(\varepsilon)d\varepsilon = 0.$$
(A1)

For $T = T_c$, and $\mu = 0$, (A1) yields

$$\mu'(T_c^+) = -\frac{1}{T} \frac{\int_0^\infty \varepsilon \rho(\varepsilon) (n_\varepsilon)^2 \exp[\varepsilon/kT] d\varepsilon}{\int_0^\infty \rho(\varepsilon) (n_\varepsilon)^2 \exp[\varepsilon/kT] d\varepsilon} .$$
(A2)

From Eq. (6) it can be shown that

$$\Delta C(T_c) = C(T_c^-) - C(T_c^+)$$

= $\frac{-\mu'(T_c^+)}{4kT_c} \int_0^\infty \frac{\varepsilon \rho(\varepsilon)}{\sinh^2(\varepsilon/2kT_c)} d\varepsilon$. (A3)

To obtain $\Delta C(T_c)$ we make use of the values for $\mu'(T_c^+)$ given in Eq. (A2).

If $\Delta C(T_c) = 0$ we look for discontinuity in $(\partial C/\partial T)_{T_c}$. In this case Eq. (6) yields

$$\Delta \left[\frac{\partial C}{\partial T} \right]_{T=T_c} = \left[\frac{\partial C}{\partial T} \right]_{T=T_c^-} - \left[\frac{\partial C}{\partial T} \right]_{T=T_c^+} \\ = \frac{-\mu''(T_c^+)}{4kT_c} \int_0^\infty \frac{\varepsilon \rho(\varepsilon)}{\sinh^2(\varepsilon/2kT_c^0)} d\varepsilon , \quad (A4)$$

where $\mu''(T_c^+)$ can be calculated by taking the derivative with respect to temperature of Eq. (A1). The result is

$$\mu''(T_c^+) = -\frac{1}{kT_c^3} \left[\left[\int_0^\infty \frac{\varepsilon^2 \rho(\varepsilon)}{\sinh^3(\varepsilon/2kT_c)} \cosh(\varepsilon/2kT_c) d\varepsilon \right] \left[\int_0^\infty \frac{\rho(\varepsilon)}{\sinh^2(\varepsilon/2kT_c)} d\varepsilon \right] - \left[\int_0^\infty \frac{\varepsilon \rho(\varepsilon) d\varepsilon}{\sinh^2(\varepsilon/2kT_c)} \right] \left[\int_0^\infty \frac{\varepsilon \rho(\varepsilon)}{\sinh^3(\varepsilon/2kT_c)} \cosh(\varepsilon/2kT_c) d\varepsilon \right] \right] \right] \left[\int_0^\infty \frac{\rho(\varepsilon) d\varepsilon}{\sinh^2(\varepsilon/2kT_c)} \right]^2.$$
(A5)

APPENDIX B: CALCULATION OF THE DENSITY

The density of particles of a Bose gas in an external potential is given by

$$n(\mathbf{r}) = \sum_{\varepsilon} n_{\varepsilon} |\Psi_{\varepsilon}|^2 , \qquad (B1)$$

where Ψ_{ε} is the wave function of the state of the potential $U(\mathbf{r})$ having energy ε . However, for most potentials Eq. (B1) is difficult to evaluate. A useful approximation can be obtained without using (B1). Equation (3) assumes the semiclassical approximation

$$dN = \frac{1}{h^3} n_\varepsilon d^3 p d^3 r .$$
 (B2)

It is convenient to write

$$n(\mathbf{p},\mathbf{r}) = \{ \exp[(p^2/2M + U(\mathbf{r}) - \mu)/kT] - 1 \}^{-1} .$$
 (B3)

The density of particles with momentum between p and p + dp, at position **r**, is

$$\left[\frac{dN}{dV}\right]_{\mathbf{p},\mathbf{r}} = \frac{1}{h^3} n(\mathbf{p},\mathbf{r}) d^3 p \quad . \tag{B4}$$

The total density is found by integrating (B4) with the result

$$\left|\frac{dN}{dV}\right|_{\mathbf{r}} = \frac{4\pi}{h^3} \int_0^\infty n(\mathbf{p}, \mathbf{r}) p^2 dp \quad . \tag{B5}$$

By making a change of variable Eq. (B5) becomes

$$n(\mathbf{r}) = \frac{2}{\sqrt{\pi}} \frac{1}{\Lambda^3} \int_0^\infty x^{1/2} \{ \exp[x + U(\mathbf{r})/kT + \mu/kT] - 1 \}^{-1} dx ,$$

$$= \frac{2}{\sqrt{\pi}} \frac{1}{\Lambda^3} \sum_{t=0}^\infty e^{-t} [U(\mathbf{r})/kT - \mu/kT] \int_0^\infty \exp\left[-x(t+1) - \frac{U(\mathbf{r})}{kT} - \mu/kT\right] x^{1/2} dx ,$$
(B6)

where we have used the series $1/(1-y) = \sum_{t=0}^{\infty} y^t$ (for y < 1). The integral can be carried out with the result

$$n(\mathbf{r}) = \frac{1}{\Lambda^3} \sum_{t=1}^{\infty} \exp\{t[\mu - U(\mathbf{r})]/kT\} \frac{1}{t^{3/2}} .$$
(B7)

This result, found by using Eq. (B1) for a harmonic oscillator, has been used previously¹³ in calculations of BEC.

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