Density profile of the weakly interacting Bose gas confined in a potential well: Nonzero temperature

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A theory is developed for the density profile of a weakly interacting Bose gas confined within an arbitrary potential well at nonzero temperature. This problem is of interest in connection with magnetically confined spin-aligned atomic hydrogen (H↓). The approach taken is conceptually simpler and of comparable accuracy as compared to previous approaches. It is based on the statement of constancy of the chemical potential in equilibrium. This in turn involves the internal chemical potential, a functional of the density, which we treat in a local-density approximation. For a given temperature we develop a form for the local internal chemical potential for a wide range of density using known low-density, intermediate-density (i.e., near the Bose-condensation density), and high-density analytic forms, with appropriate smooth interpolants connecting these three profiles are evaluated within the Bogoliubov approximation for the local internal chemical potential for parameters appropriate to magnetically confined H↓ for both symmetric linear and quadratic one-dimensionally varying wells. Comparison is made to previous work. The nonanalytic region of the density profile near the Bose-condensation density is analyzed. We also calculate density profiles including the next-highest-order interaction correction (i.e., beyond Bogoliubov) in the internal chemical potential. For conditions relevant to hypothetical H↓ at moderate densities this leads to a small but discernable effect on the density profile.

I. INTRODUCTION

This paper presents a general theory of the low-temperature density profile of a weakly nonideal Bose gas trapped within an arbitrary potential well. Studies of this problem at zero temperature have been reported earlier.[1,2] This subject is of interest in respect to low-temperature atomic hydrogen gas stabilized in a strong nonuniform magnetic field.[3] Spin-aligned hydrogen (H↓), a Bose system, is believed to remain gaseous at low to moderate densities down to temperature $T=0$.[4] Another possible application of this theory is to the excitonic Bose gas in nonuniformly stressed semiconductor crystals.[5]

Studies of the confined, weakly interacting Bose gas at finite temperature have been reported earlier. Both Goldman, Silvera, and Legget[6] (GSL) and Huse and Sigga[7] developed extensions of the Gross-Pitaevskii theory of the weakly interacting inhomogeneous Bose gas to finite temperatures. They utilized Hartree-Fock and Bogoliubov approximations and obtained density profiles of magnetically confined H↓. Condat and Guyer examined this system via a Ginzburg-Landau approach and achieved results rather comparable to those of GSL.[8]

The present approach is based on thermodynamic, i.e., macroscopic considerations. It is conceptually simpler and as accurate as compared to previous approaches. It utilizes the principle that for a nonuniform system in diffusive equilibrium the chemical potential is constant throughout the system. In turn the chemical potential is the sum of the internal chemical potential [a functional of the density $n(r)$] and the external potential energy of one particle. Here we evaluate the internal chemical potential within the local-density approximation (LDA). Thus the internal chemical potential is taken as a local functional of $n(r)$ of the same form as for the chemical potential of a uniform system of density n. Such a functional is developed here for the weakly nonideal Bose gas at finite temperature.

This paper is organized as follows: Sec. II presents the overall model and indicates the program for solving for the LDA density profile. Section III is concerned with the development of an appropriate local internal chemical-potential functional which for a given nonzero temperature is to be valid for the higher-density quantum regime (usually near the well minimum), the much-lower-density classical regime (usually away from the well minimum), and the intermediate-density regime. Account is taken of Bose condensation. The local internal chemical potential away from these limiting regimes is obtained by means of appropriate interpolations between the known "high"-density and near-Bose-condensation transition forms and between the latter and the known "low"-density form. The density dependence of the local internal chemical potential near the Bose-condensation transition density is discussed. Section IV presents results for the nonzero temperature-density profiles for two symmetric power-law wells. We consider both the leading-order (in interaction strength) Bogoliubov form for the local internal chemical potential and the effect of including in the latter the next-highest-order interaction correction. The higher-order interaction effects have not been considered in previous studies. Numerical results are given for conditions appropriate to H↓. Comparison is made to previous work. Section V contains a conclusion.

II. MODEL AND LDA FORMULATION

We consider a gas comprised of a large number N of particles each of mass m. We assume that the particles interact with an arbitrary purely repulsive short-range potential energy $U(r)$ (with r the interparticle distance), such that $U(r) \rightarrow 0$ monotonically, for $r \rightarrow \infty$, while $U(r) \rightarrow \infty$, monotonically, as $r \rightarrow 0$. (These requirements could be relaxed to include interparticle potentials with an attractive part provided the system remains gaseous throughout under conditions of interest.)

We take the gas to be confined to the interior of an effectively infinitely long cylinder of cross sectional area A and with arbitrary cross-sectional shape. The cross-sectional area and shape are assumed to be such that the density is independent of positional variations perpendicular to the cylindrical axis.

The particles are taken to move in a potential energy well $V(z)$, with the z axis parallel to the cylindrical axis. The form of $V(z)$ is arbitrary except that we impose the following three conditions: (i) $V(0)=0$, (ii) $V(z)$ is even, and (iii) $V(z)$ monotonically increases without bound as $|z| \rightarrow \infty$.[9] Thus we expect that the gas will be confined to the region of the minimum of $V(z)$, i.e., the density will fall off as $|z| \rightarrow \infty$. We note that the conditions on $V(z)$ just described effectively encompass those of the experimental arrangements used in the investigation of H↓.

The statement of constancy of the chemical potential of a nonuniform system in diffuse equilibrium reads

$$\bar{\mu}[n(z)]+V(z)=\mu \ . \tag{1}$$

Here μ is the chemical potential, $n(z)$ is the density profile, and $\bar{\mu}$ is the internal chemical potential, generally a nonlocal functional of the density profile $n(z)$. If the density varies sufficiently slowly we may use the LDA, i.e., we replace the nonlocal functional $\bar{\mu}[n(z)]$ by the local-density form $\bar{\mu}_0(n(z))$, which is the chemical potential of a corresponding uniform system of density $n=n(z)$. We note that functionals $\bar{\mu}_0(n)$ do exist in the literature for the weakly interacting Bose gas for certain T,n ranges.

$$\bar{\mu}_0(n(z))+V(z)=\mu \ , \tag{2a}$$

$$\Longrightarrow n(z)=\bar{\mu}_0^{-1}(\mu-V(z)) \ , \tag{2b}$$

where $\bar{\mu}_0^{-1}$ is the inverse local internal chemical-potential function. The value of μ is determined from the normalization of $n(z)$:

$$N=2A\int_0^\infty n(z)dz=2A\int_0^\infty \bar{\mu}_0^{-1}(\mu-V(z))dz \ . \tag{3}$$

Once having determined μ from Eq. (3) we substitute back into Eq. (2b) to obtain $n(z)$. This program for determining $n(z)$ has been carried out at zero temperature.[1,2] It was found that the LDA density profile exhibits sharp cutoffs at $\pm z_0$ with z_0 finite. This is a consequence of the vanishing of the local internal chemical potential in the zero-density limit at zero temperature. At nonzero temperature on the other hand the local internal

chemical potential for a general Bose gas will diverge in the zero-density, i.e., ideal limit. For the ideal case the local internal chemical potential $\bar{\mu}_{0c}$ is given by[10]

$$\bar{\mu}_{0c}=kT\ln\left[n\left[\frac{2\pi\hbar^2}{mkT}\right]^{3/2}\right] \ , \tag{4}$$

where k is Boltzmann's constant; $\bar{\mu}_{0c}$ clearly diverges as the density tends to zero. The divergence of $\bar{\mu}_{0c}$ (toward $-\infty$) as $n \rightarrow 0$ implies, via Eq. (2a), by the properties of $V(z)$, and by the thermodynamic inequality[10,11]

$$\left.\frac{\partial\bar{\mu}_0}{\partial n}\right|_{V,T}>0 \tag{5}$$

that $n(z)$ will not have a sharp cutoff, but will monotonically decrease from a maximum value of $n(0)$ toward zero as $z \rightarrow \pm\infty$. Thus the nonzero temperature LDA density profile is qualitatively different from the zero-temperature profile.

III. FINITE-TEMPERATURE CHEMICAL POTENTIAL OF THE UNIFORM WEAKLY INTERACTING BOSE GAS

We develop in this section an approximate though relatively accurate form for the finite-temperature local internal chemical potential function for the weakly interacting Bose gas.

We first consider the behavior of $\bar{\mu}_0(n)$ at finite T in the vicinity of the condensation density n_c.[12] The free energy of the uniform weakly nonideal Bose gas near n_c was analyzed by Huang, Yang, and Luttinger[13] (HYL). They used a lowest-order (in the s-wave scattering length) perturbation-theoretic approach to obtain the quasiparticle energies and then evaluated the partition function. They assumed the following conditions:

$$an^{1/3}\ll 1 \ , \tag{6a}$$

$$\bar{k}a\ll 1 \ , \tag{6b}$$

$$a/\lambda\ll 1 \ , \tag{6c}$$

$$a\lambda^2 n\ll 1 \ , \tag{6d}$$

where a is the s-wave scattering length for the interparticle potential, $\bar{k}$ is the mean relative wave number of any pair of particles, and λ is the thermal de Broglie wavelength, given by

$$\lambda=\left[\frac{2\pi\hbar^2}{mkT}\right]^{1/2} \ . \tag{7}$$

The criteria Eqs. (6) are satisfied for the possible experimental conditions of H↓ discussed below.

HYL obtained for the free energy per unit volume F/V (to first order in a/λ and $a\lambda^2 n$):

$$\frac{F}{V} = -kTn \begin{cases} \dfrac{1}{\lambda^3 n} g_{5/2}(y) - \ln y - 2a\lambda^2 n, & n \leq n_c \\[4mm] \dfrac{1}{\lambda^3 n} g_{5/2}(1) - 2a\lambda^2 n \left[1 - \dfrac{1}{2}\left[1 - \dfrac{g_{3/2}(1)}{n\lambda^3}\right]^2\right], & n \geq n_c \end{cases}$$

(8a)

(8b)

Here n_c is given by the ideal-gas result

$$n_c = \left[\frac{mkT}{3.31\hbar^2}\right]^{3/2} . \tag{9}$$

This result applies for n not too far from n_c. Here the functions $g_l(x)$ are defined via

$$g_l(x) \equiv \sum_{m=1}^{\infty} \frac{x^m}{m^l} . \tag{10}$$

We further have the special values: $g_{3/2}(1) = 2.612$, $g_{5/2}(1) = 1.342$. In Eqs. (8), y is determined as the solution of

$$g_{3/2}(y) = \lambda^3 n . \tag{11}$$

We note that $g_{3/2}(x)$ is monotonically increasing from $x = 0$ to $x = 1$, and has infinite first derivative at $x = 1$. Also, $x = 1$ corresponds to $n = n_c$.

The chemical potential $\bar{\mu}_{0,\text{bc}}$ within the HYL approach, i.e., near the Bose-condensation density is readily calculated from Eq. (8):

$$\bar{\mu}_{0,\text{bc}}(n) = \frac{\partial}{\partial n}\left[\frac{F}{V}\right]\bigg|_{V,T} = kT \begin{cases} \dfrac{n}{y}\dfrac{dy}{dn} - \dfrac{1}{\lambda^3}\dfrac{d}{dn}g_{5/2}(y) + \ln y + 4a\lambda^2 n, & n \leq n_c \\[4mm] 2a\left[\lambda^2 n + g_{3/2}(1)\dfrac{1}{\lambda}\right], & n \geq n_c \end{cases}$$

(12a)

(12b)

where again y satisfies Eq. (11). In deriving Eq. (12) we have made use of

$$\frac{d}{dx}g_{5/2}(x) = \frac{1}{x}g_{3/2}(x) . \tag{13}$$

Using Eq. (9) in Eqs. (12) we find for $n = n_c$:

$$\bar{\mu}_{0,\text{bc}}(n_c) = 4.17a\left[\frac{m}{\hbar^2}\right]^{1/2}(kT)^{3/2} . \tag{14}$$

We find for the first derivative of $\bar{\mu}_{0,\text{BC}}$ with respect to n, just below and just above n_c the following results:

$$\frac{d\bar{\mu}_{0,\text{bc}}(n)}{dn}\bigg|_{n_c^-} = 4a\lambda^2 kT , \tag{15a}$$

$$\frac{d\bar{\mu}_{0,\text{bc}}(n)}{dn}\bigg|_{n_c^+} = 2a\lambda^2 kT , \tag{15b}$$

In deriving Eqs. (15) we have made use of the following: Eq. (13), the result [which follows from Eq. (11)]:

$$\frac{dy}{dn} = \frac{\lambda^3}{\dfrac{d}{dy}g_{3/2}(y)} , \tag{16}$$

and the divergence of $d[g_{3/2}(y)]/dy$ at $y = 1$. Thus, the first derivative of $\bar{\mu}_{0,\text{BC}}$ with respect to n is discontinuous at n_c: the derivative drops by a factor of two as n increases through n_c. This nonanalyticity in the chemical potential will translate to a nonanalyticity in the nonuni-

form density profile (below).

We turn next to the form of the local internal chemical potential $\bar{\mu}_{0q}$ in the higher density quantum regime. For the dilute case we have

$$\bar{\mu}_{0q} = bna(1 + b_1(na^3)^{1/2}) - \bar{b}a^{1/2}\frac{T^2}{n^{1/2}} , \tag{17a}$$

with

$$b = \frac{4\pi\hbar^2}{m} , \tag{17b}$$

$$b_1 = \frac{32}{3\pi^{1/2}} , \tag{17c}$$

$$\bar{b} = \frac{\sqrt{\pi}}{6}\frac{m}{\hbar^2}k^2 . \tag{17d}$$

The first two terms on the right hand side of Eq. (17a) comprise the zero temperature result out to order $na(na^3)^{1/2}$, first evaluated by Lee and Yang[14] [the term bna is the Bogoliubov[15] result]. The temperature dependent term in Eq. (17a) is the approximate leading order temperature dependent correction evaluated within a mean field approach.[16]

The limiting low density form of the local internal chemical potential $\bar{\mu}_{0c}$ has been given in Eq. (4).

Finally we adopt the following form for the nonzero temperature local internal chemical potential over the relevant density range:

$$\bar{\mu}_0(n) = \begin{cases} \bar{\mu}_{0c}(n) = kT\ln\left[n\left[\dfrac{2\pi\hbar^2}{mkT}\right]^{3/2}\right], & n \leq n_l, \quad (18a) \\[2ex] \bar{\mu}_{0l}(n) = c_{l1} + c_{l2}\ln n + c_{l3}n^{1/4} + c_{l4}n^{1/2}, & n_l \leq n \leq n_c, \quad (18b) \\[2ex] \bar{\mu}_{0u}(n) = c_{u1} + c_{u2}n + c_{u3}n^2 + c_{u4}n^3, & n_c \leq n \leq n_u, \quad (18c) \\[2ex] \bar{\mu}_{0q}(n) = bna(1 + b_1(na^3)^{1/2}) - \bar{b}a^{1/2}\dfrac{T^2}{n^{1/2}}, & n_u \leq n \leq n_u'. \quad (18d) \end{cases}$$

Here n_l, n_u, and n_u' are appropriate cutoffs for the applicability of the classical and quantum forms for $\bar{u}_0$ (see below). The function $\bar{\mu}_{0l}(n)$ is an interpolant whose coefficients c_{lj}, $j = 1, \ldots 4$, are chosen to insure the following continuity conditions:

$$\bar{\mu}_{0l}(n_l) = \bar{\mu}_{0c}(n_l), \quad (19a)$$

$$\frac{d}{dn}\bar{\mu}_{0l}\bigg|_{n_l} = \frac{d}{dn}\bar{\mu}_{0c}\bigg|_{n_l}, \quad (19b)$$

$$\bar{\mu}_{0l}(n_c) = \bar{\mu}_{0,\mathrm{bc}}(n_c), \quad (19c)$$

$$\frac{d}{dn}\bar{\mu}_{0l}\bigg|_{n_c} = \frac{d}{dn}\bar{\mu}_{0,\mathrm{bc}}\bigg|_{n_c^-}. \quad (19d)$$

Similarly $\bar{\mu}_{0u}(n)$ is an interpolant whose coefficients c_{uj}, $j = 1, \ldots 4$, are chosen to insure the following continuity conditions:

$$\bar{\mu}_{0u}(n_u) = \bar{\mu}_{0q}(n_u), \quad (20a)$$

$$\frac{d}{dn}\bar{\mu}_{0u}\bigg|_{n_u} = \frac{d}{dn}\bar{\mu}_{0q}\bigg|_{n_u}, \quad (20b)$$

$$\bar{\mu}_{0u}(n_c) = \bar{\mu}_{0,\mathrm{bc}}(n_c), \quad (20c)$$

$$\frac{d\bar{\mu}_{0u}}{dn}\bigg|_{n_c} = \frac{d}{dn}\bar{\mu}_{0,\mathrm{bc}}\bigg|_{n_c^+}. \quad (20d)$$

Thus the two interpolants smoothly connect the immediate near Bose condensation density regime to, respectively, the limiting classical and quantum regimes. Note from Eqs. (19), (20), and (15) that the interpolants build in the correct discontinuous density derivative of $\bar{\mu}_{0,\mathrm{bc}}$ at $n = n_c$.

The cutoffs n_l, n_u, and n_u' are chosen as follows: The classical expression $\bar{\mu}_{0c}$ will be valid in the ideal limit when $e^{\bar{\mu}_{0c}/kT} \ll 1$, i.e., when the single particle state occupations are small. This then gives the condition [using Eq. (4)]:[10]

$$n\left[\frac{2\pi\hbar^2}{mKT}\right]^{3/2} \ll 1. \quad (21)$$

We choose for n_l the value for which the left hand side of Eq. (21) equals 0.01:

$$n_l = 0.01\left[\frac{mkT}{2\pi\hbar^2}\right]^{3/2}. \quad (22)$$

This estimate of n_l should be reasonable for the case of weak interactions present as well.

The criterion for n_u is such that for $n = n_u$ the temperature dependent term in Eq. (18d) is a small fraction (we choose 0.1) of the first zero temperature term. For densities appreciably lower than this n_u, the temperature dependent term, which is inversely proportional to $n^{1/2}$, will become too large for approximation Eq. (17a) to be valid. Furthermore, for this choice of n_u the omitted correction to the approximate $\bar{\mu}_{0q}$ [Eqs. (17)] will be roughly of order ~ 0.01 of the retained form for $n = n_u$. We thus find from Eqs. (17):

$$n_u = \left[\frac{1}{2.4\pi^{1/2}\lambda^{1/2}}\left[\frac{m^2k^2}{\hbar^4}\right]T^2\right]^{2/3}. \quad (23)$$

The choice of n_u' is such that the interaction correction involving b_1 in Eq. (17a) is of the order of ~ 0.1 times the leading order $T = 0$ term. We obtain from Eqs. (17):

$$n_u' = 0.01\left[\frac{3\pi^{1/2}}{32}\right]^2\frac{1}{a^3} = 2.76\times10^{-4}\frac{1}{a^3}. \quad (24)$$

For n greater than n_u' we would have to include terms in $\bar{\mu}_{0Q}$ beyond those of Eq. (17a).

Figure 1 gives plots of $\bar{\mu}_0(n)$ for temperatures 30 and 100 mK. We choose, appropriate for H↓, the value $a = 7.4\times10^{-11}$ m. The plots are over a large density range which spans from the classical region, through the cross over region (encompassing the Bose condensation density regime), and into the quantum region. Values of n_l, n_c, and n_u are indicated in the figure. The discontinuity in the first density derivative at n_c is barely in evidence in the semilog plot. The main difference between the two curves is in the low density region well below n_c. For densities rather greater than n_u, the two curves become very close indicating the decreasing importance of the temperature in this relatively high density quantum regime. Both curves are confined to $n < n_u' \approx 6.8\times10^{26}$ m^{-3}. We note that in the vicinity of n_c, $\bar{\mu}_0(n)$ exhibits a marked flattening.
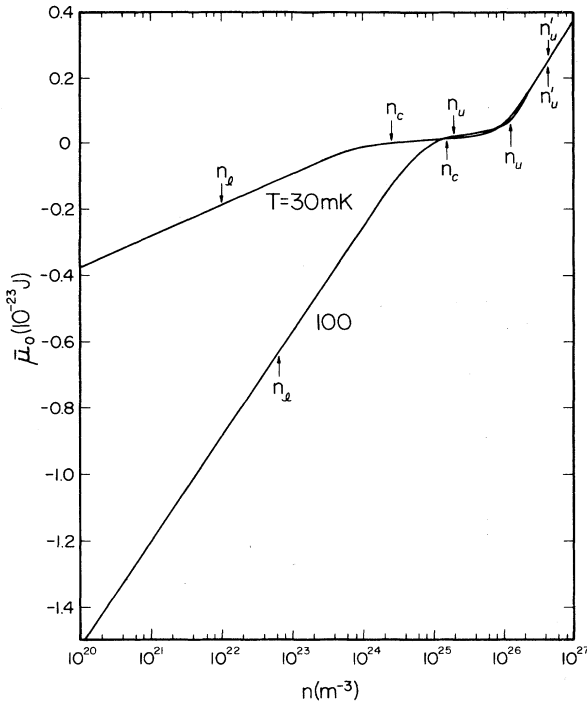
FIG. 1. Chemical potential of a uniform weakly interacting Bose gas (Bogoliubov approximation) for temperatures 30 and 100 mK. Parameter values are appropriate to $H\downarrow$ (see text). Values of n_l, n_c, n_u and n_u' are indicated for the two curves [downward (upward) arrows for 30 mK (100 mK)]; n_u' value is same for both curves.

IV. LDA PROFILE OF THE CONFINED WEAKLY INTERACTING BOSE GAS AT NONZERO TEMPERATURE

We implement the program of Sec. II using the internal chemical potential form of Sec. III. We consider confining potential energies of the form

$$V(z) = V_0 \left[\frac{|z|}{z_s} \right]^\nu , \qquad (25)$$

where V_0, z_s, and ν are all positive constants. We initially consider the extreme dilute limit wherein we can ignore the higher order interaction correction term involving b_1 in Eq. (17a), i.e., the Bogoliubov case.

We choose parameters which model typical arrangements for magnetic confinement of $H\downarrow$. Thus, as with GSL,[6] we use $m = 1.67 \times 10^{-27}$ kg, $a = 7.4 \times 10^{-11}$ m, $A = 10^{-6}$ m^2, $N = 10^{16}$. Further we set $V_0 = \mu_B B_0$, with magnetic field parameter $B_0 = 10$ T, with μ_B the electron Bohr magneton, and $z_s = 5.1 \times 10^{-2}$ m. We consider two potential well forms: $\nu = 1, 2$.

Now the H-atom $1s$ energy level will split in a magnetic field into four hyperfine levels.[3] For relevant large fields the splitting of the lowest two hyperfine levels ΔE is[2,17]

$$\Delta E \approx 2(\alpha_H + \tfrac{1}{2} g_p \mu_N B) , \qquad (26a)$$

$$= 3.4 \times 10^1 \text{mK} + (2.0 \text{ mK/T}) B , \qquad (26b)$$

where $4\alpha_H$ is a zero field hyperfine splitting, $g_p = 5.58$ is the proton g factor, and μ_N is the nuclear Bohr magneton; the magnetic field B is in Tesla. We analyze the system on the assumption that the parameters are such that only the lowest hyperfine level is appreciably occupied. This may require the application of a large uniform field B_u in addition to the nonuniform confining field.

Figure 2 shows density profiles for the above system for the symmetric, "linear" potential well ($\nu = 1$) and for four temperatures. The $T = 0$ profile was analyzed earlier and found to be linear for $z_0 > |z| > 0$.[2] We then see the effect of increasing temperature is to deplete the region near $z = 0$, and to redistribute the particles out to larger z; in fact, as noted above, the density is nonzero for all z. This contrasts with the $T = 0$ LDA profile which goes to zero at a finite $z = \pm z_0$.

The $T = 0$ profile is largely associated with nearly complete Bose condensation into the lowest single-particle state within each thin (on the scale of z_0) slab normal to the z axis;[18] this is referred to as condensate broadening.[1] As temperature increases a thermal depletion of the condensate occurs. The Bose condensation densities are indicated in the three nonzero temperature curves. We note that the profiles for 60 and 80 mK ("intermediate" temperatures) exhibit a relatively steep portion for $n > n_c$ and a flatter portion for $n < n_c$. Moreover there is a discontinuity in dn/dz at n_c (see below). The condensate fraction decreases to zero as n decreases to n_c. For sufficiently large T (e.g., for $T = 100$ mK in Fig. 2) the condensate is absent and the profile tends to the thermally dominated classical form.

We next turn to the case of the quadratic potential well ($\nu = 2$). Figure 3 shows density profiles at four temperatures. Again, at $T = 0$ the profile is dominated by the condensate.[1,2] The effect of going from the symmetric linear to the quadratic well (keeping V_0 and z_s fixed) is to
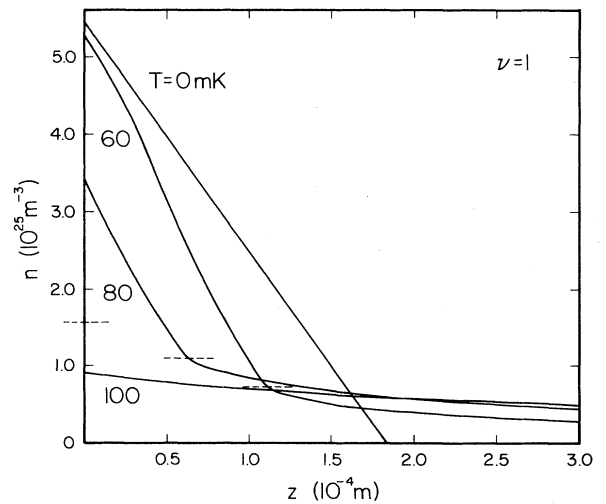

FIG. 2. Density profiles of a weakly interacting Bose gas (Bogoliubov approximation), confined to a symmetric linear potential energy well for several temperatures. GSL parameter values (appropriate to magnetically confined $H\downarrow$). Horizontal dashed lines are at density n_c. Note: for $T = 100$ mK, $n_c > n(0)$.
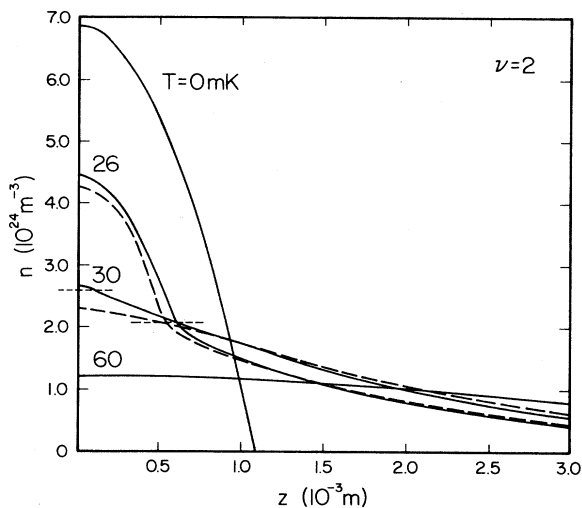
FIG. 3. Density profiles of a weakly interacting Bose gas (Bogliubov approximation), confined to a quadratic potential energy well for several temperatures. GSL parameter values (appropriate to magnetically confined H↓). Solid lines are present theory; dashed lines are GSL theory. Horizontal dashed lines are at density n_c. Note: right dashed line is for $T = 26$ mK.

allow the gas to extend out to larger z. For $T = 26$ mK the condensate is significantly thermally depleted and the lower density tail is large. For $T = 30$ mK the curve evidences a very weak residual condensate whereas for $T = 60$ mK there is no condensation. Comparison is made in Fig. 3 to the GSL calculation for the same parameters (at $T = 26$, 30 mK). We see that the GSL curves are a few percent lower than the present curves for the higher n central region while lying just above the present curves in the outer tail region of the profile.

We consider the legitmacy of the single hyperfine level occupancy assumption for the above two cases. At zero temperature it is appropriate to consider a "Bose temperature" T_{B_0} which is the temperature corresponding to the mean energy per particle at the density maximum;[2,19] this reflects the interactions in the system and vanishes in the $T = 0$ ideal limit. For the above parameters for $\nu = 1,2$ it is found that $T_{B_0} = 12.1$ (1.54) mK for $\nu = 1$ (2).[19] From Eq. (2b) we find with an additional uniform field $B_u = 200$ T an additional splitting of $\Delta E \approx 430$ mK. This is much greater than T_{B_0} for $\nu = 1,2$ and in fact is somewhat greater than kT for the temperatures considered. Thus single band occupation is effectively realizable.

We mention that the discontinuity in the derivative of $\bar{\mu}_0$ with respect to n [Eqs. (15)] implies the above noted discontinuity in the density profile: We readily find from Eq. (2a), with Eqs. (15), and using the continuity of $V(z)$:

$$\frac{(dn/dz)\,|\,z_c^-}{(dn/dz)\,|\,z_c^+} = 2 \ , \tag{27}$$

where z_c is the z value at which $n = n_c$. Note the result Eq. (27) is independent of both $V(z)$ and T. Indeed the ν and T independence of this slope ratio is evident in Figs.

2 and 3.

We next consider the effect of including the next higher-order term in the interaction strength in the local internal chemical potential in the quantum regime [i.e., including the term involving b_1, in Eq. (17a)]. We expect that this correction will have the effect of decreasing the density in the higher density $(z \approx 0)$ region and (to conserve particles) increasing the density in the larger $|z|$ region. For our model calculation we use the above GSL parameters except that we use $N = 2 \times 10^{19}$ in order to increase the importance of the correction. Density profiles for the quadratic well for three temperatures are given in Fig. 4. For each temperature we show the curves with and without the higher order interaction correction. The effect of the additional interaction term is greatest for the $T = 0$ case; this follows since the $T = 0$ curve has the largest peak density. By the time the temperature has increased to 1.3 K the effect of the interaction correction on the profile is negligible. Note that the $T = 1.05$ K interaction correction curve is just slightly above the Bogoliubov curve for $z \gtrsim 1 \times 10^{-2}$ m.

We check the single band occupancy assumption for the higher N considered here. We find for $T = 0$, $T_{B_0} \approx 244$ mK; thus $B_u = 500$ T $\Longrightarrow \Delta E \approx 1000$ mK will give single band occupancy at $T = 0$. For this B_u, ΔE is of the order of the largest kT considered. Our highest T
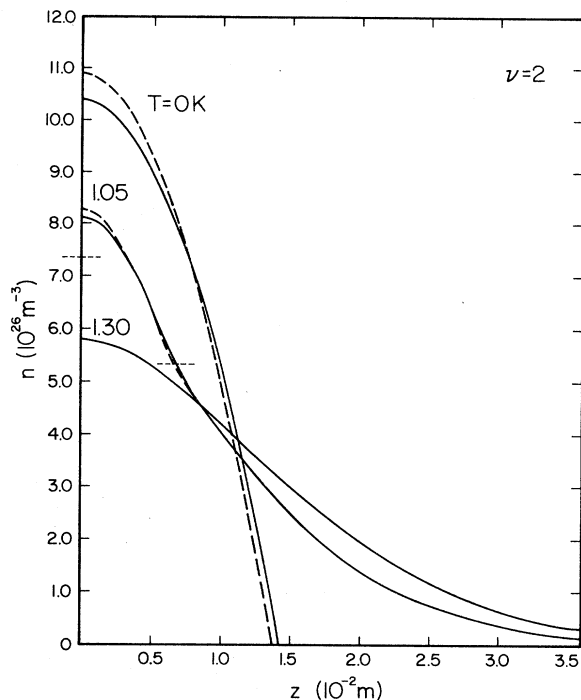

FIG. 4. Density profiles of a weakly interacting Bose gas confined to a quadratic potential energy well for several temperatures: effect of higher order interactions. Dashed line is Bogoliubov result; solid line includes next interaction correction beyond Bogoliubov term in internal chemical potential. GSL parameter values except $N = 2 \times 10^{19}$ (appropriate to magnetically confined H↓). Horizontal dashed lines are at density n_c. Note: for $T = 1.30$ K, $n_c > n(0)$.

results are thus compatible with single band occupation for $B_u \gtrsim 2000$ T. Naturally at somewhat lower T a somewhat lower value of B_u can be used.

Note that it would not be justified to use Eq. (17a) (including the $\sim b_1$ term) for significantly higher N, i.e., higher peak profile density, since $n_u' \sim 10^{27}$ m^{-3}. That is, roughly beyond the density at the peak of the $T=0$ curve, the quantum expression Eq. (17a) for $\bar{\mu}_{0q}$ loses validity.

Finally we briefly comment on the applicability of the LDA. Firstly, this issue has been considered in the same detail for the case of $T=0$.[2] Of particular concern for the case of $T=0$ was the near surface region of the profile. It was concluded that for relevant parameters of interest the $T=0$ LDA profile was justified over all the profile except a generally very small (macroscopically) region near the surface. For finite temperature the surface does not exist and thus the special concerns at $T=0$ do not enter. The peaked condensate part of the profile at finite temperature should be fairly accurately given in LDA since it is comparable to the $T=0$ profile (away from the surface), which generally, again, is well given within LDA. The nearby lower density thermal tail region with its relatively slow density variation should also be handled accurately in LDA.

V. CONCLUSION

We have analyzed the nonzero temperature density profile of a weakly interacting Bose gas confined within a potential well. Our approach starts with the principle of the constancy of the chemical potential in a nonuniform system in equilibrium. In turn we make use of a local density approximation in treating the internal chemical potential. The latter is approximately evaluated using known low density, intermediate, (i.e., near condensation) density, and high density forms with appropriate interpolants connecting these three forms. The approach taken here differs from those of previous studies.

Density profiles $n(z)$ were calculated in the Bogoliubov approximation for the local internal chemical potential for parameters appropriate to H$\downarrow$ for both symmetric linear and quadratic well. We compared to GSL (who examined the quadratic case only) and found very close agreement. A general conclusion was reached that dn/dz was discontinuous at $z=z_c$ (i.e., where $n=n_c$), with the magnitude of the left derivative there twice that of the right derivative, independent of the potential or temperature. We also investigated the effect of including the next highest interaction term in the internal chemical potential. For a higher density model of H$\downarrow$ we found that this led to a noticeable drop in density near the well minimum. An assessment of the LDA was also given.

A next natural step in this effort would be to incorporate higher-order interaction corrections in the internal chemical potential (e.g., in the higher-density quantum region and near n_c). Density profiles with higher peak densities could then be investigated.

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