The Density Distribution of a Weakly Interacting Bose Gas in an External Potential*

David A. Huse and Eric D. Siggia

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York

The Gross–Pitaevskii equations are generalized to finite temperatures by means of the self-consistent Hartree–Fock and Bogolyubov approximations that are derived through a variational principle for the optimal set of one-particle eigenstates. A number of sample density profiles are provided for spin-polarized atomic hydrogen when the external potential depends on the z coordinate only.

1. INTRODUCTION

Spin-polarized atomic hydrogen (H↓) at densities less than or of order 10^{19} cm^{-3} is a weakly interacting Bose gas.[1] To stabilize the atoms against recombination into molecules requires a strong magnetic field. In practice the magnetic field is nonuniform and serves to confine the gas.[2,3] It is of interest, therefore, to study theoretically the behavior of a weakly interacting Bose gas in an inhomogeneous potential.

This problem has of course been examined previously, in the context of superfluid ^{4}He, both at low temperatures, where the mean field equations of Gross and Pitaevskii apply, and near the critical point $T = T_c$, where scaling ideas are used.[4] In ^{4}He away from T_c healing lengths are very small and of largely theoretical interest. In H↓, however, Walraven and Silvera pointed out that the change in the density profile that accompanies Bose condensation is dramatic and susceptible to direct experimental measurement.[2,5] Our goal in this paper will therefore be to generalize the Gross–Pitaevskii theory to finite temperatures but avoid temperatures so close to T_c that critical fluctuations are important.

This is naturally accomplished through the finite-temperature self-consistent Hartree–Fock equations that we derive variationally in Section 2.

Within this approximation, Bose condensation corresponds to the macroscopic occupancy of the lowest one-particle eigenstate. Neither the derivation nor the results of Hartree–Fock are entirely trivial and the correct equations are rather more complicated than the corresponding theory for an inhomogeneous Fermi system. For physically reasonable parameters below T_c, one finds a nearly discontinuous change in density near the condensate edge and a pseudo-gap in the density of states of order the mean interparticle potential that would be visible in the low-temperature specific heat. Both these features are unphysical and disappear when we derive the Bogolyubov–Hartree–Fock theory in Section 3. The resulting equations are sufficiently complicated, however, that quantitative density profiles appear to require considerable numerical analysis.

We will ignore the hyperfine structure of H↓ here and treat it as a spinless boson. It would be relatively easy, though, to include the second hyperfine state which would necessarily be part of the "normal" fluid. It was argued in Ref. 6 that if the conditions necessary for both hyperfine states individualy to condense were ever achieved, rapid phase separation would ensue.

Some of the results of Section 2 were obtained simultaneously by Goldman et al.[10]

2. HARTREE–FOCK APPROXIMATION

The Hamiltonian for an interacting Bose gas in a potential $u(\mathbf{r})$ is, in second quantized notation,

$$H = \int d^3 r\, \hat{\psi}^\dagger(\mathbf{r})[-(\hbar^2/2m)\nabla^2 + u(\mathbf{r})]\hat{\psi}(\mathbf{r})$$

$$+ \tfrac{1}{2} \int d^3 r\, d^3 r'\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \tag{1}$$

We will approximate the interparticle potential as a delta function with weight $v = \hbar^2 4\pi a/m$, where a is the s-wave scattering length. For H↓ the triplet potential has $a = 0.72$ Å.[7] The variational principle says that for a given temperature T $(\beta = 1/k_B T)$ and chemical potential μ the grand potential

$$\Omega = -k_B T \ln (\text{Tr } e^{-\beta(H-\mu N)}) \tag{2}$$

satisfies $\Omega \le \tilde{\Omega}(H_t)$ for any trial Hamiltonian H_t, where

$$\tilde{\Omega}(H_t) = \Omega_t + \langle H \rangle_t - \langle H_t \rangle_t \tag{3}$$

Ω_t is the grand potential of the system obeying the trial Hamiltonian, and

$\langle \mathcal{O} \rangle_t$ is the expectation value of $\mathcal{O}$ in the ensemble defined by H_t. A trial Hamiltonian with many free parameters may be used and the best approximation to the true system is obtained by minimizing $\tilde{\Omega}(H_t)$.*

We first consider a general one-body trial Hamiltonian in diagonal form,

$$H_t = \sum a_k^{\dagger} \varepsilon_k a_k \tag{4}$$

where

$$a_k = \int d^3 r \, \psi_k(\mathbf{r}) \hat{\psi}(\mathbf{r}) \tag{5}$$

and the $\{\psi_k\}$ are a complete orthogonal set of single-particle wave functions normalized to unity. To avoid macroscopic density fluctuations in our trial ensemble when the system is Bose-condensed, the lowest energy single-particle state must be treated specially; the trial ensemble will have the restriction $a_0^{\dagger} a_0 = N_0$. In the thermodynamic limit ($n_k/N = 0$ for all $k \neq 0$) we obtain

$$\tilde{\Omega}(H_t, N_0) = k_B T \sum_{k \neq 0} \ln\left(1 - e^{-\beta(\varepsilon_k - \mu)}\right) + N_0(\langle 0|H_0|0\rangle - \mu)$$

$$+ \sum_{k \neq 0} n_k(\langle k|H_0|k\rangle - \varepsilon_k) + \tfrac{1}{2}N_0^2 \langle 00|V|00\rangle$$

$$+ 2N_0 \sum_{k \neq 0} n_k \langle 0k|V|0k\rangle + \sum_{j \neq 0} \sum_{k \neq 0} n_j n_k \langle jk|V|jk\rangle \tag{6}$$

where $n_k = \{\exp[\beta(\varepsilon_k - \mu)] - 1\}^{-1}$ are the usual boson occupation numbers, H_0 is the one-body part of the Hamiltonian,

$$\langle j|H_0|k\rangle = \int d^3 r \, \psi_j^*[-(\hbar^2/2m)\nabla^2 + u(\mathbf{r})]\psi_k(\mathbf{r}) \tag{7a}$$

and V involves the interparticle interactions,

$$\langle jk|V|lm\rangle = v \int d^3 r \, \psi_j^*(\mathbf{r})\psi_k^*(\mathbf{r})\psi_l(\mathbf{r})\psi_m(\mathbf{r}) \tag{7b}$$

Note that the integral in (7b) is of order an inverse volume. We define the condensate density to be $\rho_0(\mathbf{r}) = N_0|\psi_0(\mathbf{r})|^2$, while the total density is $\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r})$, where

$$\rho_1(\mathbf{r}) = \sum_{k \neq 0} n_k|\psi_k(\mathbf{r})|^2 \tag{8}$$

When $\tilde{\Omega}$ is minimized with respect to N_0 and ε_k we obtain

$$\langle 0|H_0 + 2v\rho_1 + v\rho_0|0\rangle = \mu \tag{9}$$

*This is done in detail for the uniform system in Ref. 8.

and, for $k \neq 0$,

$$\langle k|H_0 + 2v\rho|k\rangle = \varepsilon_k \qquad (10)$$

respectively, where $\langle j|v\rho_0|k\rangle \equiv N_0\langle j0|V|k0\rangle$ and

$$\langle j|v\rho_1|k\rangle \equiv \sum_{l \neq 0} n_l\langle jl|V|kl\rangle \qquad (11)$$

The wave functions $\{\psi_k\}$ are also free "parameters" in H_t subject to the constrain that they remain a complete orthonormal set. It is not practical to consider arbitrary variations in the $\{\psi_k\}$ and then impose the orthonormality constraints by a sufficient number of Lagrange multipliers because for arbitrary $\{\psi_k\}$ the trial Hamiltonian is not necessarily diagonal, so $\tilde{\Omega}$ is difficult to obtain. The *permitted* variations in the $\{\psi_k\}$ are basis changes that leave H_t diagonal. We therefore demand that $\tilde{\Omega}$ be stationary under an arbitrary infinitesimal basis change of the form

$$\psi_k \to \psi_k + \sum_j \eta_{jk}\psi_j \qquad (12)$$

with $\eta_{jk}^* = -\eta_{kj}$ for unitarity and $|\eta_{jk}| \ll 1$. The resulting equations are

$$\langle k|H_0 + 2v\rho_1 + v\rho_0|0\rangle = \mu\delta_{k0} \qquad (13)$$

and, for $j \neq 0$ and $k \neq 0$,

$$\langle j|H_0 + 2v\rho|k\rangle = \varepsilon_k\delta_{jk} \qquad (14)$$

The above two sets of equations may be satisfied if the single-particle states are all eigenstates of the effective single-particle Hamiltonian

$$H_{\text{eff}} = H_0 + 2v\rho - |0\rangle\langle 0|v\rho_0 - v\rho_0|0\rangle\langle 0| + |0\rangle\langle 0|v\rho_0|0\rangle\langle 0| \qquad (15)$$

with $H_{\text{eff}}|k\rangle = \varepsilon_k|k\rangle$ and $\varepsilon_0 = \mu$. Note that H_{eff} is a nonlocal operator. The condensate, however, is also an eigenstate of a local operator, namely

$$(H_0 + 2v\rho - v\rho_0)|0\rangle = \mu|0\rangle \qquad (16)$$

To summarize, in position space we have the following infinite set of self-consistent integrodifferential equations:

$$-(\hbar^2/2m)\nabla^2\psi_0(\mathbf{r}) + [u(\mathbf{r}) + 2v\rho_1(\mathbf{r}) + vN_0|\psi_0(\mathbf{r})|^2]\psi_0(\mathbf{r}) = \mu\psi_0(\mathbf{r}) \qquad (17)$$

$$-(h^2/2m)\nabla^2\psi_k(\mathbf{r}) + \{u(\mathbf{r}) + 2v[\rho_1(\mathbf{r}) + N_0|\psi_0(\mathbf{r})|^2]\}\psi_k(\mathbf{r})$$

$$-vN_0\psi_0(\mathbf{r})\{[|\psi_0(\mathbf{r})|^2 - \int d^3r' \, |\psi_0(\mathbf{r}')|^4]$$

$$\times \int d^3r'' \, \psi_0^*(\mathbf{r}'') \, \psi_k(\mathbf{r}'')$$

$$+ \int dr' \, \psi_0^*(\mathbf{r}')|\psi_0(\mathbf{r}')|^2\psi_k(\mathbf{r}')\} = \varepsilon_k\psi_k(\mathbf{r}) \tag{18}$$

The effective Hamiltonian (15) may be written as $H_{\text{eff}} = H_0 + 2v\rho + H_1$ and the nonlocal part H_1 may be treated as a perturbation. In fact, in a macroscopic system H_1 is an extremely small perturbation for all but possibly a very few $k \neq 0$ single-particle states. Therefore we will ignore the perturbation for all states other than the condensate. Formally, however, it must be included to guarantee that $\langle k|0\rangle = 0$. In a macroscopic system with a smooth potential the kinetic energy of the condensate in (17) is also negligible, so we may approximate the condensate density as

$$v\rho_0(\mathbf{r}) = [\mu - u(\mathbf{r}) - 2v\rho_1(\mathbf{r})]\theta(\mu - u(\mathbf{r}) - 2v\rho_1(\mathbf{r})) \tag{19}$$

everywhere except near the edge of the condensate, where the argument of the above theta function vanishes. The validity of this approximation is examined below.

Let us adopt a further approximation suggested by recent experiments[2,3] and assume that the external potential $u(\mathbf{r})$ is a function only of z. This approximation may be used because the sample chamber confines the gas to the vicinity of the z axis. Since the true potential is proportional to a magnetic field with zero curl, however, it will have an x and y dependence, and the absolute minimum, where the condensate will first appear on cooling, must be on the surface of the chamber.

If the potential is a function of z only and varies on a sufficiently slow scale it is sensible to use the semiclassical or WKB approximation for the wave functions $\{\psi_k, k \neq 0\}$. The errors inherent in using this approximation are significant only near the edge of the condensate and are examined below. Assuming periodic boundary conditions in the x–y plane, each single-particle state is identified by a momentum $\hbar k$ in the x–y plane and an energy eigenvalue ε_z for the motion in the z direction. The wave function to first order in the WKB approximation is

$$\psi_{\mathbf{k},\varepsilon}(\mathbf{r}) \propto [\exp(i\mathbf{k}\cdot\mathbf{r})]\{2m[\varepsilon_z - u_{\text{eff}}(z)]/\hbar^2\}^{-1/4} \tag{20}$$

where the local effective potential is

$$u_{\text{eff}}(z) = u(z) + 2v\rho(z) - \mu \tag{21}$$

In integrating Eq. (8) with the above expression for the wave functions, the

density of states and normalization of the wave function conveniently cancel, leaving

$$\rho_1(z) = \frac{m}{2\pi^2\hbar} \int_0^\infty k \, dk \int_{u_{\text{eff}}(z)}^\infty \frac{d\varepsilon_z \{2m[\varepsilon_z - u_{\text{eff}}(z)]\}^{-1/2}}{\{\exp[\beta(\varepsilon_z + \hbar^2 k^2/2m)]\} - 1} \quad (22)$$

$$= \lambda^{-3} g_{3/2}(\exp[-\beta u_{\text{eff}}(z)]) \quad (23)$$

where $\lambda = (2\pi\hbar^2/mk_B T)^{1/2}$ is the thermal de Broglie wavelength and $g_{3/2}(z)$ is the usual Bose function.[9]

The first-order WKB approximation will not be valid at z for the states with the lowest ε_z, say for $\varepsilon_z - u_{\text{eff}}(z) \lesssim \tilde{\varepsilon}(z)$. Assuming that the error made in (20) is then a factor of order unity, the error in the above expression for $\rho_1(z)$ may be estimated as

$$\delta\rho_1(z) \approx \mathcal{O}\left(\frac{m}{\hbar} \int_0^\infty k \, dk \int_{u_{\text{eff}}(z)}^{u_{\text{eff}}(z)+\tilde{\varepsilon}(z)} \frac{d\varepsilon_z \{2m[\varepsilon_z - u_{\text{eff}}(z)]\}^{-1/2}}{\{\exp[\beta(\varepsilon_z + \hbar^2 k^2/2m)]\} - 1}\right)$$

$$\approx \mathcal{O}\left(\frac{[2m\tilde{\varepsilon}(z)]^{1/2}}{\hbar\lambda^2}\right) \quad (24)$$

The last estimate follows from the assumption $\beta[u_{\text{eff}}(z) + \tilde{\varepsilon}(z)] \ll 1$, which is appropriate in the regions where this error may be significant.

Within certain approximations we then have a relatively simple set of coupled equations for the local densities, namely (19), (21), and (23). The derivation of Eq. (23) depended on having translational invariance in the x–y plane. However, the same equation (with $\mathbf{r}$ substituted for z) may be obtained in a somewhat less rigorous fashion for an arbitrary, albeit smooth and gradual, potential by using a Thomas–Fermi-like approach.

The theta function in Eq. (19) separates the solutions of the coupled equations into two types. Those with $\rho_0(z) = 0$ are only possible for

$$u(z) \geq u(z_a) \equiv \mu - 2v\lambda^{-3}\zeta(3/2) \quad (25)$$

because $\rho_1(z)$ is bounded above by $\zeta(3/2)/\lambda^3$, where $\zeta(3/2) = \sum n^{-3/2} \simeq 2.612$. For $\rho_0(z) \neq 0$ we see that $u_{\text{eff}}(z) = v\rho_0(z)$. Three examples of solutions to the coupled equations for the densities are shown in Fig. 1. The quadratic potential of Walraven and Silvera[2] $u(z) = \mu_e B_0(z^2/l^2 - 1)$ has been used, with $B_0 = 10$ T and $l = 5.1$ cm. The discontinuities in the densities are discussed below.

Our analysis is only valid for a *dilute* Bose gas, which means $v\rho \ll k_B T_c$, where T_c is the Bose condensation temperature. Thus in the region where $\rho_0 \neq 0$, we have $\beta u_{\text{eff}} = \beta v\rho_0 < \beta v\rho \ll T_c/T$, so we may assume $\beta u_{\text{eff}} \ll 1$ as long as the temperature is not too far below T_c. For $\beta u_{\text{eff}}(z) \ll 1$ ·the expansion[9] $g_{3/2}(e^{-\alpha}) = \zeta(3/2) - 2(\pi\alpha)^{1/2} + \cdots$ may be used in Eq. (23) and
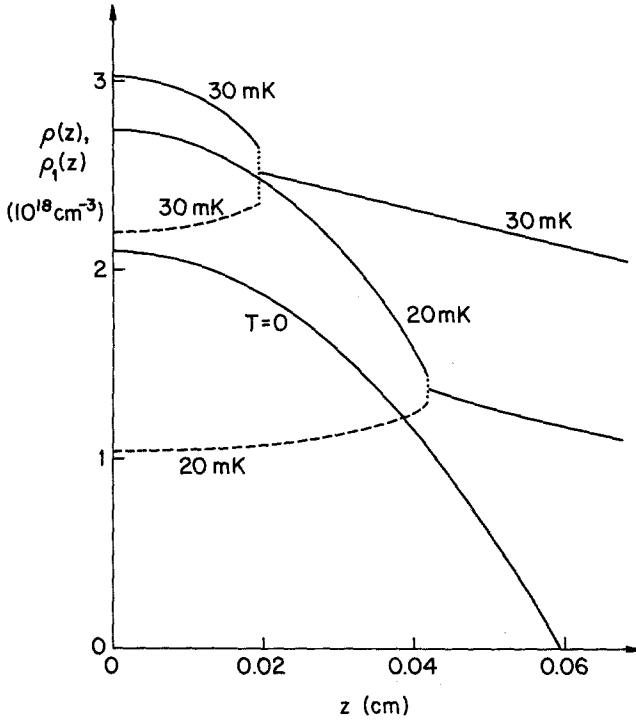
Fig. 1. Density profiles of a weakly interacting Bose gas in a quadratic potential as calculated in the finite-temperature self-consistent Hartree–Fock approximation. Three different temperatures and total amounts of gas are illustrated, using the potential of Walraven and Silvera,[2] $u(z) = \mu_e B_0(z^2/l^2 - 1)$, with $B_0 = 10$ T and $l = 5.1$ cm. The solid lines denote the total density $\rho(z)$, while the dashed lines indicate $\rho_1(z)$, the density of particles not in the Bose condensate.

the coupled equations for the densities are thereby reduced to a single quadratic equation in the dimensionless variable $[\hbar^2\lambda^4 u_{\text{eff}}(z)/2mv^2]^{1/2}$. As noted above, there are two types of solutions. When inequality (25) is satisfied there is a solution with $\rho_0 = 0$ and

$$\left[\frac{\hbar^2\lambda^4 u_{\text{eff}}(z)}{2mv^2}\right]^{1/2} = \left\{1 + \frac{\hbar^2\lambda^4}{2mv^2}\left[u(z) + \frac{2mv}{\hbar^2\lambda^3}\zeta\left(\frac{3}{2}\right) - \mu\right]\right\}^{1/2} - 1 \quad (26)$$

There are also solutions with $u_{\text{eff}}(z) = v\rho_0(z) \neq 0$ and

$$\left[\frac{\hbar^2\lambda^4 u_{\text{eff}}(z)}{2mv^2}\right]^{1/2} = 1 \pm \left\{1 - \frac{\hbar^2\lambda^4}{2mv^2}\left[u(z) + \frac{2mv}{\hbar^2\lambda^3}\zeta\left(\frac{3}{2}\right) - \mu\right]\right\}^{1/2} \quad (27)$$

When the inequality (25) is violated the solution with the plus sign in (27) is

unique. However, for z such that

$$u(z_a) \leq u(z) \leq u(z_b) \equiv u(z_a) + 2mv^2/\hbar^2\lambda^4 \qquad (28)$$

all three solutions to the coupled equations for the density are present. This is illustrated in Fig. 2. For $u(z) > u(z_b)$ only the solution (26) exists. Somewhere between z_a and z_b the densities must therefore have a discontinuity of order $mv/\hbar^2\lambda^4$. Precisely where this discontinuity occurs is determined by searching for the *minimum* of $\tilde{\Omega}$ in (6) rather than just an extremum. In doing so one notes that the "middle" solution, the minus sign in Eq. (27), corresponds to a maximum in the free energy and so is not
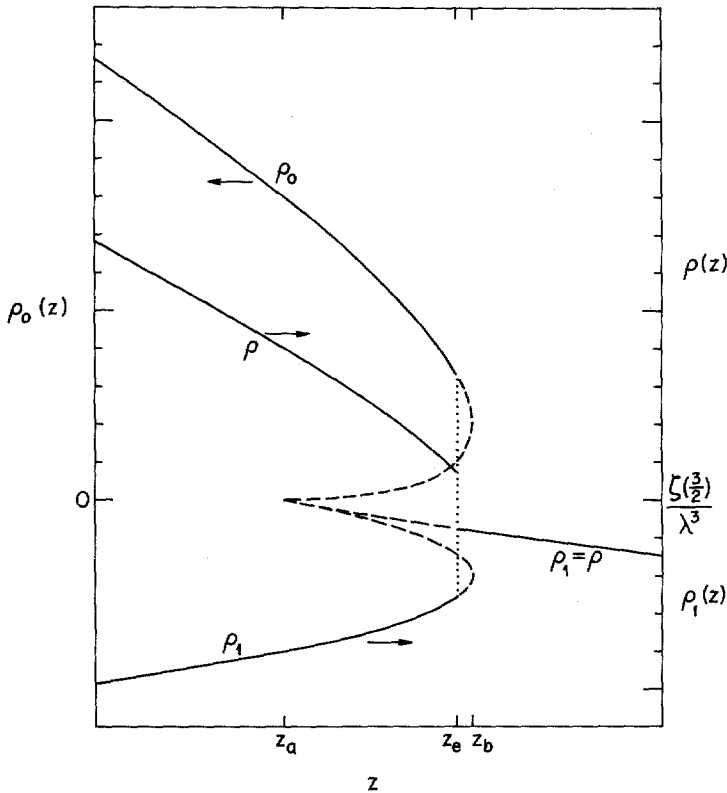

Fig. 2. Detail of the density profile at the edge of the Bose condensate in the Hartree–Fock approximation for a sufficiently gradual potential that may be approximated as a linear function in the region shown. The points z_a and z_b are defined in (25) and (28). The actual condensate edge lies at z_e. The dashed lines represent the continuation of an extremal solution of $\tilde{\Omega}$ into a region where it is no longer a minimum. The solid lines represent realizable densities as marked.

physical. The result obtained is that the discontinuity is at z_e, where $u(z_e) = u(z_a) + (0.92)2mv^2/\hbar^2\lambda^4$, at which point the total density $\rho(z)$ jumps by $1.5mv/\hbar^2\lambda^4$. Clearly, a *true* discontinuity cannot occur. Therefore we now examine our approximations to see just where they are consistent with the results obtained.

The first approximation made was to ignore the kinetic energy of ψ_0 in (17). This is clearly appropriate except where $\psi_0 \sim 0$. To estimate the error made near the edge of the condensate at $z = z_e$ we can use $\psi_0(z)$ from Eq. (27),

$$vN_0\psi_0^2(z) = \mathcal{O}(mv^2/\hbar^2\lambda^4 + |(z - z_e)\nabla u|) \tag{29}$$

where ∇u is evaluated at $z = z_e$, the edge of the condensate. We therefore see that the local kinetic energy near $z = z_e$ is

$$-\frac{\hbar^2}{2m}\left[\frac{\nabla\psi_0(z)}{\psi_0(z)}\right]^2 = \mathcal{O}\left(\frac{\hbar^2}{m}\left[\frac{|\nabla u|}{v\rho_0(z)}\right]^2\right)$$

The assumption that it may be ignored then amounts to

$$\frac{\hbar^2}{m}\left(\frac{|\nabla u|}{v\rho_0(z)}\right)^2 \ll v\rho_0(z)$$

If $\hbar^2\lambda^2/mv \ll (m|\nabla u|/\hbar^2)^{-1/3}$, this is satisfied for all z. Otherwise it is satisfied only for $z \gg (m|\nabla u|/\hbar^2)^{-1/3}$. In the latter case the discontinuity in the densities is not to be taken seriously. In the former case, which corresponds to the $T \neq 0$ plots shown in Fig. 1, the discontinuity in $\rho_0(z)$ will occur on a length scale of order the "healing length" of Eq. (17),

$$\left[\frac{mv\rho_0(z_e)}{\hbar^2}\right]^{-1/2} = \frac{\hbar^2\lambda^2}{mv} = (1.7 \times 10^{-5} \text{ cm})\left(\frac{20 \text{ mK}}{k_B T}\right)$$

and the density profile indeed features a slightly rounded step.

The error in the WKB approximation for $\rho_1(z)$ was estimated as $\mathcal{O}([m\tilde{\varepsilon}(z)]^{1/2}/\hbar\lambda^2)$. The above analysis that leads to (26) and (27) depends on knowing $\rho_1(z)$ accurately to order $[mu_{\text{eff}}(z)]^{1/2}/\hbar\lambda^2$. Thus our approximations are valid provided $\tilde{\varepsilon}(z) \ll u_{\text{eff}}(z)$. To estimate $\tilde{\varepsilon}(z)$ we recall that the first-order WKB approximation for a wave function is reasonably accurate unless one is within order one wavelength of the classical turning point or of a serious discontinuity in the effective potential. Noting that $|\nabla u_{\text{eff}}| \approx \mathcal{O}|\nabla u|$, we then obtain

$$\tilde{\varepsilon}(z) = \mathcal{O}\left(\max\left\{\frac{\hbar^2}{m|z - z_e|^2}, \left[\frac{\hbar^2|\nabla u|^2}{m}\right]^{1/3}\right\}\right)$$

Therefore, Eqs. (26) and (27) are insensitive to the errors in the WKB approximation provided

$$\max\left\{\frac{\hbar^2}{m|z-z_e|^2},\left[\frac{\hbar^2|\nabla u|^2}{m}\right]^{1/3}\right\}\ll\frac{mv^2}{\hbar^2\lambda^4}+|(z-z_e)\nabla u| \tag{30}$$

Condition (30), which is identical to the condition derived in the preceding paragraph that justified the neglect of $\nabla^2\psi_0$ in (17), can be rewritten as

$$|z-z_e|\gg\min\left\{\frac{\hbar^2\lambda^2}{mv},\left[\frac{m|\nabla u|}{\hbar^2}\right]^{-1/3}\right\} \tag{31}$$

It must be noted that the discontinuity in the densities at the edge of the condensate arises due to properties of the very low-lying single-particle states. Figure 3 shows the effective single-particle potential u_{eff} corresponding to the $T = 30$ mK density profile in Fig. 1. It is clear that the lowest lying single-particle states do not penetrate into the region occupied by the condensate. This explains the drop in ρ_1 and the consequent step up in ρ_0 as one enters the condensate.

It is also apparent from Fig. 3 that the uncondensed eigenstates with energies, measured from μ, less than v times some average of ρ_0 will be localized on the surface of the condensate. Thus the low-temperature specific heat will be effectively proportional to the sample area and not its
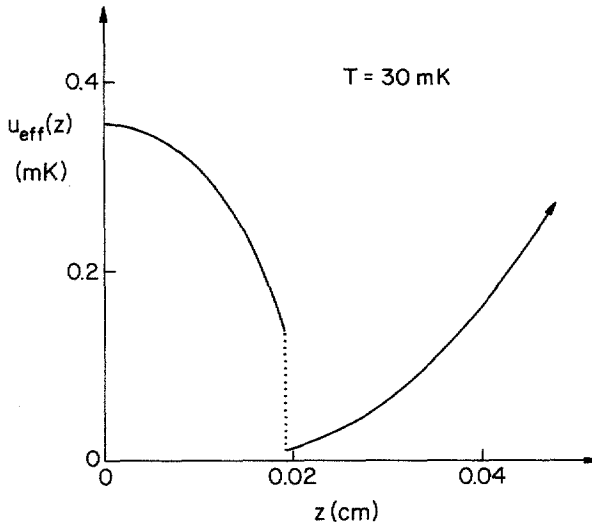

Fig. 3. The effective single-particle potential $u_{\text{eff}}(z)$, (21), corresponding to the $T = 30$ mK density profile in Fig. 1.

volume. Even in a translationally invariant Bose system, the Hartree–Fock equations are inadequate for $k_B T \lesssim v\rho_0$ since they predict a gap in the spectrum of excitations of order $v\rho_0$. The Bogolyubov generalization of Hartree–Fock developed in the next section eliminates both the discontinuities in the densities and the curious density of states.

3. BOGOLYUBOV–HARTREE–FOCK APPROXIMATION

Let us now consider a more general trial Hamiltonian that allows "quasiparticles." The quasiparticles are bosons with creation operator

$$b_k = a_k \operatorname{ch} \theta_k + a^+_{-k} \operatorname{sh} \theta_k \tag{32}$$

where a_k is the usual particle creation operator and $\psi_{-k} = \psi^*_k$. The trial Hamiltonian is then

$$H_t - \mu N = \sum_{k \neq 0} b^+_k E_k b_k \tag{33}$$

and the restriction on the ensemble is now $N_0 = \langle a^+_0 a_0 \rangle_t = \langle a_0 a_0 \rangle_t$. The trial ensemble is diagonal, so

$$\langle b^+_k b_k \rangle_t \equiv N_k = (e^{\beta E_k} - 1)^{-1} \tag{34}$$

which results in

$$\langle a^+_k a_k \rangle_t \equiv n_k = (N_k + \tfrac{1}{2}) \operatorname{ch} (2\theta_k) - \tfrac{1}{2} \tag{35}$$

and

$$\langle a_k a_{-k} \rangle_t = \langle a^+_k a^+_{-k} \rangle_t = -(N_k + \tfrac{1}{2}) \operatorname{sh} (2\theta_k) \tag{36}$$

(The hyperbolic sine, cosine, and tangent are denoted by sh, ch, and th, respectively.)

In the thermodynamic limit we then obtain

$$\tilde{\Omega}(H_t, N_0) = k_B T \sum_{k \neq 0} \ln (1 - e^{-\beta E_k}) + N_0(\langle 0|H_0|0 \rangle - \mu)$$

$$+ \sum_{k \neq 0} [n_k(\langle k|H_0|k \rangle - \mu) - N_k E_k] + \tfrac{1}{2}N_0^2 \langle 00|V|00 \rangle$$

$$+ N_0 \sum_{k \neq 0} \langle 0k|V|0k \rangle [2n_k - (N_k + \tfrac{1}{2}) \operatorname{sh} (2\theta_k)]$$

$$+ \sum_{j \neq 0} \sum_{k \neq 0} \langle jk|V|jk \rangle [n_j n_k + (N_j + \tfrac{1}{2})$$

$$\times \operatorname{sh} (2\theta_j)(N_k + \tfrac{1}{2}) \operatorname{sh} (2\theta_k)] \tag{37}$$

Demanding that $\tilde{\Omega}$ be stationary under variation of N_0, E_k, θ_k, and the $\{\psi_k\}$

results in

$$\langle 0|H_0 + 2v\rho - v(\rho_0 + \bar\rho)|k\rangle = \mu\delta_{0k} \qquad (38)$$

$$E_k^2 = \langle k|H_0 + 2v\rho - \mu|k\rangle^2 - \langle k|v(\rho_0 - \bar\rho)|k\rangle^2 \qquad (39)$$

$$\text{sh }2\theta_k = \langle k|v(\rho_0 - \bar\rho)|k\rangle/E_k \qquad (40)$$

and, for $j \neq k \neq 0 \neq j$,

$$\langle j|H_0 + 2v\rho - f_{jk}v(\rho_0 - \bar\rho)|k\rangle = 0 \qquad (41)$$

where

$$f_{jk} = \frac{(n_j + \tfrac{1}{2})\text{ th }(2\theta_j) - (n_k + \tfrac{1}{2})\text{ th }(2\theta_k)}{n_j - n_k} \qquad (42)$$

and

$$\bar\rho(z) = \sum_{k \neq 0} |\psi_k(z)|^2 (N_k + \tfrac{1}{2})\text{ sh }(2\theta_k) \qquad (43)$$

Since our calculation is to first order in the interparticle interaction v, and $\bar\rho$ is higher order in v than ρ_0, the $\bar\rho$'s in the above equations should be neglected. The equation for the condensate wave function (38) then becomes the same as in the Hartree–Fock approximation (16). The remaining single-particle wave functions are more elusive. How to solve a set of equations like (41) is unclear. However, a first approximation would be

$$(H_0 + 2v\rho - f_k v\rho_0)|k\rangle = \varepsilon_k|k\rangle \qquad (44)$$

where f_k to lowest order is just the limit of (42) as $j \to k$. [Note that (44) defines ε_k.] We then note that for the lowest lying states, with $\varepsilon_k \ll \langle v\rho_0\rangle$, n_k is very large, th $2\theta_k \approx 1$, so $f_{jk} \approx 1$ for almost all j. Thus we expect these lowest lying states to see an effective single-particle potential almost identical to that seen by the condensate (16). Consequently, they are not localized just outside of the condensate as is the case in the Hartree–Fock approximation. It is precisely these lowest lying single-particle states that cause the discontinuities in the densities seen in the last section. We therefore believe that these discontinuities are merely an artifact of the Hartree–Fock approximation and are not physical.

The nonlocal Hartree–Fock equations for the single-particle wave functions (18) were approximately solved by ignoring the nonlocal part, resulting in an expression very similar to (44), namely $(H_0 + 2v\rho)|k\rangle = \varepsilon_k|k\rangle$. For $\varepsilon_k \gg \langle v\rho_0\rangle$ it is clear that to leading order the $\{\psi_k(z)\}$ and the $\{n_k\}$ obtained will be the same in the Bogolyubov-Hartree–Fock approximation as in the Hartree–Fock approximation. As was noted earlier, for a dilute Bose gas at temperatures not too far below T_c the Bose condensation

temperature, we have $k_B T \gg \langle v\rho_0 \rangle$, so the strong discrepancy between the two treatments will always involve only a minority of the single-particle states, affecting neither the condensate nor states with $\varepsilon_k \gg \langle v\rho_0 \rangle$. Thus we believe the density profiles of Fig. 1 obtained from the Hartree–Fock approximation are indeed correct to leading order, but features that are higher order in the interaction v, namely the depression of ρ_1 within the condensate and, of course, the discontinuities at the edge of the condensate, are probably incorrect. A distinctive feature that we believe to be correct and that might help in identifying Bose condensation is the change in the gradient of the total density at the edge of condensate by a factor of order two.

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