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JP Fernandez

WJ Mullin
mullin@physics.umass.edu

The Two-Dimensional Bose-Einstein Condensate

Juan Pablo Fernández and William J. Mullin
Department of Physics, University of Massachusetts, Amherst, MA 01003, U.S.A.
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We study the Hartree-Fock-Bogoliubov mean-field theory as applied to a two-dimensional finite trapped Bose gas at low temperatures and find that, in the Hartree-Fock approximation, the system can be described either with or without the presence of a condensate; this is true in the thermodynamic limit as well. Of the two solutions, the one that includes a condensate has a lower free energy at all temperatures. However, the Hartree-Fock scheme neglects the presence of phonons within the system, and when we allow for the possibility of phonons we are unable to find condensed solutions; the uncondensed solutions, on the other hand, are valid also in the latter, more general scheme. Our results confirm that low-energy phonons destabilize the two-dimensional condensate.

I. INTRODUCTION

In a recent paper [1], one of the groups that pioneered the formation and detection of Bose-Einstein condensation (BEC) in harmonically trapped atomic gases [2, 3, 4] reports the creation of (pseudo-) two-dimensional condensates. These have been produced by taking a three-dimensional condensate of ^{23}Na atoms and carrying out two independent processes on it: 1) Initially, one of the confining frequencies (that in the z direction, ω_z, in order to minimize the effects of gravity) is increased until the condensate radius in that dimension is smaller than the healing length associated with the interaction between atoms (taken here to be repulsive and parametrized by the two-body scattering length a). This is not sufficient to reduce the dimensionality, however, since the atoms, each of which has mass m, will literally squeeze into the third dimension if there are more than

$$N = \sqrt{\frac{32\hbar}{225ma^2}}\sqrt{\frac{\omega_z^3}{\omega_x^2\omega_y^2}} \tag{1}$$

of them in the trap. 2) Consequently, the number of atoms in the condensate must be reduced; this is achieved by exposing the condensate to a thermal beam. The reduction in effective dimensionality becomes apparent when the aspect ratio of the condensate, which is independent of N in 3D, starts to change as the number of atoms is gradually reduced. The condensates thus produced have a number of atoms that ranges between 10^4 and 10^5.

This constitutes an important experimental contribution to the long-standing debate about the existence of BEC in two dimensions. It is a well-known fact (and a standard textbook exercise) that BEC cannot happen in a 2D homogeneous ideal gas; a rigorous mathematical theorem [5] extends this result to the case where there are interactions between the bosons. When the system is in a harmonic trap, on the other hand, BEC can occur in two dimensions [6] below a temperature $k_{\mathrm{B}}T_c = \hbar\omega\sqrt{6N/\pi^2}$, but the theorem is once again valid when interactions between the bosons are considered [7]: while there is a BEC in the 2D system, it occurs at $T = 0$.

The preceding discussion is valid only in the thermodynamic limit, which in the particular case of an isotropically trapped system consists of making $N \to \infty$ and $\omega \to 0$ in such a way that $N\omega^2$ remains finite [7, 8]. The question remains whether a phenomenon resembling BEC—that is, the accumulation of a macroscopic number of particles in a single quantum state—occurs or not when the system consists of a *finite* number of particles confined by a trap of finite frequency, as is certainly the case in experimental situations. If there is such a phenomenon, one would like to know more about the process by which this "condensate" is destabilized at finite temperatures as N grows.

Some authors [9, 10] have considered, in the finite homogeneous 2D case, the possibility of a BEC. A similar analysis [11] was considered for a quasi-2D trapped gas; the latter reference finds that the phase fluctuations in the condensate vary with temperature and particle number as

$$\langle(\delta\phi)^2\rangle \propto T\log N \tag{2}$$

which diverges for finite temperature as $N \to \infty$, as one would expect. For finite N, on the other hand, the fluctuations are tempered at very low temperature; since the coherence length, though finite, is still larger than the characteristic length imposed on the system by the trap [12] or by walls, one can speak of a "quasicondensate." It is this quasicondensation that we wish to study in this paper. Reference [13] reports the observation of a quasicondensate in a homogeneous system of atomic hydrogen adsorbed on ^{4}He; at this point we cannot tell if the condensates reported in Ref. [1] are actually quasicondensates.

One can approach the study of the 2D Bose gas by employing mean-field theory, which in this context refers to the Hartree-Fock-Bogoliubov (HFB) equations and various simplifications thereof that we will review in quantitative detail and classify in the present work. The HFB theory has been remarkably successful in treating the 3D case; though we give a few representative references below, we refer the reader to Ref. [14], which includes a comprehensive review and an exhaustive list of references, and will henceforth concentrate on the work that has been carried out in 2D.

The HFB theory assumes from the outset that the system is partially condensed, and proposes separate equations to describe the condensate and the uncondensed (thermal) component. The condensate is described by a macroscopic wavefunction that obeys a generalized Gross-Pitaevskiĭ (GP) equation [15, 16], while the noncondensate consists of a superposition of Bogoliubov quasiparticle and "quasihole" excitations weighted by a Bose distribution. The expression for the noncondensate can be simplified by neglecting the quasihole excitations (the Hartree-Fock scheme) [17, 18], by performing a semiclassical WKB approximation [19], or by combining both of these [20, 21, 22]. Each one of the above schemes can be further simplified, when the thermodynamic limit is approached, by neglecting the kinetic energy of the condensate: this is the Thomas-Fermi limit [23, 24]. Finally one can neglect the interactions between thermal atoms, arriving at the semi-ideal model [25, 26].

The semi-ideal model has been implemented in 2D [27, 28], but has been found to yield unphysical results as the interaction strength becomes sizable. The full-blown HFB model does not appear to be much more successful, at least when considered in the semiclassical limit. In a previous paper [29] one of us found that, below a certain temperature, the introduction of a condensate in the Thomas-Fermi limit (corresponding to the thermodynamic limit) renders the HFB equations incompatible, with the noncondensate density becoming infinite at every point in space. The singularity occurs at the low end of the energy spectrum, indicating that the condensate is being destabilized by long-wavelength phonons; this interpretation in terms of phase fluctuations had already been proposed for the homogeneous system [5, 30]. In this work we also report our inability to find self-consistent semiclassical solutions to the HFB model when a finite trapped system is considered.

Moreover, it was recently discovered [31, 32] that it is possible, in the 2D case exclusively, to solve the HFB equations semiclassically at *any* temperature without even having to invoke the presence of a condensate (thus obtaining what we will call an "uncondensed" solution). In other words, it is possible to simply cross out the condensate component and solve for the system to a temperature close to $T = 0$. The solution thus obtained shows an accumulation of atoms at the center of the trap and yields a bulge in density similar to that caused by the presence of a condensate, even though no state is macroscopically occupied.

These results appear to reinforce the conclusion that BEC cannot happen in the two-dimensional trapped system. However, we are still confronted with the experimental results described above. Furthermore, two different Monte Carlo simulations [33, 34] show significant concentrations of particles in the lowest energy state for finite N, though it must be said that this method provides little information about the types of excitations that contribute to the disappearance of the condensate, and that it is difficult to carry out such simulations on very large systems.

The HFB model cannot be discounted at this stage either: when we restrict ourselves to the Hartree-Fock approximation, it is possible to find self-consistent solutions (henceforth referred to as "condensed") involving a condensate, both for finite systems and in the thermodynamic limit, when using either the discrete set of equations [35] or the WKB approximation [36] to treat the noncondensate. The Hartree-Fock approximation neglects phononlike excitations, so it is not surprising that it yields solutions. However, one may be able to justify its usefulness.

It is known that, in the infinite homogeneous system, infrared singularities occur but are renormalized by interactions, providing, in essence, a cutoff at a low wavenumber $k_0 \approx \sqrt{nmU}$ [37, 38, 39], where n is the density, m the particle mass, and U the effective interaction strength. Indeed, it is possible to estimate the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature by simply cutting off the ideal-gas density expression at this k_0 [38]. Presumably a similar situation occurs in the trapped case. The Hartree-Fock approach provides a convergent theory by cutting off the singularities at a wavenumber similar to that of more rigorous theories. Whether such an approach gives a reasonable estimate of the BKT transition temperature, the superfluid density, or a quasicondensate density for the finite system will need to await a more rigorous theoretical approach to the interacting 2D trapped gas [40].

Given the above limitations, we analyze the character of the BEC in the 2D trapped system by solving the coupled equations of the theory. We find that, in the Hartree-Fock scheme, it is possible to find both condensed and uncondensed solutions for the two-dimensional equations. We also calculate the free energy corresponding to each one and find that the condensed solution has a lower free energy at all temperatures, which appears to imply that, at least at this level of approximation, the uncondensed solution is unphysical or metastable. The condensed solution will be "preferred" over the uncondensed one, and we assume that the solution represents an approximation to a quasi-condensate.

It is evident from our discussion that our approach to BEC in 2D trapped systems is a preliminary one and that a further analysis that takes fully into account the BKT transition is necessary. A start to answering this need has been presented in Ref. [40], and we intend to return to this problem ourselves in the future.

II. THE MODEL

A. The Hartree-Fock-Bogoliubov equations

Throughout this paper we use a dimensionless system of units in which all lengths are scaled by the oscillator length $x_0 \equiv \sqrt{\hbar/m\omega}$ and all energies are expressed in terms of the one-dimensional ground-state energy of

the oscillator, $\hbar\omega/2$. Dimensionless variables will in general carry a tilde: for example, the total density n becomes $\tilde{n} \equiv x_0^2 n$ and the chemical potential $\tilde{\mu} \equiv \mu/\frac{1}{2}\hbar\omega$.

The HFB equations [14, 21, 41, 42] result from assuming that 1) the (repulsive) interactions between atoms consist exclusively of two-body low-energy collisions that can be described by a delta-function pseudopotential [43] of strength g (related to its dimensionless counterpart $\tilde{\gamma}$ through $g \equiv \frac{1}{2}\hbar\omega x_0^2\tilde{\gamma}$), that 2) the many-body field operator Ψ can be decomposed via

$$\Psi = \langle\Psi\rangle + \tilde{\psi} \equiv \tilde{\Phi} + \tilde{\psi}, \tag{3}$$

where the ensemble average $\tilde{\Phi}$ is a real macroscopic wavefunction that describes the condensate (reflecting the imposition of macroscopic long-range order on the condensed system), and that 3) products of noncondensate operators can be simplified using a finite-temperature version of Wick's theorem [44]. If we insert (3) into the many-body grand-canonical Hamiltonian

$$\tilde{H} = \int d^2x\, \Psi^\dagger(\tilde{\Lambda} + \frac{\tilde{\gamma}}{2}\Psi^\dagger\Psi^\dagger\Psi)\Psi, \tag{4}$$

where $\tilde{\Lambda} = -\tilde{\nabla}^2 + x^2 - \tilde{\mu}$, and neglect anomalous averages via the Popov approximation [21], we obtain an expression that can be diagonalized and yields an infinite set of coupled differential equations.

On one hand, the macroscopic wavefunction mentioned above is the square root of the dimensionless condensate density n_0 and obeys the generalized Gross-Pitaevskiĭ equation,

$$\tilde{\Lambda}\tilde{\Phi} + \tilde{\gamma}(\tilde{n}_0 + 2\tilde{n}')\tilde{\Phi} = 0, \tag{5}$$

where $\tilde{n}' \equiv \tilde{n} - \tilde{n}_0$ is the noncondensate density. The factor of 2 in (5) and hereafter is a consequence of the direct (Hartree) and exchange (Fock) terms being identical, which follows from the fact that the delta-function interaction that we are considering has zero range [42]. (The term involving the condensate does not include that factor; this is a consequence of the restricted grand-canonical ensemble that we are using. See the end of the next section.)

The noncondensate, in turn, is described by an infinite number of pairs of functions that obey [41]

$$\begin{pmatrix} \tilde{\Lambda} + 2\tilde{\gamma}\tilde{n} & -\tilde{\gamma}\tilde{n}_0 \\ -\tilde{\gamma}\tilde{n}_0 & \tilde{\Lambda} + 2\tilde{\gamma}\tilde{n} \end{pmatrix} \begin{pmatrix} u_j \\ v_j \end{pmatrix} = \tilde{\epsilon}_j \begin{pmatrix} u_j \\ -v_j \end{pmatrix} \tag{6}$$

and which generate the noncondensate density via

$$\tilde{n}'(\mathbf{x}) = \sum_j \left(\left(|u_j|^2 + |v_j|^2\right) f_j + |v_j|^2 \right), \tag{7}$$

where we have introduced the Bose-Einstein distribution factor $f_j \equiv (e^{\tilde{\epsilon}_j/t} - 1)^{-1}$, which appears when the free energy of the system is minimized, and the dimensionless temperature $t \equiv k_{\rm B}T/\frac{1}{2}\hbar\omega$. The last term of (7) describes the zero-temperature depletion of the condensate, which accounts for less than 1% of the particles and is therefore negligible [21]. This self-consistent set of equations is closed, and the chemical potential found, by imposing that the total number of particles remain fixed:

$$N = N_0 + N' = \int d^2x\, \tilde{n}(\mathbf{x}) = \int d^2x\, (\tilde{n}_0 + \tilde{n}')\,. \tag{8}$$

At temperatures such that $k_{\rm B}T \gg \hbar\omega$, one can use the semiclassical (WKB) approximation [19] that results from taking $u_j \approx u(\mathbf{x})e^{i\phi}$ and $v_j \approx v(\mathbf{x})e^{i\phi}$. The phase common to both defines a quasiparticle momentum through $\boldsymbol{\kappa} = \tilde{\boldsymbol{\nabla}}\phi$; u, v, and $\boldsymbol{\kappa}$ vary sufficiently slowly with $\mathbf{x}$ that their spatial derivatives can be neglected [21]. The distribution factor is now $f_j \approx f(\mathbf{x}, \boldsymbol{\kappa})$, infinite sums are transformed into momentum integrals—which in two dimensions can be solved in closed form [29]—and the equations become algebraic, yielding the Bogoliubov energy spectrum [21]

$$\tilde{\epsilon}_{\rm HFB}(\boldsymbol{\kappa}, \mathbf{x}) = \sqrt{(\kappa^2 + x^2 + 2\tilde{\gamma}\tilde{n} - \tilde{\mu})^2 - \tilde{\gamma}^2\tilde{n}_0^2} \tag{9}$$

and the following integral expression for the noncondensate density:

$$\begin{aligned} \tilde{n}'(\mathbf{x}) = &\ \frac{t}{4\pi} \int_{((x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})^2 - \tilde{\gamma}^2\tilde{n}_0^2)^{1/2}/t}^{\infty} \frac{d\xi}{e^\xi - 1} \\ = &-\frac{t}{4\pi} \log\left(1 - e^{-(\sqrt{(x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})^2 - \tilde{\gamma}^2\tilde{n}_0^2})/t}\right). \end{aligned} \tag{10}$$

At high enough temperatures there is no condensate, and the density on the left-hand side of (10) is just the total density. We thus have to solve a single self-consistent equation,

$$\tilde{n}'(\mathbf{x}) \to \tilde{n}(\mathbf{x}) = -\frac{t}{4\pi} \log\left(1 - e^{-(x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})/t}\right); \tag{11}$$

the chemical potential is once again calculated by requiring N to be fixed. Equation (11) has been found by the authors of Ref. [31] to be soluble at *all temperatures*, a result that we confirm in the present work. Reference [29] had mistakenly concluded that it was impossible to solve (11) below a certain temperature.

The Hartree-Fock approximation [17, 21, 23] amounts to neglecting the v_j in (6) and, when combined with the semiclassical treatment, results in the disappearance of the last term within the square root of Eq. (9). The energy spectrum now becomes

$$\tilde{\epsilon}_{\rm HF} \equiv \tilde{\epsilon} = \kappa^2 + x^2 + 2\tilde{\gamma}\tilde{n} - \tilde{\mu} \tag{12}$$

and the noncondensate density turns into

$$\tilde{n}'(\mathbf{x}) = -\frac{t}{4\pi} \log\left(1 - e^{-(x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})/t}\right), \tag{13}$$

an expression that differs from (11) in that the left-hand side corresponds only to the noncondensate density. The three-dimensional version of this equation, coupled

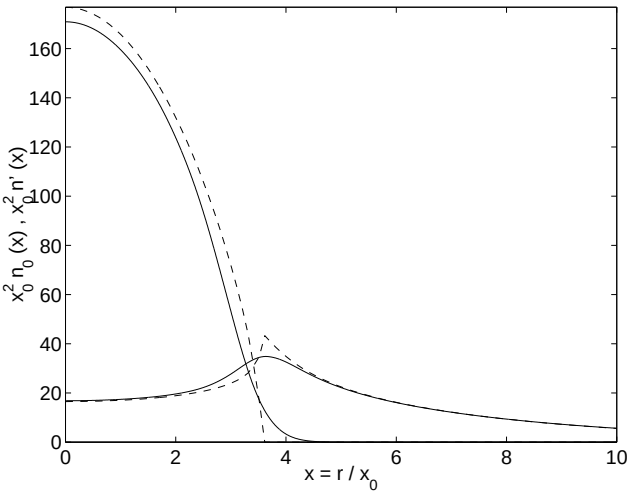

FIG. 1: Condensate and noncondensate density profiles of a two-dimensional gas with $N = 10^4$ and $\tilde{\gamma} = 0.1$ at $T = 0.7T_c$, where T_c is the ideal-gas transition temperature. The Goldman-Silvera-Leggett model (dashed lines) treats the condensate in the Thomas-Fermi limit (14), while the Hartree-Fock model (full lines) uses the full Gross-Pitaevskiĭ equation (5). Both models use Eq. (13) to describe the noncondensate.

with (5) and (8), has been frequently used in the literature to study the three-dimensional gas. Reference [22], for example, exhibits a detailed comparison of its predictions to those of Monte Carlo simulations and finds excellent agreement between the two.

In two dimensions, the Hartree-Fock equations have been solved without resorting to the WKB approximation [35]. The authors of this reference succeeded in finding self-consistent density profiles and used them to study the temperature dependence of the condensate fraction. Our results [36], which do take advantage of the semiclassical approximation, agree quite well with theirs (see Fig. 1).

B. The Thermodynamic Limit

When N is large we can neglect the kinetic energy of the system, which in 2D can be shown to be of order $1/N$ [29], and obtain the Thomas-Fermi approximation [24]

$$\tilde{\gamma}\tilde{n}_0 = (\tilde{\mu} - x^2 - 2\tilde{\gamma}\tilde{n}')\Theta(\tilde{\mu} - x^2 - 2\tilde{\gamma}\tilde{n}'), \qquad (14)$$

where $\Theta(x)$ is the Heaviside step function, introduced to ensure that the density profile is everywhere real and positive. Also, since the thermodynamic limit requires that $\omega \to 0$, the WKB approximation becomes rigorous and can be used with confidence. Thus we can insert expression (14) in the Bogoliubov energy spectrum (9) and show that the latter reduces to

$$\tilde{\epsilon}_{\rm HFB}(\boldsymbol{\kappa}, \mathbf{x}) \approx \kappa\sqrt{\kappa^2 + 2\tilde{\gamma}\tilde{n}_0} \approx \kappa\sqrt{2\tilde{\gamma}\tilde{n}_0} \qquad (15)$$

for small quasimomenta. The fact that it is linear clearly shows us that, in this approximation, the low end of the energy spectrum corresponds to phononlike quasiparticles. Now, if we introduce (14) into the noncondensate density (10), we can see that the argument of the logarithm vanishes at all temperatures, making the density diverge at every point in space. The first line of (10) shows that the divergence in the integral is caused at its lower limit; this restates the conclusion arrived at in Ref. [29]: low-energy phonons destabilize the condensate in the two-dimensional thermodynamic limit when the noncondensate quasiparticles obey the Bogoliubov spectrum.

In the Hartree-Fock approximation, on the other hand, the energy spectrum tends in this limit to $\tilde{\epsilon} \approx \kappa^2 + \tilde{\gamma}\tilde{n}_0$ and predicts single-particle excitations whose minimum energy is $\tilde{\gamma}\tilde{n}_0$; this can be interpreted equivalently by assigning a minimum value $\kappa_c^2 = \tilde{\gamma}\tilde{n}_0$ for the excitation quasimomentum. This cutoff is consistent with those proposed in the past [9, 10, 37, 38, 39] and removes the infrared singularity in the HFB equations.

This momentum cutoff is robust enough that it enables one to carry out Hartree-Fock calculations even in the thermodynamic limit: in fact, as was first found in Ref. [23], the introduction of this limit actually simplifies the calculations, and it is possible to find self-consistent solutions by simultaneously treating the noncondensate in the Hartree-Fock approximation and the condensate in the Thomas-Fermi limit [35, 36]. This model cannot provide realistic density profiles at every point in space, since the condensate density (14) has a discontinuous derivative at its edge, but predicts quite reasonable results outside of this region, as can be seen in Fig. 1.

C. The Free Energy

We have seen that in 2D the mean-field-theory BEC equations admit solutions both with and without a condensate. The unphysical solution should be that with the highest free energy, since equilibrium at finite temperatures occurs when the grand potential attains a minimum; in fact, the Bose-Einstein distribution factor in Eq. (7) comes from minimizing this quantity [17, 45], which in our dimensionless units adopts the form

$$\Omega = (U - \mu N - TS)/\frac{1}{2}\hbar\omega \equiv \int d^2x\,(\Upsilon - \tilde{\mu}\tilde{n} - t\Sigma). \qquad (16)$$

At this point we have to keep in mind that the grand-canonical free energy is a function of $\tilde{\mu}$, not of N; in order to make a meaningful comparison of these energies at the same N, then, we have to compare the Helmholtz free energies, given by $\tilde{A} = \Omega + \tilde{\mu}N$. The expressions given below have all been derived in the grand-canonical

ensemble and thus contain the chemical potential; we will eliminate this dependence on $\tilde{\mu}$ by adding $\tilde{\mu}N$ to the expressions we obtain.

In the Hartree-Fock approximation, the grand-canonical energy density of the system is given by [21]

$$\Upsilon - \tilde{\mu}\tilde{n} = \tilde{\Phi}(\tilde{\Lambda} + \frac{\tilde{\gamma}}{2}\tilde{n}_0)\tilde{\Phi} + \frac{1}{(2\pi)^2}\int \frac{d^2\kappa\,\tilde{\epsilon}}{e^{\tilde{\epsilon}/t}-1} - \tilde{\gamma}\tilde{n}'^2; \quad (17)$$

the first term corresponds to the condensate energy, while the second one is the sum, weighted by the Bose-Einstein distribution, of the energies of the excited states; this last expression includes an extra term $\tilde{\gamma}\tilde{n}'^2$ that has to be subtracted explicitly, as is usually the case in Hartree-Fock calculations [44]. We can simplify (17) further by invoking Eq. (5):

$$\Upsilon - \tilde{\mu}\tilde{n} = -\tilde{\gamma}\tilde{n}^2 + \frac{\tilde{\gamma}}{2}\tilde{n}_0^2 + \frac{1}{(2\pi)^2}\int \frac{d^2\kappa\,\tilde{\epsilon}}{e^{\tilde{\epsilon}/t}-1}. \quad (18)$$

The entropy of the system can be found from the combinatorial expression [44, 46]

$$S = -k_{\rm B}\sum_i (f_i \log f_i - (f_i+1)\log(f_i+1)), \quad (19)$$

which in the WKB and Hartree-Fock approximations yields the entropy density [21]

$$t\Sigma = \frac{1}{(2\pi)^2}\int \frac{d^2\kappa\,\tilde{\epsilon}}{e^{\tilde{\epsilon}/t}-1} - \frac{t}{(2\pi)^2}\int d^2\kappa\,\log(1-e^{\tilde{\epsilon}/t}). \quad (20)$$

The first term in (20) cancels with the last one in (18), and the other term can be integrated in closed form, yielding

$$\tilde{A}_{\rm c} = \tilde{\mu}N - \int d^2x\,\big(\tilde{\gamma}(\tilde{n}^2 - \frac{1}{2}\tilde{n}_0^2) + \frac{t^2}{4\pi}\,g_2(e^{-(x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})/t})\big) \quad (21)$$

for the free energy of the condensed solution. (Here we have introduced the Bose-Einstein integral $g_\sigma(x) \equiv \sum_{k=1}^{\infty} x^k/k^\sigma$. Note that $g_1(x) = -\log(1-x)$, a function that repeatedly appears above.) As $T \to 0$, this expression reduces to the correct value in the homogeneous case [18]. In the thermodynamic limit, we can find an expression for the free energy per particle at $T = 0$ using the Thomas-Fermi density profile:

$$\frac{\tilde{A}_{\rm TF}}{N} = \frac{2}{3}\sqrt{\frac{2}{\pi}}\,\sqrt{N\tilde{\gamma}}. \quad (22)$$

The free energy of the uncondensed solution is found by simply crossing out the condensate density in (21):

$$\tilde{A}_{\rm u} = \tilde{\mu}N - \int d^2x\,\left(\tilde{\gamma}\tilde{n}^2 + \frac{t^2}{4\pi}\,g_2(e^{-(x^2+2\tilde{\gamma}\tilde{n}-\tilde{\mu})/t})\right). \quad (23)$$

Equations (21) and (23), of which more-general versions are derived in Ref. [47] by a different method [17], can be easily seen to become identical at temperatures high enough that the condensate density can be neglected. On the other hand, their low-temperature limits differ, since Eq. (23) tends to a higher value than that attained by (21). This can be traced back to the fact that the grand-canonical ensemble has to be changed in order for it to correctly describe the particle-number fluctuations at low temperatures [47, 48]. Now, a 2D Bose system has a condensate at least at $T = 0$, so the two free energies should coincide there; however, we must keep in mind that the semiclassical approximation used to derive Eq. (23) requires that $k_{\rm B}T \gg \hbar\omega$; thus the method we are using *cannot* describe the appearance of the zero-temperature condensate in the uncondensed solution. At the end of the next section we will study further consequences of this distinction.

III. NUMERICAL METHODS AND RESULTS

There is a time-honored prescription [21, 42] for finding the self-consistent solution of the Hartree-Fock equations in the presence of a condensate: Initially, we assume that only the condensate is present and solve the Gross-Pitaevskiĭ equation (5) for $\tilde{n}' = 0$. The wavefunction and eigenvalue that result are fed into the Hartree-Fock expression for the density (13), which, when integrated over all space, yields also a value for the noncondensate fraction N'; one can then readjust the condensate fraction and solve the Gross-Pitaevskiĭ equation that results. The process is then iterated until the chemical potential and the particle fractions stop changing.

By far the most difficult part of this process is the solution of the nonlinear eigenvalue problem (5). Different methods exist in the literature; we have obtained identical results by solving it as an initial value problem [49] and, much more efficiently, by employing the method of spline minimization [22, 50]. This method uses the fact that Eq. (5) is the Euler-Lagrange equation that minimizes the functional

$$J[\tilde{\Phi}] = \int d^2x\,\left[(\tilde{\boldsymbol{\nabla}}\tilde{\Phi})^2 + \tilde{\Phi}(x^2 + 2\tilde{\gamma}\tilde{n}(\mathbf{x}))\tilde{\Phi} + \frac{\tilde{\gamma}}{2}\,\tilde{\Phi}^4\right]. \quad (24)$$

After setting a small, nonuniform grid of fixed abscissas that represent the coördinate x, we take the corresponding ordinates, which represent $\tilde{\Phi}$, as the parameters to be varied until (24) attains its smallest possible value. Since we only have information about the value of the function at a discrete set of points, in order to calculate the necessary derivatives and to integrate we perform a cubic-spline interpolation; the integral is found using ten-point Gauss-Legendre quadrature. The minimization is carried out using the Nelder-Mead method.

We checked our code by comparing its predictions in three dimensions to previously published results. For the case studied in Ref. [22], the condensate fractions we

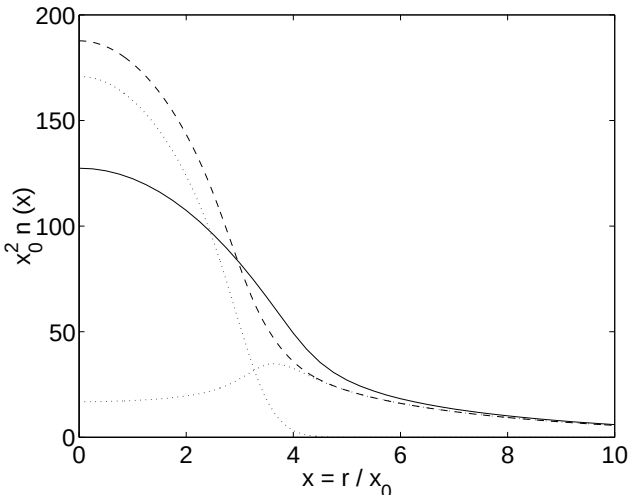

FIG. 2: Total density profiles of a two-dimensional gas with the same parameters as in Fig. 1. In this case we exhibit both the uncondensed (full line) and the condensed (dashed line) solutions; the latter we have broken once again into its condensate and noncondensate parts (dotted lines).

found differed from those in the paper by less than one part in 10^4. The code also reproduced previously known results for the ideal gas, including finite-size effects [7].

Figure 1, already discussed above, shows one of the solutions that we have found using the Hartree-Fock approximation. The gas has $N = 10^4$ atoms; the coupling constant $\tilde{\gamma}$ has been chosen so that the system has approximately the same radius as the three-dimensional gas studied in Ref. [22], where parameters resembling those of the original JILA trap [2] are used. The system is shown at $T = 0.7T_c$, where T_c is the condensation temperature for the ideal gas. We have also found solutions for the Goldman-Silvera-Leggett model, which corresponds to the large-N limit of the GP equation. This was done by treating the problem as a simultaneous system of nonlinear equations on a uniform grid and solving it with a least-squares method.

When $N = 10^4$, as in Fig. 1, it is not possible to find a self-consistent solution for the condensed equations beyond $T \approx 0.8T_c$, since $\tilde{\epsilon}_{\rm HF}$ becomes negative; this had already been noted in Ref. [22] for three dimensions, where it was interpreted as a finite-size effect, and occurs at even lower temperatures for 2D. The limitation becomes more severe as N increases: for $N = 10^6$ we cannot find solutions beyond $T \approx 0.5T_c$. The authors of Ref. [35] report predictions at temperatures very close to the transition by using a finite-size correction to the chemical potential [51]. Our inability to work above certain temperatures might be a consequence of using the semiclassical approximation, though we point out that the Popov approximation is expected to break down close to the transition temperature [14, 21].

We also found self-consistent three-dimensional solutions using the more general Bogoliubov spectrum by applying the same method and using the Hartree-Fock solutions as a starting point for the iteration. We find that these solutions exhibit an enhanced depletion of the condensate, in agreement with those found by other authors [51]. It was impossible, however, to find this kind of solution in two dimensions, even for systems with N as low as 100: after a few iterations, the chemical potential became too large, the Bogoliubov energies became imaginary, and the noncondensate density diverged. When the possibility of phononlike excitations is allowed, then, the condensate is destabilized, just as had been found in the Thomas-Fermi limit [29].

The uncondensed case, on the other hand, gives us solutions in these conditions, and to it we now turn. Equation (11) along with the particle-conservation condition (8) for all temperatures is most easily solved by rewriting (11) as

$$Ze^{-x^2/t} = 2\, e^{-(\pi-\tilde{\gamma})\nu(\mathbf{x})} \sinh \pi\nu(\mathbf{x}) \tag{25}$$

where have introduced the fugacity $Z = e^{\tilde{\mu}/t}$ and $\nu(\mathbf{x}) \equiv 2\tilde{n}(\mathbf{x})/t$. Given Z, t, and $\tilde{\gamma}$ it is possible to find ν at every point using a standard root-finding algorithm. One then wants to find the value of Z such that the total number of particles is N. It is better, however, to write Eq. (25) at the origin,

$$Z = 2\, e^{-(\pi-\tilde{\gamma})\nu_0} \sinh \pi\nu_0, \tag{26}$$

eliminate Z between (25) and (26), and solve for $\nu_0 = \nu(0)$, the density at the center of the trap, using the same root finder.

In Fig. 2 we show the (Hartree-Fock) condensed and uncondensed solutions that we have obtained. They are similar in shape and exhibit identical behavior for large x. The uncondensed solution has a lower value at the origin and predicts a wider radial density profile.

We also calculated the free energy corresponding to each solution; the results are shown in Fig. 3, which shows $\tilde{A}/N$ as a function of temperature for both cases when $N = 10^3$ and $N = 10^4$. The free energies appear to coincide at high temperatures; this was to be expected, since Eqs. (21) and (23) become identical at temperatures high enough for the condensate density $\tilde{n}_0$ to be neglected. As for the low-temperature limit, we have already noted that the free energy of the condensed solution tends to the value predicted by the zero-temperature Thomas-Fermi limit, while that of the uncondensed solution tends to a higher value. This value can actually be calculated: it is easy to show [31] that the low-T limit of Eq. (25) is

$$2\tilde{\gamma} n(\mathbf{x}) = \tilde{\mu} - x^2, \tag{27}$$

the Thomas-Fermi limit but with $\tilde{\gamma}$ replaced by $2\tilde{\gamma}$; a larger interaction strength, as we can see from (22), implies a higher free energy. Interestingly, when we compare a given Hartree-Fock solution to an uncondensed solution with half the interaction strength, we find that

the density profiles become very similar (and are indistinguishable at $T = 0$), while the free energies coincide almost exactly for a wide range of temperatures; attractive as this possibility might be, however, it has a serious flaw: the free energies start to differ as the temperature increases, where they should coincide by definition. This tells us that the factor of 2, which turns out to be the same one discussed after Eqs. (5) and (23), has to be retained; the WKB approximate expression for the uncondensed state is valid *only* for $k_{\rm B}T \gg \hbar\omega$, so dropping the factor of 2 in order to match the $T = 0$ condensate is invalid. (The authors of Ref. [31], in fact, omit this factor from their paper, although they address this question in a subsequent publication [32]). It is in fact this factor that guarantees that the uncondensed solution has a higher free energy than the condensed one at all temperatures; this, despite our inability to find condensed solutions using the Bogoliubov energy spectrum, leads us to conclude that, at least at this level of approximation, the uncondensed solution is unphysical and the two-dimensional finite trapped system will exhibit some sort of condensation at finite temperature.

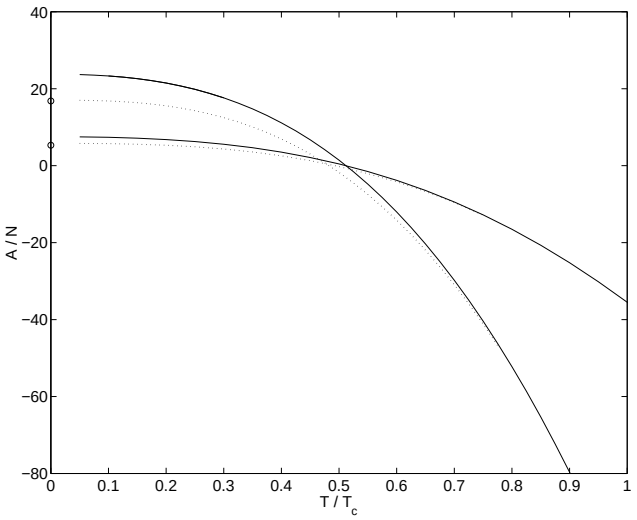

FIG. 3: Free energies per particle for the condensed (dashed line) and uncondensed (full line) solutions. The curves with higher value at $T = 0$ correspond to $N = 10^4$ atoms, while those with the lower value at $T = 0$ correspond to $N = 10^4$. The coupling constant is $\tilde{\gamma} = 0.1$ in both cases. The open circles on the vertical axis are the Thomas-Fermi predictions given by Eq. (22) for $T = 0$. The free energies seem to be converging in the high-temperature limit; the low-temperature limit, on the other hand, shows the discrepancy that results from restricting condensate fluctuations (see discussion after Eq. (23)). Note that T_c, the transition temperature for the ideal 2D trapped gas, depends on N; thus the x axis for each N represents a different actual temperature.

IV. CONCLUSION

We have found solutions to the two-dimensional HFB equations in the Hartree-Fock approximation, both for finite numbers of atoms and in the thermodynamic limit; still, when we try to go beyond this scheme and consider the whole Bogoliubov excitation spectrum, the low end of which is described by phonons, we are unable to find self-consistent solutions for finite—even low—values of N. We have seen that it is possible to describe the system as having no condensate at all, but these solutions, at least for the parameter combinations that we have studied, have a higher free energy than their partly-condensed counterparts; this leads us to conclude that the 2D system will have some kind of condensate at low enough temperatures, insofar as the Hartree-Fock approach can successfully describe the quasicondensate that we expect to find in a finite system.

One could argue that the whole mean-field approach we have adopted is wrong in two dimensions, since a condensation into a single state is being assumed from the start. However, an alternative treatment [52] that does not make this assumption ends up with equations identical to (6), so we are left none the wiser. We have also bypassed the fact that the interaction strength g is not really constant in 2D, but rather depends logarithmically on the relative momentum [11, 53]; this, however, has been found to be of little consequence [32]. Another possibility is that condensation occurs into a band of states, forming a "smeared" or generalized condensate [54, 55]; this alternative situation is not ruled out by the standard proof of Hohenberg's theorem [56].

Monte Carlo simulations *do* seem to predict the presence of a condensate in two dimensions [33, 34]. Furthermore, two-dimensional condensates appear to have been produced in the laboratory [1, 13]. Presumably the MC simulations show both the effects of a quasicondensation of a finite system and the BKT transition to the superfluid state. Our attempt here has been to test the possibility of representing these Bose effects by a relatively simple set of HFB or Hartree-Fock equations. While no solutions can be found for the HFB set, even for a finite system, the Hartree-Fock equations do provide a description of a condensed state. We feel there is reason to believe that this description should be a fair representation of the actual situation.

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