Finite-temperature theory of the trapped two-dimensional Bose gas

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We present a Hartree-Fock-Bogoliubov (HFB) theoretical treatment of the two-dimensional trapped Bose gas and indicate how semiclassical approximations to this and other formalisms have lead to confusion. We numerically obtain results for the quantum-mechanical HFB theory within the Popov approximation and show that the presence of the trap stabilizes the condensate against long wavelength fluctuations. These results are used to show where phase fluctuations lead to the formation of a quasicondensate.

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The question of whether a weakly interacting Bose gas can undergo Bose-Einstein condensation (BEC) when confined to an effectively two-dimensional (2D) geometry has gained significant topical interest with the advent of recent experiments [1]. It is well known that a 2D homogeneous ideal gas of bosons does not undergo BEC at finite temperature [2]. Indeed it has been rigorously shown that even when interactions between the particles are included [3] there is no BEC phase transition at finite temperature, although a superfluid phase transition in the form of a Kosterlitz-Thouless (KT) transition [4] can be shown to take place. The KT transition occurs because of the enhanced importance of fluctuations in the 2D system yielding a quasicondensate state where the length scale for phase coherence is small compared to the system size. The observation of such a phase transition has been reported recently [5] for a 2D gas of dilute hydrogen on a liquid helium surface. For the noninteracting gas, Bagnato and Kleppner [6] showed that an ideal gas in a 2D harmonic trap does exhibit a BEC phase. Petrov *et al.* [7] included interactions and showed within the Thomas-Fermi approximation, that well below T_c there exists a true condensate while at higher temperatures a quasicondensate forms. We are interested in the phase diagram at temperatures below and within this fluctuation regime to investigate both the true BEC state and the onset of phase fluctuations that lead to the destruction of the BEC.

In 3D, the finite temperature Hartree-Fock-Bogoliubov (HFB) treatment of the trapped Bose gas has proved very successful [8–10]. It is therefore natural to develop this approach for the 2D gas. Remarkably the quantum-mechanical HFB formalism has, to the best of our knowledge, never been implemented in 2D, the development of which is the central result of this article. First let us consider however, a simplification to the fully quantum-mechanical implementation of HFB that has been used to conclude previously that there is no BEC in an interacting 2D Bose gas.

In 2D, with a cylindrically symmetric trapping potential of frequency ω_0, the grand-canonical many-body Hamiltonian is given by

$$H=\int d^2r\,\hat{\psi}^\dagger(r)\left(-\frac{\hbar^2\nabla^2}{2m}+\frac{m\omega_0^2}{2}r^2-\mu+\frac{g(r)}{2}\hat{\psi}^\dagger(r)\hat{\psi}(r)\right)\hat{\psi}(r), \quad (1)$$

where we have assumed a spatially dependent coupling parameter, introduced by the many-body T-matrix for the trapped case as proposed in Refs. [11,12].

In a manner identical to the development of the theory in 3D [13] we assume that the many-body Bose field operator can be decomposed into a mean, condensate part and a fluctuating field operator part such that $\hat{\psi}=\langle\hat{\psi}\rangle+\tilde{\psi}\equiv\phi+\tilde{\psi}$. The above Hamiltonian can then be diagonalized provided the condensate order parameter ϕ obeys the generalized Gross-Pitaevskii equation (GPE)

$$\left(-\frac{\hbar^2\nabla^2}{2m}+\frac{m\omega_0^2}{2}r^2-\mu+g(n_c+2\tilde{n})\right)\phi=0, \quad (2)$$

and the quasiparticle excitations obey the Bogoliubov-de Gennes (BdG) equations

$$\hat{\mathcal{L}}u_i-gn_cv_i=E_iu_i,$$

$$\hat{\mathcal{L}}v_i-gn_cu_i=-E_iv_i, \quad (3)$$

where $\hat{\mathcal{L}}=-(\hbar^2\nabla^2/2m)+(m\omega_0^2/2)r^2-\mu+g(2n_c+2\tilde{n})$, $n_c=\phi^*\phi$ is the condensate density and $\tilde{n}$ the noncondensate density, which is evaluated by populating the quasiparticle levels according to the usual Bose distribution. In the derivation of these equations we have used the canonical transformation $\tilde{\psi}=\Sigma_i[u_i\hat{\alpha}_i-v_i^*\hat{\alpha}_i^\dagger]$ where the $\hat{\alpha}_i$ satisfy the usual Bose commutation relations and we have taken the so-called Popov approximation, neglecting anomalous pair averages of the fluctuating field operator.

Together, the GPE and BdG equations form a closed set and can be solved numerically using techniques analogous to those developed in 3D. This we will describe shortly, but first let us attempt to obtain a semiclassical solution of these equations. This is the approach taken by previous authors [14].

Let us assume that the temperature is large compared to the energy-level spacing in the trap. We can now replace the quasiparticle amplitudes such that $u_i\approx ue^{i\theta}$ and $v_i\approx ve^{i\theta}$ where the common phase θ defines a quasiparticle momentum, $\mathbf{p}=\hbar\boldsymbol{\nabla}\theta$. Neglecting spatial derivatives of u, v, and $\mathbf{p}$ (local-density approximation) and making a continuum approximation for the Bose distribution function, the quasiparticle excitation spectrum is found to be given by

$$E_{sc}(\mathbf{p},\mathbf{r}) = \sqrt{\Lambda_{sc}^2 - (gn_c)^2}, \tag{4}$$

where $\Lambda_{sc} = (\mathbf{p}^2/2m) + \frac{1}{2}m\omega_0^2 r^2 - \mu + 2gn_c + 2g\tilde{n}$ and the condensate density is still calculated via the GPE. The density of excited state particles can now be integrated in closed form to give

$$\tilde{n} = \frac{1}{\lambda^2}\left\{-\ln[1-\exp(-\sqrt{t^2-s^2})] + \frac{t}{2} - \frac{1}{2}\sqrt{t^2-s^2}\right\}, \tag{5}$$

where $\lambda^2 = \hbar^2/2\pi mkT$, $s = gn_c/kT$, and $t = (1/kT)(\frac{1}{2}m\omega_0^2 r^2 - \mu + 2gn_c + 2g\tilde{n})$. These semiclassical HFB equations form a closed set and it is this set of equations that previous authors have attempted to solve self-consistently. This is not possible however, as the semiclassical approximation can only be used consistently at low energy if combined with a Thomas-Fermi approximation for the condensate [15]. There are therefore no solutions to these equations.

It is trivial to show that in the Thomas-Fermi limit $t = s$ and the expression for the semiclassical thermal density is undefined. Indeed, even for low particle numbers, it can be shown that the arguments of the square roots always contain values at some spatial point that are negative (and approach zero from below in the Thomas-Fermi limit) and hence this expression is never well defined. The origin of this problem lies in the expression for the semiclassical excitation spectrum. At low energies, or equivalently long wavelengths, Eq. (4) yields imaginary energies. This has been used to conclude that in 2D BEC cannot take place since the condensate is destabilized by long wavelength fluctuations [14]. This is simply incorrect. What one is seeing is a failure of the semiclassical approximation. If the discrete nature of the excitation spectrum for the finite-size trap is not retained for the low-energy excitations, and this is the case within the semiclassical approximation, there comes a point where the magnitude of the chemical potential exceeds the magnitude of the effective potential and the argument in Eq. (4) becomes negative for low **p**. Just because the semiclassical treatment of the HFB formalism fails does not mean that the quantum-mechanical theory will also. In this case the long wavelength oscillations, corresponding to the $\mathbf{p} = \mathbf{0}$ limit in the semiclassical case, are precluded by the finite size of the trap. Therefore, to determine whether BEC can take place in 2D, the full, numerically expensive, discrete calculation must be undertaken.

As an aside, it is possible to obtain a well-defined semiclassical theory of the trapped 2D gas if one makes the further Hartree-Fock approximation [16]. This consists of setting the $v(\mathbf{r},\mathbf{p})$ terms in the semiclassical HFB treatment to zero everywhere. The Hartree-Fock excitation spectrum is now single particlelike and is just given by Λ_{sc} rather than by the phononlike Bogoliubov spectrum of Eq. (4). There is therefore no problem with the infrared divergence seen previously and one can integrate to obtain the semiclassical Hartree-Fock thermal density,

$$\tilde{n} = -\frac{1}{\lambda^2}[\ln(1 - e^{-[(1/2)m\omega_0^2 r^2 + 2gn_c + 2g\tilde{n} - \mu]/kT})], \tag{6}$$

which can be solved self-consistently together with the GPE to obtain a Bose condensed solution. Interestingly, if one omits the ground state from the calculation, effectively demanding that condensation *does not* occur, then it is still possible to obtain a self-consistent solution for the thermal density at all temperatures. Therefore, at the level of the semiclassical Hartree-Fock approximation, one might conclude that there is no BEC in the thermodynamic limit for a 2D gas of trapped, interacting bosons.

By removing the lowest-lying state however, one has truncated the available state space and so one may expect that the thermodynamically stable state is the condensed phase. This is confirmed by calculating the free energies for the two states. Above the BEC transition temperature the free energy of the condensed and uncondensed solutions are virtually indistinguishable, but below the critical temperature the free energy for the condensed solution is lower, confirming that within the Hartree-Fock approximation, BEC is the thermodynamically favored state [14].

We now proceed to solve the quantum-mechanical, discrete, HFB equations [Eq. (2) and Eq. (3)] self-consistently. The method of solution is described in detail elsewhere [13], but is outlined here for completeness.

First, the GPE equation is solved using an expansion in some appropriate basis set with the condensate and noncondensate densities set to zero. The solution for the condensate wave function is then used to construct n_c and the process iterated to find a converged solution. One now needs to calculate the noncondensate density. To do this one decouples the BdG equations by making the transformation to the auxillary functions $\psi_i^{(\pm)} \equiv u_i \pm v_i$. One can thus obtain equations for $\psi_i^{(+)}$ and $\psi_i^{(-)}$ separately. These are solved using a further basis set expansion, for which we use the basis of excited states of the GPE to ensure orthogonality with the condensate and to simplify the construction of the matrix elements. The noncondensate density is then constructed by populating the quasiparticle states. This value of $\tilde{n}$ is inserted into the GPE and the whole process repeated iteratively until convergence.

In contrast to the semiclassical HFB treatment we have no difficulty in finding self-consistent solutions to the quantum, discrete HFB equations and typical results are presented below. In the numerical solution we nondimensionalize our equations using the natural harmonic-oscillator units. In this case we take our Rydberg of energy to be $\hbar\omega_0/2$ and in these units the nondimensional interaction parameter $g(r)$ takes values between 0.09 and 0.1. This parameter, in 3D, depends only upon the *s*-wave scattering length *a* however, in 2D, *g* also depends upon the strength of the confining potential in the third dimension. The 2D gas thus represents a system where the interparticle interaction strength can be tuned by

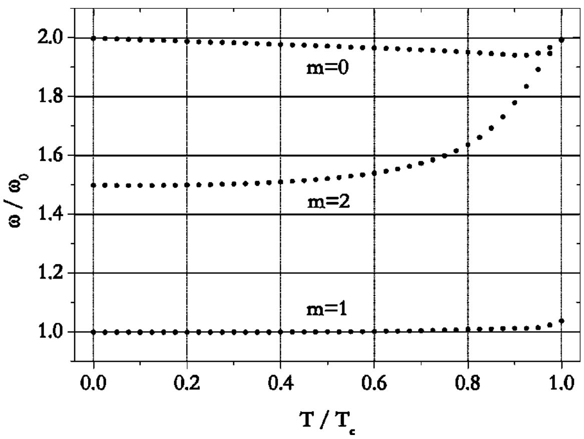

FIG. 1. Quasiparticle excitation frequencies as a function of temperature for $N=2000$ atoms and the full spatially dependent coupling parameter.

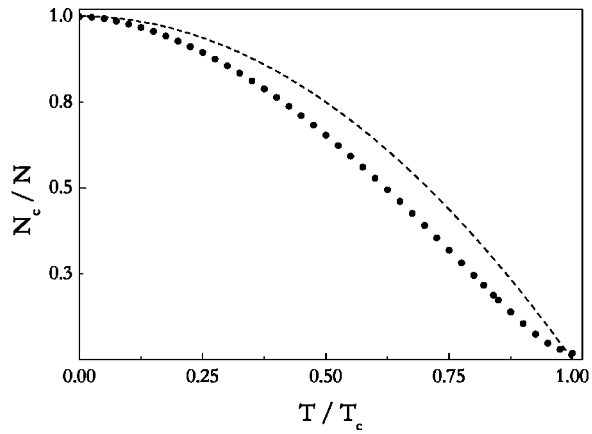

FIG. 2. Fraction of atoms in the condensate as a function of temperature. The dotted line corresponds to the noninteracting gas for comparison.

modulating the confining potential in the z direction in a manner analogous to the use of the Feshbach resonance in 3D [17]. It has even been suggested that the sign of the interaction strength (and hence whether the interactions are attractive or repulsive) can be changed by tuning the confining potential in the third direction [7].

In Fig. 1 we display the low-lying excitation spectrum as a function of temperature for the trapped gas of 2000 ^{87}Rb atoms. Shown are the lowest lying $m=1$, $m=2$, and $m=0$ quasiparticle, or collective, modes up to the critical temperature. We point out that the results shown are those of the HFB-Popov equations. In three dimensions, in the presence of significant direct driving of the thermal cloud, the theory fails to predict shifts in the frequencies above about $0.6T_c$ [18]. These are related to the dynamics of the thermal cloud not included in this theory. The excitation spectrum shown should be valid in experiments where the condensate is driven directly.

In the three-dimensional asymmetric case this approximation is valid only below $0.6T_c$. However, we include the higher temperatures for the symmetrical case where the theory in 3D does not fail. The $m=1$ mode is the Kohn mode [19] and clearly satisfies the generalized Kohn theorem to within our resolution, apart from a slight deviation near the critical temperature. The quadrupole ($m=2$) and breathing ($m=0$) modes are well defined and nowhere look like going soft (approaching zero frequency as an indication of an instability). We therefore conclude there are well defined solutions to the quantum-mechanical HFB equations, in a manner exactly the same as in 3D, for all temperatures below the critical temperature.

It is important to note that, at low temperatures, the frequency of the lowest-lying $m=0$ mode, or breathing mode, is at precisely $2\omega_0$, independent of the interaction strength. This result was predicted some time ago by Pitaevskii and Rosch [20], purely from symmetry arguments. Indeed, they show rigorously that the existence of $2\omega_0$ oscillations is ensured by the underlying SO(2,1) symmetry of the *full quantum theory Hamiltonian* for the interacting harmonically confined 2D gas with a contact interaction. It is therefore noteworthy (and critical) that our calculations confirm this result numerically at low temperatures. At higher temperatures the result is still valid, however the excitations are those for a condensate in an effective potential which is modified by the addition of the potential $2g\tilde{n}$ from the static thermal cloud. The condensate effectively sees a weaker harmonic potential and hence the $m=0$ mode has a slightly lower frequency. Above the critical temperature, the excitation frequencies, of course, go over to those of the thermal gas. Similarly, at high temperatures (near the critical temperature) the $m=1$ mode no longer satisfies the Kohn theorem precisely. This is again due to the presence of the potential from the thermal cloud. The effective potential in which the condensate oscillates is no longer harmonic and the Kohn theorem broken. As discussed previously [13], if the full dynamics of the thermal cloud were included, then the Kohn theorem would be satisfied at all temperatures.

In Fig. 2 we show the condensate fraction as a function of temperature. It is clear that at temperatures below the critical temperature we obtain a macroscopic occupation of the ground state, which implies BEC. This however is not sufficient. For true condensation we require a well-defined phase over the entire condensate. In 3D this is true for all temperatures below T_c except for a small region near the critical temperature often referred to as the Ginzburg region. In this region phase fluctuations prohibit the formation of a true condensate. In a uniform 2D gas this region extends all the way to $T=0$ and is what prevents the formation of a BEC. In Fig. 3 we plot the off-diagonal correlation function, $g^{(1)}(0,r)$ [21] showing that only at low temperatures is there a *coherent* condensate with a correlated phase spanning the condensate. As the temperature is increased the coherence begins to decay on a length scale less than the dimensions of the gas. In analogy with Petrov *et al.* [7], if we expand the field operator as $\hat{\psi}=\phi+\delta\hat{\psi}=\sqrt{\hat{n}}e^{i\hat{\phi}}$ then we can express the noncondensate density as $\tilde{n}=\langle\delta\hat{\psi}^{\dagger}\delta\hat{\psi}\rangle=\langle(\delta\hat{n}^2/4n_c)+i[\delta\hat{n},\hat{\phi}]/2+n_c\hat{\phi}^2\rangle$. At low temperatures density fluctuations are suppressed and this yields $\tilde{n}/n_c\sim\langle\hat{\phi}^2\rangle$. Using the Thomas-Fermi approximation Petrov *et al.* conclude that

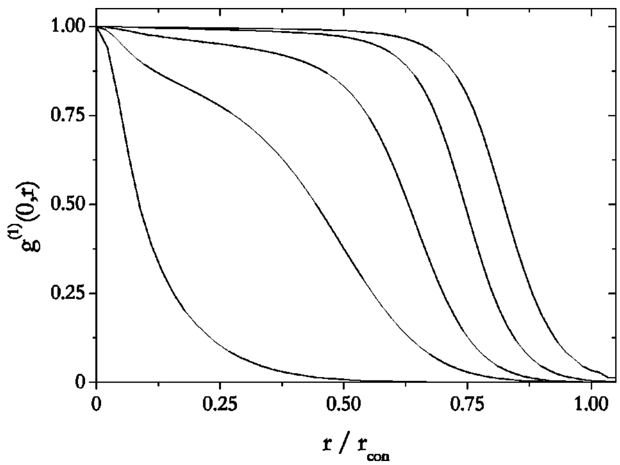

FIG. 3. Single-particle correlation function for the 2D Bose gas as a function of position at 0.05, 0.1, 0.35, 0.75, and 0.925T_c from right to left, showing decreasing correlation length as a function of temperature. Lengths are scaled with the size of the condensate r_{con} at each temperature.

phase fluctuations lead to the formation of a quasicondensate at temperatures of around $T=T_c/2$ for our parameters. In our case we find that the condensate persists to approximately this temperature, but above this the phase becomes ill defined and the system is best described as a quasicondensate. This is consistent with our numerical calculation of the correlation function. An alternate treatment of the 2D gas which coulddescribe the quasicondensate has recently been formulated [22], but has yet to be implemented.

In conclusion, we have shown that the presence of the trap stabilizes the condensate against long wavelength fluctuations. This is true not only for density fluctuations, but for phase fluctuations as well, which are included in our formalism via the contribution to the noncondensate density from low-energy quasiparticles. Our work is consistent with Petrov *et al.* [7]. A 2D trapped dilute gas of weakly interacting bosons therefore does undergo BEC, forming a pure condensate at temperatures below a transition region near T_c. Although this conclusion has been reached by, among others, Petrov *et al.* [7] and Bagnato and Kleppner [6], the converse conclusion has also appeared in the literature [14]. The prospect of performing the HFB calculation has been proposed as a means of clarifying the issue (in addition to the above references, see for example, Bayindir and Tanatar [23]), but to this point no one had done so. We have now performed this calculation and unambiguously shown that BEC does occur for the 2D trapped interacting gas when the discrete nature of the energy spectrum is taken into consideration.

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