Phase Fluctuations in Atomic Bose Gases

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We improve on the Popov theory for partially Bose-Einstein condensed atomic gases by treating the phase fluctuations exactly. As a result, the theory becomes valid in arbitrary dimensions and is able to describe the low-temperature crossover between three-, two-, and one-dimensional Bose gases, which is currently being explored experimentally. We consider both homogeneous and trapped Bose gases.

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Introduction.—One of the most important features of the trapped Bose-Einstein condensed atomic gases is the remarkable control that can be achieved experimentally over the relevant physical parameters. As a result, these gases can be studied in various physically distinct regimes, where their properties are quite different. The latest achievement in this respect is the experiment by Görlitz *et al.* [1], in which one- and two-dimensional Bose-Einstein condensates were created by reducing the temperature and the average interaction energy of the atoms below the energy splitting of either two or one of the directions of the harmonic trapping potential, respectively.

As is well known, the physics of one- and two-dimensional systems is fundamentally different from the physics in three dimensions. This difference is, for instance, illustrated by the famous Mermin-Wagner-Hohenberg theorem [2,3], which states that in one dimension Bose-Einstein condensation in a homogeneous Bose gas never occurs, whereas in two dimensions a condensate can exist only at zero temperature. In both cases, this is due to the enhanced importance of phase fluctuations. The Mermin-Wagner-Hohenberg theorem is valid only in the thermodynamic limit and does not apply to finite-size systems. In one- or two-dimensional trapped Bose gases a condensate can therefore exist if the external trapping potential sufficiently restricts the size of the atomic gas cloud [4,5].

The physics of low-dimensional Bose gases is, in fact, even more interesting, because, notwithstanding the Mermin-Wagner-Hohenberg theorem, a dilute homogeneous two-dimensional Bose gas is expected to undergo at a nonzero critical temperature a true thermodynamic phase transition that is known as the Kosterlitz-Thouless transition [6]. Below the critical temperature, the gas is superfluid but has only algebraic long-range order. This so-called topological phase transition is therefore not characterized by a local order parameter, but by the unbinding of vortex pairs and the resulting destruction of superfluidity. Since the Mermin-Wagner-Hohenberg theorem forbids a true Bose-Einstein condensate in two dimensions, the superfluid phase is characterized only by the existence of a so-called "quasicondensate." This important concept was first introduced by Popov [7] and roughly speaking corresponds to a condensate with a fluctuating phase.

Although introduced theoretically as early as in 1972, the actual observation of such a quasicondensate has only very recently been made in a spin-polarized atomic hydrogen adsorbed on a superfluid ^{4}He surface by Safonov *et al.* [8]. In particular, this experiment measures the three-body (dipolar) recombination rate of a spin-polarized atomic hydrogen gas and observes a reduction in the associated rate constant due to the presence of a quasicondensate. Qualitatively, this reduction was anticipated by Kagan, Svistunov, and Shlyapnikov, but the magnitude of the effect turns out to be much larger than predicted [9]. The reason for this discrepancy is still not fully understood, although a physical mechanism for the additional reduction was already suggested by Stoof and Bijlsma before its observation [10].

In the context of trapped atomic Bose gases, the possibility of observing a quasicondensate has been explored by Petrov *et al.* [11,12]. Although this presents an important first step towards understanding the physics of low-dimensional Bose gases, the approach can be justified only close to zero temperature. The reason for this is that density fluctuations are neglected from the outset. As a result, depletion of the quasicondensate, due to either quantum or thermal fluctuations, cannot be properly accounted for. In particular, the approach does not lead to an equation of state for the Bose gas.

The main aim of the present Letter is to overcome this problem and to formulate a microscopic theory that includes both density and phase fluctuations of the Bose gas. It is similar in spirit to the successful Popov theory for three-dimensional Bose-Einstein condensed gases, and can be used to study in detail the thermodynamic behavior of low-dimensional degenerate Bose gases. Moreover, it describes also the crossover between three-, two-, and one-dimensional Bose gases. To explain most clearly how this can be achieved, we first discuss the homogeneous case. After that, we generalize the theory to inhomogeneous gases.

Modified Popov theory.—Formulating a microscopic theory for lower-dimensional Bose gases is complicated by the fact that mean-field theory is plagued with infrared divergences. To facilitate the discussion of how to deal with these divergences, we first recapitulate the expressions for the density n and the chemical potential μ that follow from the usual Popov theory for partially Bose-Einstein condensed gases. For a Bose gas in a box with volume V they read [7,13]

$$n = n_0 + \frac{1}{V}\sum_{\mathbf{k}}\left[\frac{\epsilon_{\mathbf{k}} + n_0 V_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} + \frac{\epsilon_{\mathbf{k}} + n_0 V_0}{\hbar\omega_{\mathbf{k}}} N(\hbar\omega_{\mathbf{k}})\right], \quad (1)$$

$$\frac{\mu}{V_0} = n_0 + \frac{1}{V}\sum_{\mathbf{k}}\left[\frac{2\epsilon_{\mathbf{k}} + n_0 V_0 - 2\hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} + \frac{2\epsilon_{\mathbf{k}} + n_0 V_0}{\hbar\omega_{\mathbf{k}}} N(\hbar\omega_{\mathbf{k}})\right]. \quad (2)$$

Here n_0 is the density of the Bose-Einstein condensate, $V_0\delta(\mathbf{x} - \mathbf{x}')$ is the bare two-body interaction potential, $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$ is the kinetic energy of the atoms, $\hbar\omega_{\mathbf{k}} = (\epsilon_{\mathbf{k}}^2 + 2n_0V_0\epsilon_{\mathbf{k}})^{1/2}$ is the Bogoliubov dispersion relation, and $N(x) = 1/(e^{\beta x} - 1)$ is the Bose-Einstein distribution function where $\beta = 1/k_{\mathrm{B}}T$ is the inverse thermal energy.

In agreement with the Mermin-Wagner-Hohenberg theorem, the momentum sums in Eqs. (1) and (2) contain terms that are infrared divergent at all temperatures in one dimension and at any nonzero temperature in two dimensions. The physical reason for these "dangerous" terms is that the above expressions have been derived by taking into account only quadratic fluctuations around the classical result n_0, i.e., by writing the annihilation operator for the atoms as $\hat{\psi}(\mathbf{x}) = \sqrt{n_0} + \hat{\psi}'(\mathbf{x})$ and neglecting in the Hamiltonian terms of third and fourth order in $\hat{\psi}'(\mathbf{x})$. As a result the phase fluctuations of the condensate give the quadratic contribution $n_0\langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x})\rangle$ to the right-hand side of the above equations, whereas an exact approach that sums up all the higher-order terms in the expansion would clearly give no contribution at all to these local quantities because $\langle e^{-i\hat{\chi}(\mathbf{x})}e^{i\hat{\chi}(\mathbf{x})}\rangle = 1 + \langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x})\rangle + \cdots = 1$. To correct for this we thus need to subtract the quadratic contribution of the phase fluctuations, which from Eqs. (1) and (2) is seen to be given by

$$n_0\langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x})\rangle = \frac{1}{V}\sum_{\mathbf{k}}\frac{n_0V_0}{2\hbar\omega_{\mathbf{k}}}[1 + 2N(\hbar\omega_{\mathbf{k}})]. \quad (3)$$

As expected, the infrared divergences that occur in the one- and two-dimensional cases are removed by performing this subtraction.

After having removed the spurious contributions from the phase fluctuations of the condensate, the resulting expressions turn out to be ultraviolet divergent. These divergences can be removed by the standard renormalization of the bare coupling constant V_0. Apart from a subtraction, this essentially amounts to replacing everywhere the bare two-body potential V_0 by the two-body T matrix evaluated at zero initial and final relative momenta and at the energy -2μ, which we denote from now on by $T^{2B}(-2\mu)$. Note that the energy argument of the T matrix is -2μ, because this is precisely the energy it costs to excite two atoms from the condensate [14,15]. In this manner, we finally arrive at

$$n = n_0 + \frac{1}{V}\sum_{\mathbf{k}}\left[\frac{\epsilon_{\mathbf{k}} - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} + \frac{n_0T^{2B}(-2\mu)}{2\epsilon_{\mathbf{k}} + 2\mu} + \frac{\epsilon_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}N(\hbar\omega_{\mathbf{k}})\right], \quad (4)$$

$$\mu = (2n - n_0)T^{2B}(-2\mu) = (2n' + n_0)T^{2B}(-2\mu), \quad (5)$$

where $n' = n - n_0$ represents the depletion of the condensate due to quantum and thermal fluctuations and the Bogoliubov quasiparticle dispersion now equals $\hbar\omega_{\mathbf{k}} = [\epsilon_{\mathbf{k}}^2 + 2n_0T^{2B}(-2\mu)\epsilon_{\mathbf{k}}]^{1/2}$. The most important feature of Eqs. (4) and (5) is that they contain no infrared and ultraviolet divergences and therefore can be applied in any dimension and at all temperatures, even if no condensate exists. How this can be reconciled with the Mermin-Wagner-Hohenberg theorem is discussed next.

One dimension.—To understand the physical meaning of the quantity n_0 in Eqs. (4) and (5), we must determine the off-diagonal long-range behavior of the one-particle density matrix. Because this is a nonlocal property of the Bose gas, the phase fluctuations contribute and in the limit $|\mathbf{x}| \to \infty$, we find

$$\langle\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{0})\rangle \simeq n_0 e^{-\langle[\hat{\chi}(\mathbf{x})-\hat{\chi}(\mathbf{0})]^2\rangle/2}. \quad (6)$$

Moreover, using Eq. (3) and carrying out the renormalization of the bare coupling constant, we obtain

$$\langle[\hat{\chi}(\mathbf{x}) - \hat{\chi}(\mathbf{0})]^2\rangle = \frac{T^{2B}(-2\mu)}{V} \times \sum_{\mathbf{k}}\left[\frac{1}{\hbar\omega_{\mathbf{k}}}[1 + 2N(\hbar\omega_{\mathbf{k}})] - \frac{1}{\epsilon_{\mathbf{k}} + \mu}\right][1 - \cos(\mathbf{k}\cdot\mathbf{x})]. \quad (7)$$

At zero temperature, the quantity $\langle[\hat{\chi}(\mathbf{x}) - \hat{\chi}(\mathbf{0})]^2\rangle$ diverges logarithmically for large distances, which leads to algebraic off-diagonal long-range order in the one-particle density matrix. In detail we can show that the leading behavior of the zero-temperature one-particle density matrix for $|\mathbf{x}| \gg \xi$ is

$$\langle\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{0})\rangle \simeq \frac{n_0}{(|\mathbf{x}|/\xi)^\eta}, \quad (8)$$

where $\eta = 1/4\pi n_0\xi$ is the correlation-function exponent and $\xi = \hbar/[4mn_0T^{2B}(-2\mu)]^{1/2}$ is the correlation length. At nonzero temperatures, $\langle[\hat{\chi}(\mathbf{x}) - \hat{\chi}(\mathbf{0})]^2\rangle$ diverges linearly for large distances, and the one-particle density matrix thus no longer displays off-diagonal long-range order.

A few remarks are in order at this point. Most importantly for our purposes, the asymptotic behavior of the one-particle density matrix at zero temperature proves that the gas is not Bose-Einstein condensed and that n_0 should be identified with the quasicondensate density. Moreover, from our equation of state we can show that in the weakly interacting limit $4\pi n\xi \gg 1$, the fractional depletion of the quasicondensate is $(n - n_0)/n = (\pi\sqrt{2}/4 - 1)/4\pi n\xi$ and therefore very small. Keeping this in mind, Eq. (8) is in complete agreement with the exact result obtained by Haldane [16]. Note that our theory cannot describe the strongly interacting case $4\pi n\xi \ll 1$, where the one-dimensional Bose gas behaves as a Tonks gas [17,18]. Finally, our results show that at nonzero temperatures not even a quasicondensate exists and we have to use the equation of state for the normal state $n = \sum_{\mathbf{k}} N(\epsilon_{\mathbf{k}} + \hbar\Sigma - \mu)/V$ to describe the gas. Here the Hartree-Fock self-energy satisfies $\hbar\Sigma = 2nT^{2B}(-\hbar\Sigma)$.

Two dimensions.—Applying the same arguments in two dimensions leads to the conclusion that at zero temperature, n_0 corresponds to the condensate density, whereas at a nonzero temperature, it represents the quasicondensate density. In particular, the correlation-function exponent is $\eta = 1/n_0\Lambda^2$ where $\Lambda = (2\pi\hbar^2/mk_BT)^{1/2}$ is the thermal de Broglie wave length. Because of the mean-field nature of the modified Popov theory, the Kosterlitz-Thouless transition is absent and a nontrivial solution of the equation of state exists even if $\eta > 1/4$. This can be corrected for by explicitly including the effect of vortex pairs in the phase fluctuations. As we show in a future paper, this is achieved by using the modified Popov theory to determine the initial values of a renormalization-group calculation for the superfluid density and the fugacity of the vortices. It should, however, be noted that for many applications we are not interested in the phase fluctuations and this additional renormalization is not very important. This is, for instance, true for the reduction of the three-body recombination rate constant of a hydrogen gas [19].

At zero temperature, the fractional depletion of the condensate in the Popov approximation was first calculated by Schick [14] and is $T^{2B}(-2\mu)/4\pi$ where the chemical potential satisfies $\mu = nT^{2B}(-2\mu)$. The corresponding result based on Eq. (4) is $(1 - \ln 2)T^{2B}(-2\mu)/4\pi$ where μ now satisfies Eq. (5). Thus the depletion is reduced by a factor of approximately 3. In two dimensions, the two-body T matrix cannot be approximated by an energy-independent constant, and this is the reason why we have been very careful about the appropriate energy of the two-body collisions [20]. The T matrix now obeys

$$T^{2B}(-2\mu) = \frac{4\pi\hbar^2}{m}\,\frac{1}{\ln(2\hbar^2/\mu m a^2)}, \tag{9}$$

where a is the scattering length.

Three dimensions.—We know that the Popov theory has been very successful in describing the properties of three-dimensional trapped Bose gases. It is therefore important to mention that, although the modification that we have performed is essential for one- and two-dimensional Bose gases, it leads only to minor changes in the three-dimensional case. This can be seen by considering the temperature dependence of the condensate density. At zero temperature, the fractional depletion that results from the Popov theory was first calculated by Lee and Yang [21] and equals $(8/3)\sqrt{na^3/\pi}$, where the T matrix is taken to be $T^{2B}(-2\mu) = 4\pi a\hbar^2/m$ and a is the scattering length. The result that follows from Eqs. (4) and (5) is $(32/3 - 2\sqrt{2}\,\pi)\sqrt{na^3/\pi}$. The fractional depletion is thus approximately 2/3 of the Popov result. This is, in fact, the largest change in the condensate depletion, since the effects of the phase fluctuations decrease at larger temperatures. The critical temperature $T_{\rm BEC}$ is found by taking the limit $n_0 \to 0$ in Eqs. (4) and (5). These expressions then reduce to the same expressions for the density and chemical potential as in the Popov theory. This implies that our critical temperature for Bose-Einstein condensation coincides with that obtained in the Popov theory and with that of an ideal Bose gas.

Trapped Bose gases.—We now generalize our mean-field theory to a Bose gas in an external potential $V^{\rm ext}(\mathbf{x})$. First, the right-hand side of Eq. (4) is expressed in terms of the Bogoliubov coherence factors $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, which are then replaced by $u_j(\mathbf{x})$ and $v_j(\mathbf{x})$. The latter satisfies the Bogoliubov–de Gennes equations [22,23]

$$\left[-\hbar\omega_j - \frac{\hbar^2}{2m}\nabla^2 - \mu(\mathbf{x}) + 2T^{2B}(-2\mu(\mathbf{x}))n(\mathbf{x})\right]u_j(\mathbf{x}) + T^{2B}(-2\mu(\mathbf{x}))n_0(\mathbf{x})v_j(\mathbf{x}) = 0, \tag{10}$$

$$\left[\hbar\omega_j - \frac{\hbar^2}{2m}\nabla^2 - \mu(\mathbf{x}) + 2T^{2B}(-2\mu(\mathbf{x}))n(\mathbf{x})\right]v_j(\mathbf{x}) + T^{2B}(-2\mu(\mathbf{x}))n_0(\mathbf{x})u_j(\mathbf{x}) = 0, \tag{11}$$

where $n_0(\mathbf{x}) = |\psi_0(\mathbf{x})|^2$ and $\mu(\mathbf{x}) = \mu - V^{\rm ext}(\mathbf{x})$. Note that we have chosen $u_j(\mathbf{x})$ and $v_j(\mathbf{x})$ to be real. In some cases, e.g., when the macroscopic wave function $\psi_0(\mathbf{x})$ contains a vortex, one cannot choose these amplitudes to be real, and our equations must be generalized to incorporate that fact. In terms of these particle and hole amplitudes, the expression for the total density in Eq. (4) reads

$$n(\mathbf{x}) = n_0(\mathbf{x}) + \sum_j \left\{[u_j(\mathbf{x}) + v_j(\mathbf{x})]^2 N(\hbar\omega_j) + v_j(\mathbf{x})[u_j(\mathbf{x}) + v_j(\mathbf{x})] + \frac{T^{2B}(-2\mu(\mathbf{x}))n_0(\mathbf{x})}{2\epsilon_j + 2\mu(\mathbf{x})}[\phi_j(\mathbf{x})]^2\right\}. \tag{12}$$

Here ϵ_j are the eigenenergies and $\phi_j(\mathbf{x})$ the eigenstates of the external trapping potential. In the large-j limit, we have that $u_j(\mathbf{x}) = \phi_j(\mathbf{x})$ and

$$v_j(\mathbf{x}) = -\frac{T^{2B}(-2\mu(\mathbf{x}))n_0(\mathbf{x})}{2\epsilon_j}\,\phi_j(\mathbf{x})\,. \tag{13}$$

As a result, the sum in the expression for the total density is ultraviolet finite since the second and third terms cancel each other in the large-j limit. Furthermore, the inhomogeneous generalization of Eq. (5) becomes the nonlinear Schrödinger equation

$$\mu\psi_0(\mathbf{x}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V^{\mathrm{ext}}(\mathbf{x}) + T^{2B}(-2\mu(\mathbf{x}))\left(2n'(\mathbf{x}) + |\psi_0(\mathbf{x})|^2\right)\right]\psi_0(\mathbf{x})\,. \tag{14}$$

Finally, the expression for the phase fluctuations in the case of a trapped Bose gas can be obtained from $\langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x}')\rangle$, which is equal to the part of

$$-\sum_j \frac{1}{\sqrt{n_0(\mathbf{x})n_0(\mathbf{x}')}}\left\{u_j(\mathbf{x})v_j(\mathbf{x}')[1 + 2N(\hbar\omega_j)] + \left[\frac{T^{2B}(-2\mu(\mathbf{x}'))n_0(\mathbf{x}')}{2\epsilon_j + 2\mu(\mathbf{x}')}\right]\phi_j(\mathbf{x})\phi_j(\mathbf{x}')\right\},$$

which is symmetric under exchange of $\mathbf{x}$ and $\mathbf{x}'$. Note that this correlation function is free of ultraviolet divergences in contrast to the long-wavelength result used in Refs. [11,12].

Discussion.—We have proposed a new mean-field theory for dilute Bose gases in arbitrary dimensions, in which the phase fluctuations are treated exactly. We reproduce exact results in one dimension, and the results in three dimensions are essentially the same as those predicted by the Popov theory. The exact treatment of the phase fluctuations has solved the long-standing problem of infrared divergences in one- and two-dimensional Bose systems. This opens up the possibility to study in the same detail as in the three-dimensional case, the physics of low-dimensional atomic gases. As previously mentioned, we can also incorporate the Kosterlitz-Thouless transition and, for instance, perform an *ab initio* calculation of the critical temperature as a function of the scattering length and the density of the gas.

The inhomogeneous generalization of the modified Popov theory describes in a self-consistent manner the density profile and the full crossover from a condensate to quasicondensate in one- and two-dimensional trapped Bose gases. In practice, however, we expect that a good approximation is obtained by simply calculating the densities $n_0(\mathbf{x})$ and $n'(\mathbf{x})$ in the Thomas-Fermi approximation, i.e., by applying Eqs. (4) and (5) locally at every point in space with a chemical potential equal to $\mu(\mathbf{x})$. Work in this direction is also in progress [19].

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