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. When applied to a degenerate two-dimensional atomic hydrogen gas, we find reasonable agreement with recent experimental data for the reduction of the three-body recombination rate.

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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 a Bose-Einstein condensation in a homogeneous Bose gas never occurs, whereas in two dimensions a condensate can only exist 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 only characterized 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 only be justified 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. We apply the theory to a two-dimensional atomic hydrogen gas and show that the additional reduction of the three-body recombination rate can be understood from the renormalization effect put forward by Stoof and Bijlsma.

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, $\hbar\omega_{\mathbf{k}} = (\epsilon_{\mathbf{k}}^2 + 2n_0 V_0 \epsilon_{\mathbf{k}})^{1/2}$ 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 $\langle e^{-i\hat\chi(\mathbf{x})}e^{i\hat\chi(\mathbf{x})}\rangle = 1 + \langle\hat\chi(\mathbf{x})\hat\chi(\mathbf{x})\rangle + \ldots = 1$. 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

$$n_0\langle\hat\chi(\mathbf{x})\hat\chi(\mathbf{x})\rangle = \frac{1}{V}\sum_{\mathbf{k}} \frac{n_0 V_0}{2\hbar\omega_{\mathbf{k}}} \left[1 + 2N(\hbar\omega_{\mathbf{k}})\right] . \quad (3)$$

As expected, the infrared divergences that occur in the one and two-dimensional case 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 $T^{2\mathrm{B}}(-2\mu)$. 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

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

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

where $n' = n - n_0$ represents the depletion of the condensate due to quantum and thermal fluctuations and the Bogoliubov quasiparticle dispersion now equals $\hbar\omega_{\mathbf{k}} = \left[\epsilon_{\mathbf{k}}^2 + 2n_0 T^{2\mathrm{B}}(-2\mu)\epsilon_{\mathbf{k}}\right]^{1/2}$. 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

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

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 $\hbar\Sigma = 2nT^{2B}(-2\hbar\Sigma)$.

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. Due to 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 [19], 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.

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.

As an example of a physical observable in which phase fluctuations are not important, we proceed to determine the reduction of the three-body recombination rate constant due to the presence of a condensate. This can be expressed as [10]

$$\frac{L(T)}{L^{MB}} = \left[\frac{T^{2B}(-2\mu)}{T^{2B}(-2\hbar\Sigma)}\right]^6 K_R^{(3)}(T)\ , \tag{9}$$

where L^{MB} is the recombination rate constant in the normal phase and the self-energy satisfies $\hbar\Sigma = 2nT^{2B}(-2\hbar\Sigma)$. The renormalized three-body correlator

$$K_R^{(3)}(T) = \frac{1}{6n^3}\left[n_0^3 + 9n_0^2n' + 18n_0(n')^2 + 6(n')^3\right] \tag{10}$$

is obtained from the expression for the correlation function $\langle\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x})\rangle$ by removing, as before, the spurious contributions from the phase fluctuations. To obtain Eq. (10), we have used that the anomalous average obeys $\langle\hat{\psi}'(\mathbf{x})\hat{\psi}'(\mathbf{x})\rangle = -n_0\langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x})\rangle$ and that the normal average is given by $\langle\hat{\psi}'^\dagger(\mathbf{x})\hat{\psi}'(\mathbf{x})\rangle = n' + n_0\langle\hat{\chi}(\mathbf{x})\hat{\chi}(\mathbf{x})\rangle$.

In two dimensions, the T-matrix depends logarithmically on the chemical potential as

$$T^{2B}(-2\mu) = \frac{4\pi\hbar^2}{m}\frac{1}{\ln(2\hbar^2/\mu ma^2)}\ , \tag{11}$$

where a is the two-dimensional s-wave scattering length. In the case of atomic hydrogen adsorbed on a superfluid helium film, the scattering length was found to be $a = 2.4a_0$ [20]. However, there is some uncertainty in this number because the hydrogen wave function perpendicular to the helium surface is not known very accurately. When comparing with experiment, we will therefore allow a to vary somewhat.

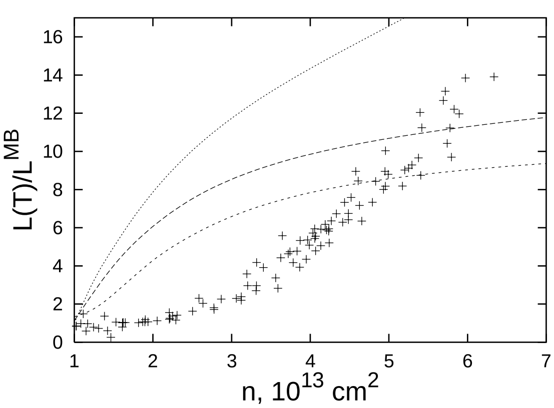

FIG. 1. Reduction of the three-body recombination rate as function of density for $T = 190$mK and three different values of the scattering length. The dotted line corresponds to $a = 2.4a_0$, the long-dashed line to $a = 1.2a_0$, and the dashed line to $a = 0.6a_0$, respectively. Data points are from Refs. [8,21].

In Fig. 1, we show the reduction of the three-body recombination rate as a function of the density at a fixed temperature $T = 190$mK for three different values of a. As can clearly be seen from Fig. 1, the reduction of the three-body recombination rate is very sensitive to the value of a. The data points shown correspond to temperatures that are in the range 180-215mK. The density and temperature of the gas were not measured directly, but inferred from the properties of the three-dimensional buffer gas by assuming a constant value for the two-dimensional T-matrix, which was fitted to be $5.1(5) \times 10^{-15}\mathrm{Kcm}^2$. Although this compares favorably with the value $7.8 \times 10^{-15}\mathrm{Kcm}^2$ obtained here with $a = 0.6a_0$ and $n = 5 \times 10^{-13}\mathrm{cm}^{-2}$, our findings show that the dependence on the chemical potential is not negligible. This results in large uncertainties in the experimental results [8,21] which are not shown in the figure. In view of this issue and the theoretical uncertainty in a, we think that there is reasonable agreement between theory and experiment at this point.

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 [22] and equals $(8/3)\sqrt{na^3/\pi}$, where the T-matrix is taken to be $T^{2\mathrm{B}} = 4\pi a\hbar^2/m$ 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 decreases at larger temperatures. In particular, the condensate density vanishes at exactly the same critical temperature, which also coincides with that of an ideal Bose gas.

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. In two dimensions. the theory is able to explain the reduction of the three-body recombination rate at low temperature, which has been a puzzle up to now. Although we have been focusing on the homogeneous Bose gas, we would like to emphasize that the theory is easily generalized to a Bose gas in an external potential $V^{\mathrm{ex}}(\mathbf{x})$. Introducing the quantity $\phi(\mathbf{x}) = \sqrt{n_0(\mathbf{x})}$, Eq. (5) becomes a modified time-independent Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2\nabla^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + 2T^{2\mathrm{B}}(-2\mu(\mathbf{x}))n'(\mathbf{x}) + T^{2\mathrm{B}}(-2\mu(\mathbf{x}))|\phi(\mathbf{x})|^2\right]\phi(\mathbf{x}) = \mu\phi(\mathbf{x}) , \qquad (12)$$

where $\mu(\mathbf{x}) = \mu - V^{\mathrm{ex}}(\mathbf{x})$ is the local chemical potential. The depletion density $n'(\mathbf{x})$ in Eq. (12) follows from Eq. (4) by expressing it in terms of the Bogoliubov coherence factors $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, and then replacing these by $u_{\mathbf{n}}(\mathbf{x})$ and $v_{\mathbf{n}}(\mathbf{x})$. The latter satisfy the usual Bogoliubov-de Gennes equations that can be derived by linearizing the above modified Gross-Pitaevskii equation. In practice, we expect that a good approximation is obtained simply by 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. Work in this direction is in progress [19].

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