

Dynamics of Fluctuating Bose-Einstein Condensates

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We present a generalized Gross-Pitaevskii equation that describes also the dissipative dynamics of a trapped partially Bose condensed gas. It takes the form of a complex nonlinear Schrödinger equation with noise. We consider an approximation to this Langevin field equation that preserves the correct equilibrium for both the condensed and the noncondensed parts of the gas. We then use this formalism to describe the reversible formation of a one-dimensional Bose condensate, and compare with recent experiments. In addition, we determine the frequencies and the damping of collective modes in this case.

The observation of Bose-Einstein condensation in ultracold trapped atomic vapors [1–3] has offered the possibility to study the equilibrium and nonequilibrium properties of these degenerate gases experimentally and to compare the results with *ab initio* calculations. The latter have as an input only the mass and scattering length of the particular atom of interest, and the parameters involved in the experimental setup. To describe the various equilibrium and nonequilibrium properties like for example topological excitations, relaxation rates, mode frequencies, damping rates and density profiles, theories have been developed at different levels of sophistication.

At the most elementary level, the Gross-Pitaevskii equation already captures many of the experimentally observed phenomena [4]. It describes in Hartree approximation the zero-temperature dynamics of the condensate, and has been used to explain and predict many features of these Bose-condensed systems. At the next level, the static and dynamic properties of the noncondensed or thermal part of the gas are to be included. This can in first instance be done by including into the Gross-Pitaevskii equation the Hartree-Fock interaction with the thermal cloud and coupling it to an equation for the dynamics of the thermal part of the gas. The latter is in good approximation given by a Boltzmann equation for the single-particle distribution function [5].

All these theories describe in essence only the average dynamics of the gas. Near the critical region however, fluctuations in the order parameter are generally much larger than the average value of the order parameter itself. Therefore, in this region, it is necessary to include fluctuations into a description of the trapped gas. Also far below the critical temperature, it can be essential in some cases to include fluctuations into a description of the dynamics of the gas. For example, to understand the phenomenon of phase diffusion [6], one needs to consider fluctuations that disturb the phase of the condensate. From a fundamental point of view, the desired dissipative generalization of the Gross-Pitaevskii equation should obey the so-called fluctuation-dissipation theorem

[7]. This guarantees that both the condensed as well as the noncondensed components of the gas will relax to thermal equilibrium. As a result, the order parameter fluctuates around its mean value, and the central quantity describing the dynamics of the condensate is not this mean value, but the actual probability distribution of the order parameter. With all this in mind, a unified theory describing the coherent dynamics of the condensate wave function, the incoherent scattering between the various components of the gas, as well as the fluctuations around the average value of the order parameter has been developed by one of us [8,9].

The purpose of this Letter is two-fold. First, we show how the coupled dynamics of the thermal cloud and the condensate can be solved in a selfconsistent way, that on the one hand leads to the correct equilibrium distribution of the trapped gas, and at the same time takes into account both mean-field effects as well as fluctuations. Second, we show that fluctuations can be of crucial importance when trying to understand recent experimental results.

In general, a theoretical description of a trapped interacting Bose gas is possible in terms of the Langevin equation

$$i\hbar \frac{\partial \Phi(\mathbf{x}, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{x}) - \mu - iR(\mathbf{x}, t) \right. \\ \left. + T^{2B} |\Phi(\mathbf{x}, t)|^2 \right] \Phi(\mathbf{x}, t) + \eta(\mathbf{x}, t). \quad (1)$$

Here \hbar is Planck's constant, m is the mass of the atom, $V_{\text{ext}}(\mathbf{x})$ is the external trapping potential, and $T^{2B} = 4\pi\hbar^2 a/m$ is the s-wave approximation to the two-body scattering matrix, with a the scattering length. This Langevin equation can be derived using a field-theoretic formulation of the Keldysh formalism [9], and describes the fluctuations as well as the mean-field effects of both the condensed and the noncondensed parts of the gas. The derivation requires that the high-energy part of the system is sufficiently close to equilibrium that it can be described as having a temperature T and a chemical potential μ , and can play the role of a 'heat bath'. This

requirement is usually well satisfied and enters through the explicit expression for the imaginary part in our generalized Gross-Pitaevskii equation, which, if the gas is sufficiently close to or below the critical temperature, can be approximated by

$$iR(\mathbf{x}, t) = -\frac{\beta}{4}\hbar\Sigma^K(\mathbf{x})\left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{x}) - \mu + T^{2B}|\Phi(\mathbf{x}, t)|^2\right]. \quad (2)$$

Here β is $1/k_B T$, with k_B Boltzmann's constant.

If $R(\mathbf{x}, t)$ has this particular form, the trapped gas will relax to equilibrium, because it enforces the fluctuation-dissipation theorem. Note that Eq. (2) is always valid for the energy levels below the chemical potential, i.e., for the condensate, but causes the energy distribution function for the noncondensed cloud to relax to its 'classical' value $N(\epsilon) = [\beta(\epsilon - \mu)]^{-1}$. Therefore, it cannot describe the exponential decay of the density of noncondensed atoms at the edges of the thermal cloud. Instead, the density of thermal atoms decays algebraically. In addition, the classical approximation overestimates the average number of atoms for the eigenstates above the chemical potential. Both defects can be cured [10], but are unimportant for the condensate and the low-energy part of the thermal cloud, where most of the atoms reside, and for which our theory is intended to be valid.

Finally, the correlations of the Gaussian noise $\eta(\mathbf{x}, t)$ in Eq. (1) are given by

$$\langle \eta^*(\mathbf{x}, t)\eta(\mathbf{x}', t') \rangle = \frac{i\hbar^2}{2}\Sigma^K(\mathbf{x})\delta(t-t')\delta(\mathbf{x}-\mathbf{x}'), \quad (3)$$

where the average denotes an average over the different realizations of the noise. The general expressions for $R(\mathbf{x}, t)$ and $\Sigma^K(\mathbf{x})$ can be found in Ref. [9], and lead to a Keldysh selfenergy $\Sigma^K(\mathbf{x})$ equal to

$$\hbar\Sigma^K(\mathbf{x}) = -\frac{4i[T^{2B}]^2}{(2\pi)^5\hbar^6}\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 \delta(\mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3) \delta(\epsilon_1 - \epsilon_2 - \epsilon_3)(1 + N_1)N_2N_3, \quad (4)$$

with $N_i \equiv N(\epsilon_i)$ the Bose distribution for the eliminated part of the gas, and $\epsilon_i = \mathbf{p}_i^2/2m + V_{\text{ext}}(\mathbf{x}) - \mu$. It determines the strength of the fluctuations through Eq. (3) and is related to the damping by means of the fluctuation-dissipation theorem.

At this point, we explain briefly the experimental setup we are considering in the rest of this Letter. It is inspired by a recent experiment by Stamper-Kurn *et al* [11], and the ideal realization of the conditions mentioned above. In the experiment we are considering, a Bose gas is trapped and cooled to a temperature above the transition temperature. Subsequently, a dimple is created in the external trapping potential, say along the z -axis, by means of optical techniques. This dimple is steep enough

such that there is only one energy level in the potential perpendicular to the z -axis. We assume the dimple to be well approximated by a harmonic potential with trapping frequency ω_\perp . Factorizing the wave function $\Phi_0(\mathbf{x}) = \Phi(x, y)\Phi(z)$, the atoms trapped inside this dimple form effectively a one-dimensional gas, with an interaction strength $g = T^{2B}/2\pi l_\perp^2$. Here, $l_\perp = \sqrt{\hbar/m\omega_\perp}$ is the harmonic oscillator length, and Φ_0 the harmonic groundstate in the dimple. By changing the depth of the dimple, its lowest energy level can become lower than the chemical potential of the noncondensed three-dimensional gas. If this situation occurs, the atoms will condense into this ground state. Notice that during this process, the noncondensed gas in the three dimensional trapping potential will remain close to equilibrium, and represents the 'heat bath'.

We now turn to a numerical solution of Eq. (1) under these conditions, using a combination of well-known techniques [13]. To ensure particle number conservation in the absence of the term $iR(\mathbf{x}, t)$, we use an implicit method that represents the time evolution operator $\exp(-iH\delta t/\hbar)$ as $(1 + iH\delta t/2\hbar)^{-1} \times (1 - iH\delta t/2\hbar)$. Here, $H = -\hbar^2\nabla^2/2m + V_{\text{ext}}(\mathbf{x}) - \mu - iR(\mathbf{x}, t) + g|\Phi(\mathbf{x}, t)|^2$, with $\Phi(\mathbf{x}, t_i)$ the selfconsistent average $[\Phi(\mathbf{x}, t_i) + \Phi(\mathbf{x}, t_i + \delta t)]/2$. The numerical method for solving Eq. (1) can now be found from its solution $\Phi(\mathbf{x}, t_i + \delta t) = \exp(-iH\delta t/\hbar)[\Phi(\mathbf{x}, t_i) - (i/\hbar)\exp(-iHt_i/\hbar)\int_{t_i}^{t_i+\delta t} dt' \exp(iHt'/\hbar)\eta(\mathbf{x}, t')] + (i/\hbar)\exp(-iHt_i/\hbar)\int_{t_i}^{t_i+\delta t} dt' \exp(iHt'/\hbar)\eta(\mathbf{x}, t')]$. The correlations of $\xi_i(\mathbf{x})$ are $\langle \xi_i^*(\mathbf{x})\xi_j(\mathbf{x}') \rangle = \frac{i\hbar^2}{2}\Sigma^K(\mathbf{x})\delta_{ij}\delta t\delta(\mathbf{x}-\mathbf{x}') + \mathcal{O}(\delta t^2)$. The spatial discretization is straightforward.

As a first application, we show in Fig. 1 that in the case of a noninteracting vapor, the density of the harmonically trapped one-dimensional gas relaxes to the correct equilibrium given by $n(z) = \sum_\alpha |\phi_\alpha(z)|^2/\beta(\epsilon_\alpha - \mu)$, where ϵ_α are the energy eigenvalues and $\phi_\alpha(z)$ the corresponding eigenfunctions of the Hamiltonian. The equilibrium is shown for several sizes of the spatial mesh, and we see that the density distribution converges towards the continuum limit given by $[2l_z^2\beta\hbar\omega_z]^{-1/2}[\beta(V_{\text{ext}} - \mu)]^{-1/2}$ where $l_z = \sqrt{\hbar/m\omega_z}$ is the harmonic oscillator length along the z -direction, only for rather small mesh sizes. This is caused by the relatively large contribution of high-energy states due to the classical behavior of the thermal cloud. We emphasize, however, that given a certain mesh size, the correct equilibrium corresponding to that particular discretization is reproduced numerically. Moreover, it is important to realize that if we do not include the noise, the density of the gas would be zero. Hence, it is clear that the fluctuation-dissipation theorem ensures that the noise and the imaginary term in Eq. (1) cooperate in order to occupy the energy levels thermally. Thus, including fluctuations is crucial in treating the effects of the thermal cloud.

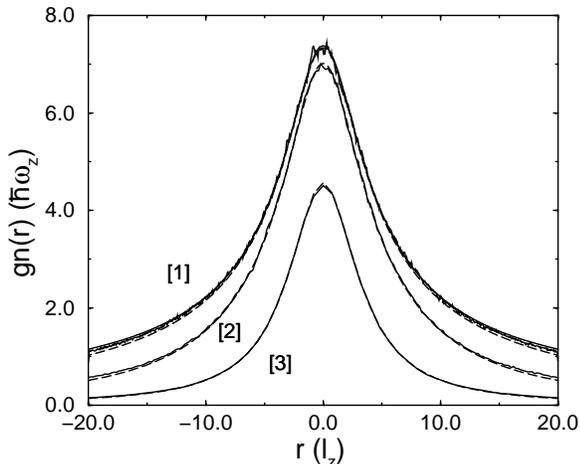


FIG. 1. Stationary density profile of a noninteracting gas above the critical temperature. The time step used is $\Delta t = 0.002 \omega_z^{-1}$, the discretization Δx used for the different lines is [1]: $\Delta x = 0.05 l_z$, [2]: $\Delta x = 0.2 l_z$, and [3]: $\Delta x = 0.8 l_z$. Also shown are the predicted classical density profiles for curves [1], [2], and [3] (dashed lines), and the continuum result (solid line). The chemical potential of the three dimensionally trapped gas is $\mu = -30 \hbar\omega_z$, and its temperature $T = 400$ nK. The trapping frequencies are $\omega_z = 2\pi \times 13$ Hz and $\omega_r = 2\pi \times 20$ Hz [11]. The trapping frequency of the dimple is $\omega_\perp = 2\pi \times 500$ Hz, and the ground state eigenvalue $\epsilon_0 = -25 \hbar\omega_z$. The atom considered is sodium, with a scattering length $a \approx 2.75$ nm.

Second, we calculate the damping of the breathing mode in a trapped one-dimensional Bose gas below the critical temperature. Shown in Fig. 2 is g times the value of the density $n(0)$ in the center of the one-dimensional trap. First, the gas relaxes towards equilibrium at an effective chemical potential $\mu - \epsilon_0 = 30 \hbar\omega_z$, where ϵ_0 is the eigenvalue of $\Phi_0(x, y)$ in the dimple. The fact that the value of $gn(0)$ does not relax to $30 \hbar\omega_z$ can be explained by realizing that mean-field effects are included in our formalism, because $\Phi(z, t)$ describes both the condensed and the noncondensed parts of the one-dimensional gas. This implies that the chemical potential for the condensed part of the gas is effectively lowered by the interaction with the noncondensed part of the gas. After allowing the gas to equilibrate, at $t = 0.61$ s the trapping frequency is instantaneously changed to $\omega'_z = 0.95 \omega_z$, and the gas starts to oscillate. The frequency ω and the damping rate γ of the oscillation are found by fitting to $n(0, t) = n_{\text{eq}}(0) + \delta n(0) \exp(-\gamma t)[1 - \cos(\omega t)]$, which describes both the relaxation of the density to its new equilibrium, as well as the excitation and damping of the oscillation. The results are $\omega = 136.84 \text{ s}^{-1}$, which is close to the result of $\sqrt{5/2}\omega_z = 129.1 \text{ s}^{-1}$ expected from the Gross-Pitaevskii equation [14], $\gamma = 12.3 \text{ s}^{-1}$, $g\delta n(0) = 0.84 \hbar\omega_z$, and $gn_{\text{eq}}(0) = 28 \hbar\omega_z$. Note that the damping is in principle caused both by the collisions with the reservoir of thermal atoms in the three-dimensional

trapping potential, which is described by $\Sigma^K(\mathbf{x})$, as well as by the nonlinear term in the Langevin equation which induces damping upon averaging over the different realizations of the noise. The latter includes collisional, as well as Landau damping.

In Fig. 3, a snapshot of the density profile is shown at several times during the initial growth of the condensate. These are taken from the simulation presented in Fig. 2. As expected, the condensate shows up as a peak in the density profile. Also shown are the Thomas-Fermi solution $[\mu - V_{\text{ext}}(z)]/g$ for the condensate density and the noninteracting result for the noncondensed part of the gas which diverges at the critical point where the effective chemical potential becomes equal to zero. This is due to the fact that in one dimension, mean-field theory completely fails near the critical temperature. Fig. 3 shows that far enough from the condensate, the noninteracting result is obtained. Again, in the center of the trap one obtains the Thomas-Fermi result only approximately due to interactions.

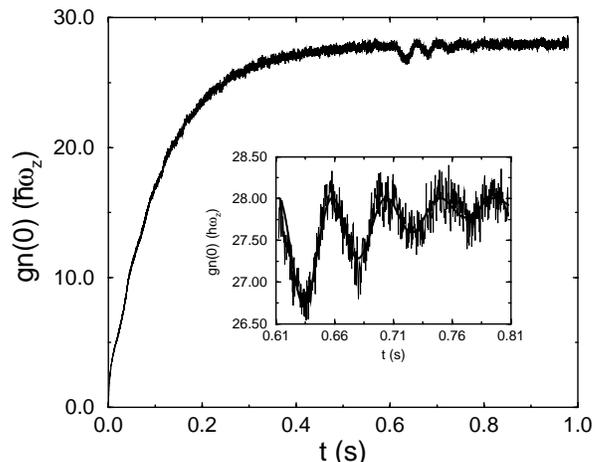


FIG. 2. Oscillations of the trapped partially Bose-condensed gas, and their damping, after a small and instantaneous change of the trapping frequency ω_z at $t = 0.61$ s. Here, we used $\Delta t = 0.002 \omega_z^{-1}$, $\Delta x = 0.05 l_z$, $\epsilon_0 = -60 \hbar\omega_z$, and $\omega_\perp = 2\pi \times 1200$ Hz. The remaining parameters are the same as in Fig. 1.

Finally, we consider the reversible formation of a one-dimensional Bose condensate, similar in spirit to the experiments by Stamper-Kurn *et al.* [11]. The dimple perturbing the external trapping potential is now oscillating in such a way, that the lowest energy level in the dimple crosses the chemical potential of the three dimensionally trapped gas several times according to $\epsilon_0 = \mu + \mu \sin(\omega t)$, with $\omega = 2\pi \text{ s}^{-1}$ and $\mu = -30 \hbar\omega_z$. The calculations have been done with and without noise. The results show that without noise, the condensate evaporation and growth cannot be described properly. Indeed, in that case, our findings depend strongly on the initial conditions. Moreover, the periodic growth occurs with decreasing ampli-

tude.

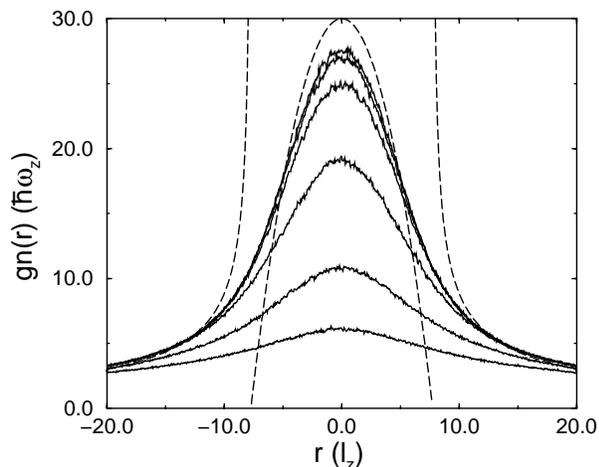


FIG. 3. This figure shows the growth of the density profile of the trapped partially Bose-condensed gas for the simulation of Fig. 2. The snapshots are taken at $t = 2 \omega_z^{-1}$, $t = 4 \omega_z^{-1}$, $t = 10 \omega_z^{-1}$, $t = 20 \omega_z^{-1}$, $t = 30 \omega_z^{-1}$, and $t = 40 \omega_z^{-1}$. The dashed lines show the equilibrium mean-field results in and outside the condensate.

To describe the growth cycles correctly, one needs to include fluctuations into the generalized Gross-Pitaevskii equation, which is to be expected since we are at times in the critical region. Notice that we quantitatively reproduce the lagging behind of the condensate as observed in an experiment performed with an essentially three-dimensional dimple. We observed a lagging behind of roughly 0.1s, whereas in experiment 0.07s was measured [11].

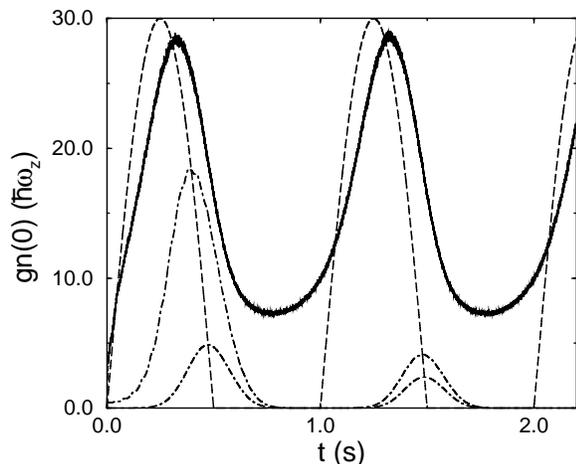


FIG. 4. Reversible formation of a condensate (solid line) because of a sinusoidal time dependence of the chemical potential in the dimple (dashed line). The time step used was $\Delta t = 0.003 \omega_z^{-1}$, the discretization $\Delta x = 0.05 l_z$, and $\omega_{\perp} = 2\pi \times 1200\text{Hz}$. The other parameters used are the same as in Fig. 1. The two dot-dashed lines correspond to simulations without noise, with 10 (top) and 0.1 (bottom) particles in the initial harmonic oscillator ground state.

In conclusion, we have shown that our generalized stochastic Gross-Pitaevskii equation consistently takes into account the dissipative dynamics of a trapped partially Bose-condensed gas, and describes the equilibrium density profile, condensate growth, coherent dynamics, and damping in a unified way. In our opinion, the one-dimensional experiment considered here would be ideal for a detailed comparison between theory and experiment in the problem of condensate growth, because the three-dimensional cloud remains in equilibrium. In addition, a numerical study of the two-dimensional case would be of interest and might be used to investigate for example the dissipative dynamics and the formation of vortices in a rotating Bose gas.

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