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Liquid-gas phase transition in Bose-Einstein condensates with time evolution

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We study the effects of a repulsive three-body interaction on a system of trapped ultracold atoms in a Bose-Einstein condensed state. The stationary solutions of the corresponding s-wave nonlinear Schrödinger equation suggest a scenario of first-order liquid-gas phase transition in the condensed state up to a critical strength of the effective three-body force. The time evolution of the condensate with feeding process and three-body recombination losses has a different characteristic pattern. Also, the decay time of the dense (liquid) phase is longer than expected due to strong oscillations of the mean-squared radius.

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The experimental evidences of Bose-Einstein condensation (BEC) in magnetically trapped weakly interacting atoms [1–3] brought considerable support to the theoretical research on bosonic condensation. The nature of the effective atom-atom interaction determines the stability of the condensed state: the two-body pseudopotential is repulsive for a positive s-wave atom-atom scattering length and attractive for a negative scattering length [4]. The ultracold trapped atom with repulsive two-body interaction undergoes a Bose-Einstein phase-transition to a stable condensed state in a number of cases found experimentally, such as for ^{87}Rb [1] and ^{23}Na [2]. However, a condensed state of atoms with negative s-wave atom-atom scattering length would be unstable for a large number of atoms [5,6]. It was indeed observed in the ^{7}Li gas [3], for which the s-wave scattering length is $a=(-14.5\pm0.4)$ Å, that the number of allowed atoms in the condensed state was limited to a maximum value between 650 and 1300, which is consistent with the mean-field prediction [5].

From a theoretical approach, the addition of a repulsive three-body interaction can extend considerably the region of stability for a condensate, even for a very weak three-body force [7–9]. As one can observe from Ref. [10], both signs for the three-body interaction are, in principle, allowed. However, in the present study we only consider the case of a repulsive three-body elastic interaction together with an attractive two-body interaction. Singh and Rokhsar [11] have also observed that above a critical value the only local minimum is a dense gas state, where the neglect of three-body collisions fails.

In this work, using the mean-field approximation, we develop the scenario of collapse, which includes two aspects of three-body interaction; that is, recombination and repulsive mean-field interaction. We begin by investigating the competition between the leading term of an attractive two-body interaction and a repulsive three-body interaction, which can happen near the Efimov limit [12], when $|a|\to\infty$. (The physics of three atoms in the Efimov limit is discussed in Ref. [13].) We should note the interesting possibility of realizing the Efimov limit. As observed in Ref. [14], it is possible in a short period of time to change the two-body interaction of excited atoms by means of light or induced magnetic fields. In this case, the Efimov limit can be reached, and the three-body T-matrix elements can present large values in magnitude due to the proximity of a weakly bound three-body state to the scattering threshold.

We first consider the stationary solutions of the corresponding extension of the Ginzburg-Pitaevskii-Gross (GPG) [15] nonlinear Schrödinger equation (NLSE), for a fixed number of particles, without dissipative terms, extending an analysis previously reported in Refs. [7,8]. Then, the time evolution of the feeding process of the condensate by an external source is obtained by solving the time-dependent NLSE with repulsive three-body interaction and dissipation due to three-body recombination processes. Our results pointed out that the mean-squared radius is an important observable to be analyzed experimentally to study the dynamics of the growth and collapse of the condensate [16,17]. In the present study, we choose the real part of the three-body interaction to be significantly larger than the magnitude of the corresponding three-body dissipative term; although, in general, they are expected to be of the same order.

The NLSE, which describes the condensed wave function in the mean-field approximation, is variationally obtained from the corresponding effective Lagrangian [8]. By considering a stationary solution, $\Psi(\vec{r},t)=e^{-i\mu t/\hbar}\psi(\vec{r})$, where μ is the chemical potential and $\psi(\vec{r})$ is normalized to the number of atoms N. By rescaling the NLSE for the s-wave solution, we obtain

$$\left[-\frac{d^2}{dx^2}+\frac{x^2}{4}-\frac{|\phi(x)|^2}{x^2}+g_3\frac{|\phi(x)|^4}{x^4}\right]\phi(x)=\beta\phi(x) \quad (1)$$

for $a<0$, where $x\equiv\sqrt{2m\omega/\hbar}\,r$ and $\phi(x)\equiv\sqrt{8\pi|a|}\,r\psi(\vec{r})$. The dimensionless parameters related to the chemical potential and the three-body strength are, respectively, given by $\beta\equiv\mu/\hbar\omega$ and $g_3\equiv\lambda_3\hbar\omega m^2/(4\pi\hbar^2 a)^2$. The normalization for $\phi(x)$ reads $\int_0^\infty dx|\phi(x)|^2=n$, where the reduced number n is related to N by $n\equiv 2N|a|\sqrt{2m\omega/\hbar}$.

In Fig. 1, considering several values of g_3 (0, 0.012, 0.015, 0.0183, and 0.02), using exact numerical calculations, we present some relevant physical quantities, in dimensionless units, as functions of the reduced number of atoms n.

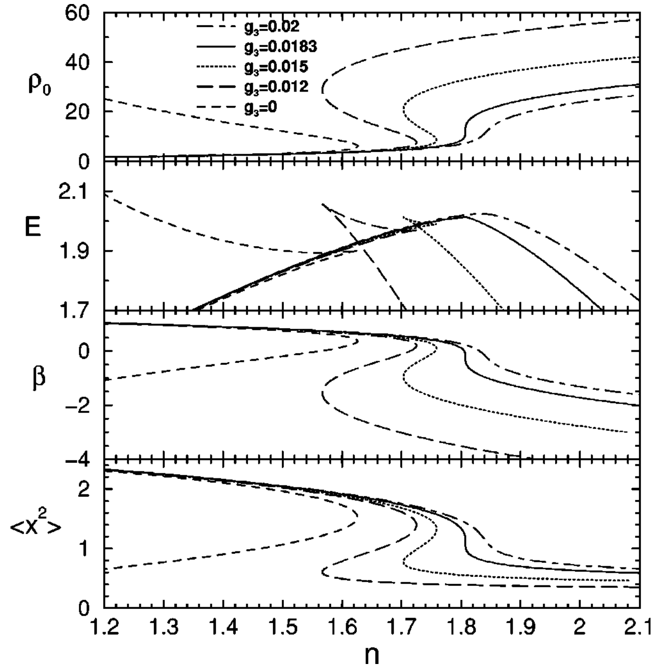

FIG. 1. Central density ρ_0, total energy E, chemical potential β, and average square radius $\langle x^2 \rangle$, in dimensionless units, as functions of the reduced number of atoms n. The three-body strengths g_3 are given in the upper frame.

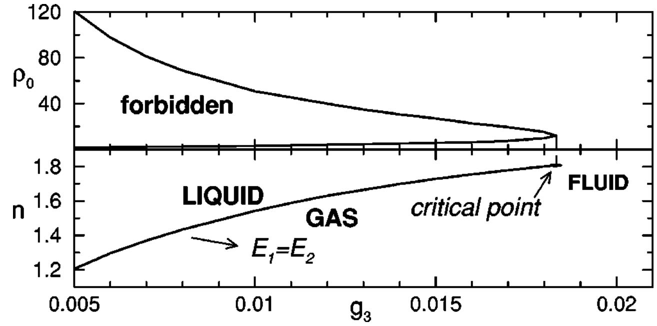

FIG. 2. Phase diagram of the Bose condensate, for the central density ρ_0 and the reduced number of atoms n, in dimensionless units.

The central density and the total energy are, respectively, given by $E_{tot}=E(N\hbar\omega/n)$ and $\rho_c=\rho_0[m\omega/(4\pi|a|\hbar)]$. For $g_3=0$, our calculation reproduces the result presented in Refs. [5,18,19], with the maximum number of atoms limited by $n_{max}\approx 1.62$ (n is equal to $|C_{nl}^{3D}|$ of Ref. [5]).

As shown in the figure, for $0<g_3<0.0183$, the density ρ_0, the chemical potential β, and the mean-squared radius $\langle x^2 \rangle$ present backbendings typical of a first-order phase transition. For each g_3, the transition point given by the crossing point in the E versus n corresponds to a Maxwell construction in the diagram of β versus n. At this point an equilibrated condensate should undergo a phase transition from the branch extending to small n to the branch extending to large n. The system should never explore the backbending part of the diagram because, as we have seen in Fig. 1, it is an unstable extremum of the energy. From this figure it is clear that the first branch is associated with large radii, small densities, and positive chemical potentials, while the second branch presents a more compact configuration with a smaller radius, a larger density, and a negative chemical potential. This justify the term gas for the first one and liquid for the second one. However, we want to stress that both solutions are quantum fluids. With $g_3=0.012$ the gas phase happens for $n<1.64$ and the liquid phase for $n>1.64$. For $g_3>0.0183$ all the presented curves are well behaved and a single fluid phase is observed. At $g_3\approx 0.0183$ and $n\approx 1.8$, the stable, metastable, and unstable solutions come to be the same. This corresponds to a critical point associated with a second-order phase transition. At this point the derivatives of β, ρ_0, and $\langle x^2 \rangle$ as a function of n all diverge. We also checked that calculations with the variational expression of $\langle x^2 \rangle$, ρ_0, and β are in good agreement with the ones depicted in Fig. 1.

In the lower frame of Fig. 2, we show the phase boundary separating the two phases in the plane defined by n and g_3 and the critical point at $n\approx 1.8$ and $g_3\approx 0.0183$. In the upper frame, we show the boundary of the forbidden region in the central density versus g_3 diagram.

The main physical characteristic of the repulsive three-body force is to prevent the collapse of the condensate for the particle number above the critical number found with only two-body attractive interaction. The three-body repulsive potential tends to overcome the attraction of the two-body potential at short distances, as described by Eq. (1), because the repulsive interaction is proportional to x^{-4}, while the two-body potential goes with x^{-2}. Thus the implosive force that shrinks the condensate at the critical number is compensated by the repulsive three-body force. The time evolution of the growth and collapse of the condensate [16] should be qualitatively modified by the presence of the repulsive three-body force. The three-body recombination effect [17], which partially ''burns'' the condensed state should be taken into account to describe quantitatively the dynamics of the condensate. In the case of only two-body attractive interaction and considering the feeding of the condensate from the nonequilibrium thermal cloud, the time evolution is dominated by a sequence of growth and collapse of the trapped condensate [17]. The collapse occurs when the condensate exceeds the critical number N_c of atoms, and it is followed by an expansion after the atoms in the high-density region of the wave function are lost due to three-body recombination processes and consequently the average attractive potential from the two-body force is weakened. The repulsion given by the three-body force will dynamically affect the compression of the condensate, weakening the implosive force and allowing more atoms to survive at high densities.

In order to quantitatively study the above features, we consider the time-dependent nonlinear Schrödinger equation corresponding to Eq. (1), including three-body recombination effects (with an intensity parameter ξ) and an imaginary linear term corresponding to the feeding of the condensate (with intensity parameter γ):

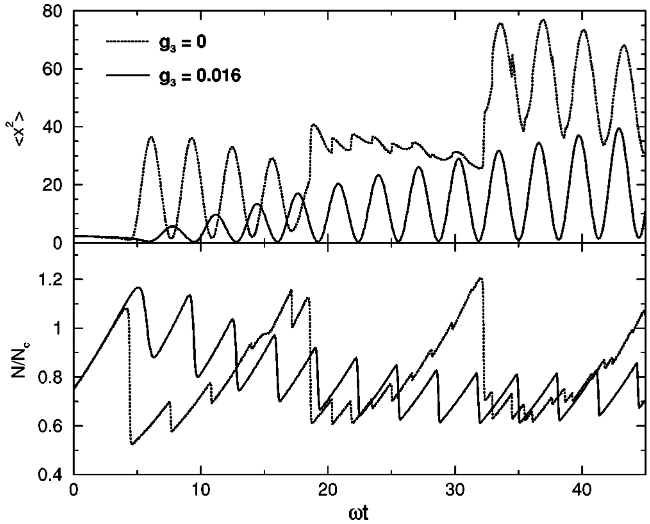

FIG. 3. Number of condensed atoms and the corresponding dimensionless mean-squared radius $\langle x^2 \rangle$, as a function of time, for $\xi=0.001$, $\gamma=0.1$. N_c is the maximum number of atoms for $g_3=0$.

$$i\frac{\partial \Phi}{d\tau}=\left[-\frac{d^2}{dx^2}+\frac{x^2}{4}-\frac{|\Phi|^2}{x^2}+(g_3-2i\xi)\frac{|\Phi|^4}{x^4}+\frac{i\gamma}{2}\right]\Phi, \tag{2}$$

where $\Phi\equiv\Phi(x,\tau)$ and $\tau\equiv\omega t$. For the parameters ξ and γ we are using the same notation as given in Ref. [17].

In Fig. 3 we show the time evolution of the number of condensed atoms, starting with $N/N_c=0.75$, found by the numerical solution of Eq. (2) with $\xi=0.001$ and $\gamma=0.1$, with and without repulsive three-body potential. We compare the results of a three-body potential with $g_3=0.016$ to the case considered in Ref. [17], with $g_3=0$. In both, N_c is the critical number for $g_3=0$. The first striking feature with repulsive three-body force is the smoothness of the compression mode in comparison with the results of $g_3=0$. This is a result of the explosive force from the repulsion, which opposes the sudden density increase and damps the loss of atoms due to three-body recombination effects. Even for g_3 lower than 0.016, and much closer to $g_3=0$, the collapses can no longer ''burn'' the same number of atoms as in the case of $g_3=0$. By extending our calculation presented in Fig. 3, for all cases with $g_3>0.01$ and for times beyond $\omega t=50$, we have checked that the number of atoms will increase considerably beyond the critical limit, while the condensate is oscillating with frequency about 2ω. In particular, the present approach indicates that the experimental recent observation of the maximum number of ^{7}Li atoms is compatible with g_3 much smaller than 0.01 [3]. The mean-squared radius for $g_3=0$, after each strong collapse (when $N>N_c$) begins to oscillate at an increased average radius. The collapse ''burns'' the atoms in the states with higher densities and explains the sudden increase of the square radius after each compression, leaving the atoms in dilute states. The inclusion of the repulsive three-body force still maintains the oscillatory mode, but the compression is not as dramatic as in the former case and, consequently, atoms in higher density states are not so efficiently burned. The remarkable increase

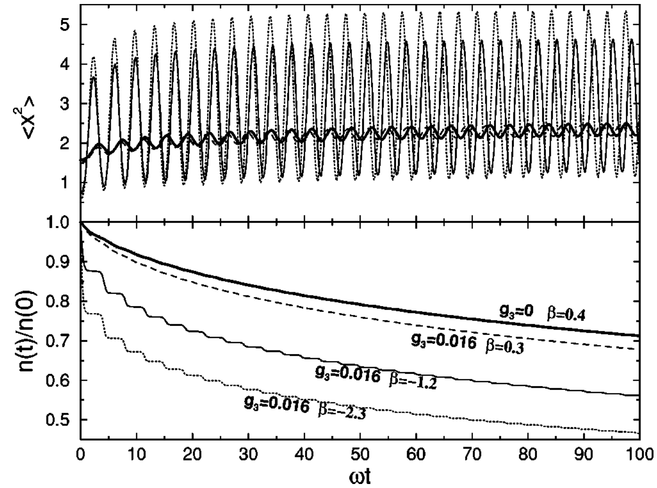

FIG. 4. Condensate decay. Number of condensed atoms and mean-squared radius as a function of ωt for $\gamma=0$ and $\xi=0.001$. The chemical potential β of the initial state and the strengths g_3 are given in the plot.

of the mean-squared radius (averaged with time) is smaller than the one found with only attractive two-body force.

Finally, we have to consider that, in the situation when the three-body repulsion dominates over the two-body attraction, the condensate can be in a denser phase where it is expected to be strongly unstable due to recombination losses. We should observe that the dynamics of the condensate is modulated by an oscillatory mode with a frequency of the order of 2ω, as also found for $g_3=0$ [17]. In case of $g_3>0$, the oscillatory mode dominates the dynamics of the condensate, implying density fluctuation, and thus the condensate does not ''burn'' as fast as expected. This will be explained in the following.

In Fig. 4 we present our study of the condensate decay, considering two different values of g_3 ($g_3=0$ and $g_3=0.016$) and $\xi=0.001$, in Eq. (2). For $g_3=0$, the initial number of atoms was such that $n(0)=1.625$, which is close to the critical limit. For $g_3=0.016$, we consider three cases: two of them starting with the same number of atoms, $n(0)=1.756$, but in different phases (the corresponding chemical potentials are $\beta=-1.2$, in a denser phase, and $\beta=0.3$); and another in an even denser phase, with $n(0)=1.965$ and $\beta=-2.3$ (see also Fig. 1). Based on the results obtained in these four different cases, we can estimate that the mean life for the condensate, which is initially in a denser phase, is not as small as expected when comparing with $g_3=0$. We observe in this case the relevant role of the oscillatory mode. In case g_3 is very close to zero, the liquid phase is expected to be destroyed before it can be observed. However, it can be detected if the lifetime is comparatively not much smaller than the period of the oscillatory mode.

The values of g_3 were chosen significantly higher than the realistic one, in case of ^{7}Li. However, the values we have used should also be considered in the perspective of a possible experimental realization of changes in the two-body scattering length [14]. In this case, near the Efimov limit, it is expected that the three-body scattering amplitude will become very large; and the proximity of the Efimov limit can be experimentally related to a first-order phase-transition in BEC. In the strict Efimov limit (infinite two-body scattering length), however, the mean-field approximation can be questioned, as the three-body characteristic interaction length, which increases with g_3, can become close to the average interparticle distance.

To summarize, our present results can be relevant in determining a possible signature of the presence of a repulsive three-body interaction in Bose condensed states. It points to an alternative type of phase transition between two Bose fluids. Because of the condensation of the atoms in a single wave function, this transition may present very peculiar fluctuations and correlation properties. As a consequence, it may fall into a different universality class than the standard liquid-gas phase transition, which is strongly affected by many-body correlations. The characterization of the two phases through their energies, chemical potentials, central densities, and radius were given for several values of the three-body parameter g_3.

Then, we develop a scenario of collapse that includes both three-body recombination and three-body repulsive interaction. It is also shown that the decay time of the condensate that begins in a denser phase can be long enough to allow observation. The observed large-amplitude oscillating states are quite different from the analyzed stationary states. The condensate radius and density also strongly oscillate, and the observed states cannot be characterized as ‘‘dense’’ or ‘‘dilute,’’ explaining the long decay time. Nevertheless, through the amplitude of the oscillations one can distinguish if the system starts in a denser phase.

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