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 ultra-cold atoms in Bose-Einstein condensed state. The stationary solutions of the corresponding $s$–wave non-linear 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 new characteristic pattern. Also, the decay time of the dense (liquid) phase is longer than expected due to strong oscillations of the mean-square-radius.

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The experimental evidences of Bose-Einstein condensation (BEC) in magnetically trapped weakly interacting atoms brought a 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 it is attractive for a negative scattering length. The ultra-cold trapped atoms with repulsive two-body interaction undergoes a Bose-Einstein phase-transition to a stable condensed state, in a number of cases found experimentally, as for $^{87}$Rb and $^{23}$Na and $^7$Li. However, a condensed state of atoms with negative $s$–wave atom-atom scattering length would be unstable for a large number of atoms. It was indeed observed in the $^7$Li gas, for which the $s$–wave scattering length is $a = (-14.5 \pm 0.4)$ 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.

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. As one can observe from Refs., 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. We will show that, due to the repulsive three-body force, new physical aspects appears in the time evolution of the condensate. In respect to the static situation, it was suggested that, for a large number of bosons the three-body repulsion can overcome the two-body attraction, and a stable condensate will appear in the trap. Singh and Rokhsar 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, which is originated from a negative two-atom $s$–wave scattering length, and a repulsive three-body interaction, which can happen in the Efimov limit, when $|a| \to \infty$. The physics of three-atoms in the Efimov limit is discussed in Refs. We first consider the stationary solutions of the corresponding extension of the Ginzburg-Pitaevskii-Gross (GPG) nonlinear Schrödinger equation (NLSE), for fixed number of particles, without dissipative terms, extending an analysis previously reported in Refs. The liquid-gas phase transition in the condensate, suggested in, was confirmed by a more detailed analysis in the present stationary calculations. 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 (given by $g_3 > 0$) and dissipation due to three-body recombination processes. The dramatic collapse and the consequent atom loss that happens at the critical number of atoms (when $g_3 = 0$) is softened by the addition of the three-body repulsive force. The decay time of the liquid-phase is also unexpectedly long, when compared with the decay time that occurs for $g_3 = 0$, which gives a clue about the possible observation of three-body interaction effects. Our results pointed out that the mean-square-radius is an important observable to be analyzed experimentally to study the dynamics of the growth and collapse of the condensate. In the present study, in order to emphasize the real part of the three-body interaction, we choose $g_3$ significantly larger than the magnitude of the dissipative term; although, in general, they are expected to be of the same order.

The NLSE, which describes the condensed wavefunction in the mean-field approximation, after considering the two-body attractive and three-body repulsive effective interaction, is variationally obtained from the corresponding effective Lagrangian (see Gammal et al. in). By considering a stationary solution, $\Psi(\vec{r}, t) = e^{-i\mu t} \psi(\vec{r})$ where $\mu$ 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 \(\phi(x) \equiv \sqrt{8\pi|a|} r\psi(r)\). 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
\[
f_0^\infty dx |\phi(x)|^2 = n \quad \text{where the reduced number } n \text{ is related to } N \text{ by } n \equiv 2N|a|\sqrt{2m\omega/\hbar}.
\]
The boundary conditions \(\phi(x)\) in Eq. (1) are given by \(\phi(0) = 0\) and \(\phi(x) \to C \exp(-x^2/4 + |\beta - \frac{1}{2}| \ln(x))\) when \(x \to \infty\). \(\triangleright\)

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 the evolution of some relevant physical quantities \(E, \mu, \rho_c\), and \(\langle r^2 \rangle\) as functions of the reduced number of atoms \(n\). For \(g_3 = 0\), our calculation reproduces the result presented in Ref. \(\triangleright\), with the maximum number of atoms limited by \(n_{\text{max}} = 1.62\) (\(n\) is equal to \(|c_m^2|\) of Ref. \(\triangleright\)).

As shown in the figure, for \(0 < g_3 < 0.0183\), the density \(\rho_c\), the chemical potential \(\mu\), and the root-mean-squared radius \(\langle r^2 \rangle\) present back bendings 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 \(\mu\) 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 back bending 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 \(\mu, \rho_c\), and \(\langle r^2 \rangle\) as a function of \(n\) all diverge. We also checked that calculations with the variational expression of \(\langle r^2 \rangle\), \(\rho_c\) and \(\mu\) 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. (3), as the repulsive interaction grows inversely to \(x^4\), while the two-body potential is proportional to \(x^{-2}\). 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 with attractive interactions [13] should be qualitatively modified by the presence of the repulsive three-body force. The three-body recombination effect [13], which “burns” partially 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, as observed by Kagan et al. [13], by 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. The collapse occurs when the number of atoms in the condensate exceeds the critical number \( N_c \); 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. It is also noticed in Ref. [13] that the condensate time evolution is dominated by an oscillatory mode of frequency \( \sim \omega \); and, as time grows and \( N \) reaches a value \( > N_c \), a huge compression takes place to implode the condensate. 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 with repulsive three-body interaction, we consider the time-dependent non-linear Schrödinger equation corresponding to Eq. (1), including three-body recombination effects (with an intensity parameter \( 2\xi \)) and an imaginary linear term corresponding to the feeding of the condensate (with intensity parameter \( \gamma \)):

\[
\frac{i}{\hbar} \frac{\partial \Phi}{\partial \tau} = \left[ -\frac{\partial^2}{\partial x^2} + \frac{x^2}{4} - \frac{|\Phi|^2}{x^2} + (g_3 - 2i\xi|\Phi|^4 + i\gamma) \frac{\Phi}{x^3} \right] \Phi, \tag{2}
\]

where \( \Phi \equiv \Phi(x, \tau) \) and \( \tau \equiv \omega t \). For the parameters \( \xi \) and \( \gamma \) we are using the same notation as given in Ref. [13].

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. [13], 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 oppose to 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 without limit while the condensate is oscillating with frequency about \( 2\omega \). 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. The mean square 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 explain the sudden increase of the square radius after each compression, remaining 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 increase of the mean square radius (averaged with time) is smaller than the one found with only attractive two-body force. This is a remarkable feature of the stabilizing effect of the repulsive three-body force allowing the presence of states with higher densities, as we found in the stationary study.

**FIG. 3.** Number of condensed atoms and the corresponding mean square radius \( \langle r^2 \rangle \) (in units of \( h/(2m\omega) \)) as a function of time, for \( \xi = 0.001, \gamma = 0.1 \). \( N_c \) is the maximum number of atoms for \( g_3 = 0 \).

Finally, we have to consider that, in the situation when the 3-body repulsion dominates over the 2-body attraction, the condensate can be in a denser phase where it is expected to be strongly unstable due to recombination losses. The decay time of the condensate in a denser phase is expected to be much smaller than the decay time of the condensate in the less dense phase. However, we should observe that the dynamics of the condensate is modulated by an oscillatory mode with a frequency of the order of \( 2\omega \), which was already identified by [13] to be \( \sim \omega \) even when \( g_3 = 0 \). In case of \( g_3 > 0 \), such oscillatory mode dominates the time evolution of the condensate. As the oscillations allow changes in the density, the condensate does not “burn” as fast as expected.

In order to study the condensate decay, we consider the original NLSE with the dissipative term and allow different possibilities for the three-body interaction \( g_3 \).
We use $\xi = 0.001$ (the same value used in Ref. [3]). In Fig. 4 we show the result of this study for $g_3 = 0$ and $g_3 = 0.016$. The initial number of atoms $N$ can be obtained from $n$, given in the figure. For $g_3 = 0$, we took $n = 1.625$, 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, $n = 1.756$, 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 $n = 1.965$ 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, related to the frequency of the trap potential, which dominates the dynamics of the condensate when $g_3 > 0$.

![Condensate decay](image)

FIG. 4. Condensate decay. Number of condensed atoms and mean square radius as function of $\omega t$, for $\gamma = 0$ and $\xi = 0.001$. The chemical potential $\beta$ of the initial state and the strengths $g_3$ are given in the plot.

To summarize, our present results can be relevant to determine a possible clear signature of the presence of a repulsive three-body interaction in Bose condensed states. It points out to a new 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 are strongly affected by many-body correlations. The characterization of the two-phases through their energies, chemical potentials, central densities and radius were also given for several values of the three-body parameter $g_3$. We develop a scenario of collapse which includes both three-body recombination and three-body repulsive interaction. From the time-dependent analysis, we show that the decay time of the condensate which begins in a denser phase is long enough to allow observation. However, the observed strongly oscillating states are quite different from the analysed stationary states. In accordance with the observed strong oscillations of the mean-squared-radius, the condensate density also strongly oscillates and the observed states cannot be characterized as “dense” or “dilute”, justifying 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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