Trapped Bose-Einstein Condensed Gas with Two and Three-Atom Interactions

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Abstract

The stability of a Bose-Einstein condensed state of trapped ultra-cold atoms is investigated under the assumption of an attractive two-body and a repulsive three-body interaction. The Ginzburg-Pitaevskii-Gross (GPG) nonlinear Schrödinger equation is extended to include an effective potential dependent on the square of the density and solved numerically for the $s$-wave. The lowest frequency of the collective mode is determined through the Fourier transform of the time dependent solution and its dependences on the number of atoms and the strength of the three-body force are studied. We show that the addition of three-body dynamics can allow the number of condensed atoms to increase considerably, even when the strength of the three-body force is very small compared with the strength of the two-body force.

Recently, the theoretical research on Bose-Einstein condensation (BEC), a phenomenon predicted by Einstein more than 70 years ago, received considerable support from the experimental evidences of BEC in magnetically trapped weakly interacting atoms \cite{1,2,3}. 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 \cite{4}. The ultra-cold trapped atoms with repulsive two-body interaction undergoes a phase-transition to a stable Bose condensed state, in a number of cases found experimentally, as for $^{87}$Rb \cite{5}, for $^{23}$Na \cite{6} and $^{7}$Li \cite{7}. However, a condensed state of atoms with negative $s$-wave atom-atom scattering length would be unstable unless the number of atoms is small enough such that the stabilizing force provided by the harmonic confinement in the trap overcomes the attractive interaction, as found on theoretical grounds \cite{8}. It was indeed observed in the $^{7}$Li gas \cite{9}.

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for which the $s$–wave scattering length is $a = (-14.5 \pm 0.4) \text{ Å}$, that the number of allowed atoms in the Bose condensed state was limited to a maximum value between 650 and 1300, which is consistent with the mean-field prediction ([1]). An earlier experiment ([2]) suggested that the number of atoms in the condensate state was significantly larger than the theoretical predictions with two-body pseudopotential. This is consistent with an addition of a potential derived from three-body interaction, which can extend considerably the region of stability for the condensate even for a very small strength of the three-body force.

Expanding our universe of possible effective interactions, it was reported in Ref. ([3]) that a sufficiently dilute and cold Bose gas exhibits similar three-body dynamics for both signs of the $s$–wave atom-atom scattering length. They concluded that the long-range three-body interaction between neutral atoms is effectively repulsive for either sign of the scattering length. Supposing that a repulsive three-body effective interaction is present in the atomic system, one can imagine that a stable condensate will be formed in the trap for a number of bosons large enough, such that they three-body interaction overcomes the attraction of the two-body interaction ([4]).

In the present work, we investigate the competition between the attractive two-body interaction, originated from a negative two-atom $s$–wave scattering length, and a repulsive three-body effective interaction. (The latter can be originated by the existence of a weakly bound three-boson state, as it will be explained.) We show that, in a dilute gas, a small repulsive three-body force added to an attractive two-body interaction is able to stabilize the condensate beyond the critical number of atoms in the trap, found just with attractive two-body force ([4]). The Ginzburg-Pitaevskii-Gross nonlinear Schrödinger equation ([5]) is extended to include an effective potential dependent on the square of the density and solved numerically for $s$–wave. The stability is studied using a weak perturbation probe and the time dependent equation is solved with the ground state as the starting point. The lowest frequency of the collective mode is determined through the Fourier transform of the time dependent solution and its dependences on the number of atoms and the strength of the three-body force are studied. In this case, a signature for a repulsive three-body force can appear with the possibility of two stable solutions, for a fixed number of atoms, even for a very small repulsive three-body interaction. Also, in this case, one stable solution is found for a large number of atoms, beyond the maximum expected with only two-body interaction.

In the following, we present the formalism, where the original Ginzburg-Pitaevskii-Gross (GPG) non-linear equation ([5]), which includes a term proportional to the density (two-body interaction), is extended through the addition
of a term proportional to the squared-density (three-body interaction). Next, after reducing such equation to dimensionless units, we study numerically the $s$–wave solution by varying the corresponding dimensionless parameters, which are related to the two-body scattering length, the strength of the three-body interaction and the number of atoms in the condensed state. As particularly observed in Ref. (11), to incorporate all two-body scattering processes in such many particle system, the two-body potential should be replaced by the many-body $T$–matrix. Usually, at very low energies, this is approximated by the two-body scattering matrix, which is directly proportional to the scattering length (6). So, to obtain the desired equation, we first consider the effective Lagrangian, which describes the condensed wave-function in the Hartree approximation, implying in the Ginzburg-Pitaevskii-Gross (GPG) energy functional (10):

$$\mathcal{L} = \int d^3r \left[ \frac{i\hbar}{2} \Psi^\dagger(\vec{r}) \frac{\partial \Psi(\vec{r})}{\partial t} - \frac{i\hbar}{2} \frac{\partial \Psi^\dagger(\vec{r})}{\partial t} \Psi(\vec{r}) + \frac{\hbar^2}{2m} \Psi^\dagger(\vec{r}) \nabla^2 \Psi(\vec{r}) - \frac{m^2}{2} \omega^2 r^2 |\Psi(\vec{r})|^2 \right] + \mathcal{L}_1. \tag{1}$$

In our description, the atomic trap is given by a rotationally symmetric harmonic potential, with angular frequency $\omega$, and $\mathcal{L}_1$ gives the effective atom interactions up to three particles.

The effective interaction Lagrangian for ultra-low temperature bosonic atoms, including two and three-body scattering at zero energy, is written as:

$$\mathcal{L}_1 = -\frac{1}{2} \int d^3r_1 d^3r_2 d^3r'_1 d^3r'_2 \Psi^\dagger(\vec{r}'_1) \Psi^\dagger(\vec{r}'_2) \Psi(\vec{r}_1) \Psi(\vec{r}_2)$$

$$\times \left\langle \vec{r}'_{12} \bigg| T^{(2)}(0) \bigg| \vec{r}_{12} \right\rangle \delta^3(\vec{r}'_1 + \vec{r}'_2 - \vec{r}_1 - \vec{r}_2)$$

$$-\frac{1}{3!} \int d^3r_1 d^3r_2 d^3r_3 d^3r'_1 d^3r'_2 d^3r'_3 \Psi^\dagger(\vec{r}'_2) \Psi^\dagger(\vec{r}'_3) \Psi(\vec{r}_1) \Psi(\vec{r}_2) \Psi(\vec{r}_3)$$

$$\times \left\langle \vec{r}'_{12} \vec{R}'_3 \bigg| T^{(3)}(0) - \sum_{j<k} T^{(2)}_{jk}(0 - K_i) \bigg| \vec{r}_{12} \vec{R}_3 \right\rangle \delta^3(\vec{R}'_{123} - \vec{R}_{123}) ,$$

where $\vec{r}_{12}$ and $\vec{R}_3$ are the relative coordinates, given by $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ and $\vec{R}_3 = \vec{r}_3 - (\vec{r}_1 + \vec{r}_2)/2$; and $\vec{R}_{123} \equiv (\vec{r}_1 + \vec{r}_2 + \vec{r}_3)$. $T^{(3)}(0)$ and $T^{(2)}_{jk}(0)$ are the corresponding three-body $T$–matrix and two-body $T$–matrix for the pair $jk$, which are evaluated at zero-energy. The two-body $T$–matrix for each pair $(jk)$ is subtracted from $T^{(3)}(0)$ to avoid double counting and $K_i$ is the kinetic energy operator for particle $i$. 

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We can approximate the above effective interaction Lagrangian at low densities by averaging the $T$-matrices over the relative coordinates, considering that the thermal wave-length is much greater than the characteristic interaction distances.

\[ \mathcal{L}_1 = -\frac{1}{2} \int d^3r_1' d^3r_1 \left\langle \vec{r}_{12} \left| T^{(2)}(0) \right| \vec{r}_{12} \right\rangle \int d^3r |\Psi(\vec{r})|^4 \]

\[ -\frac{1}{3!} \int d^3r_1' d^3R_3 d^3r_1 d^3R_3 \left\langle \vec{r}_{12} \vec{R}_3 \left| T^{(3)}(0) - \sum_{j<k} T^{(2)}_{jk}(0 - K_i) \right| \vec{r}_{12} \vec{R}_3 \right\rangle \times \int d^3r |\Psi(\vec{r})|^6 . \]  

(3)

The integrations of the $T$-matrices over the relative coordinates gives the zero momentum matrix elements:

\[ \int d^3r_1' d^3r_1 \left\langle \vec{r}_{12} \left| T^{(2)}(0) \right| \vec{r}_{12} \right\rangle = (2\pi)^3 \langle \vec{p}_{12} = 0 \left| T^{(2)}(0) \right| \vec{p}_{12} = 0 \rangle = \frac{4\pi \hbar^2 a}{m} , \]  

(4)

where $a$ is the two-body scattering length. For the connected three-body $T$-matrix, we have

\[ \int d^3r_1' d^3R_3 d^3r_1 d^3R_3 \left\langle \vec{r}_{12} \vec{R}_3 \left| T^{(3)}(0) - \sum_{j<k} T^{(2)}_{jk}(0 - K_i) \right| \vec{r}_{12} \vec{R}_3 \right\rangle \]

\[ = (2\pi)^6 \langle \vec{p}_{12} = 0; \vec{P}_3 = 0 \left| T^{(3)}(0) - \sum_{j<k} T^{(2)}_{jk}(0 - K_i) \right| \vec{p}_{12} = 0; \vec{P}_3 = 0 \rangle = 2\lambda_3 , \]  

(5)

where $\lambda_3$ is the strength of the three-body effective interaction.

The nonlinear Schrödinger equation, which describes the condensed wavefunction in the mean-field approximation, is obtained from the effective Lagrangian given in Eq. (1). By considering the interaction in Eq. (3) and the definitions in Eqs. (4) and (5), it can be written as

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{m}{2} \omega_r^2 - \frac{4\pi \hbar^2}{m} |a| |\Psi(\vec{r})|^2 + \lambda_3 |\Psi(\vec{r})|^4 \right] \Psi(\vec{r}) = \mu \Psi(\vec{r}) , \]  

(6)
where $\mu$ is the chemical potential, fixed by the number $N$ of atoms in the condensed state:

$$\int d^3r |\Psi(\vec{r})|^2 = N. \quad (7)$$

The physical scales present in Eq.(6) can be easily recognized by working with dimensionless equations. By rescaling Eq.(6) for the $s$-wave solution, we obtain

$$\left[ -\frac{d^2}{dx^2} + \frac{1}{4}x^2 - \frac{\Phi(x)^2}{x^2} + g_3 \frac{\Phi(x)^4}{x^4} \right] \Phi(x) = \beta \Phi(x), \quad (8)$$

where $x \equiv \sqrt{\frac{2m\omega}{\hbar}} r$ and $\Phi(x) \equiv \sqrt{\frac{8\pi}{a}} r \Psi(\vec{r})$. The dimensionless parameters, related to the chemical potential and the three-body strength are, respectively, given by

$$\beta \equiv \frac{\mu}{\hbar \omega} \quad \text{and} \quad g_3 \equiv \lambda \frac{\hbar \omega}{4\pi a^2}; \quad (9)$$

and the normalization for $\Phi(x)$, obtained from Eq. (8), defines a number $n$ related to the number of atoms $N$:

$$\int_0^\infty dx |\Phi(x)|^2 = n, \quad \text{where} \quad n \equiv 2N|a|^{3/2} \sqrt{\frac{2m\omega}{\hbar}}. \quad (10)$$

The boundary conditions in Eq.(8) are given by

$$\Phi(0) = 0 \quad \text{and} \quad \Phi(\infty) \sim C \exp \left[ -\frac{x^2}{4} + (\beta - 1/2) \ln(x) \right]. \quad (11)$$

The numerical solutions of Eq. (8) are obtained for several values of $\beta$, using three values of $g_3$ to characterize the solutions. We have used the Runge-Kutta (RK) and “shooting” method to obtain the corresponding solutions in each case. The stability assignment was made by studying the corresponding time dependent Schrödinger equation, using the Crank-Nicolson (CN) method [see Ref. (13)]. The numerical procedure to determine such stability was done in the following way: when applying the CN method, we started by using the static solution obtained from the RK method and observed if the modulus of the wave function remained constant. If this was occurring for a long period of time (of about 500 units of dimensionless time $\tau = \omega t$) the solution was considered stable, otherwise unstable. In another procedure we added a weak perturbation to the potential. We examined the time evolution of a selected point of the wave-function. The lowest collective oscillations ($\omega_{col}$) were determined by using the Fourier transform of such result (4).

Figures 1-4 presents our main results.
**Fig. 1** The chemical potential ($\beta$) in units of $\hbar \omega$ as a function of $n$ for three values of the non-dimensional strength of the repulsive three-body effective interaction ($g_3$). $g_3 = 0$ (dashed line); $g_3 = 0.016$ (solid line); $g_3 = 0.03$ (dot-dashed line) [see Eqs. (9) and (10)]. In the inset, for $g_3 = 0.016$, the solutions linking A and B are unstable.

**Fig. 2** Frequencies of the lowest collective excitations (with $l = 0$) as a function of $n$ for three values of the dimensionless strength $g_3$. The points A and B correspond to the points shown in the inset of Fig.1, where the frequencies go to zero.
Fig. 3 Frequencies of the lowest collective excitations ($l = 0$), as a function of $eta$ for three values of the nondimensional strength $g_3$. The points A and B correspond to the points shown in the inset of Fig.1, where the frequencies go to zero.

Fig. 4 Total energy of the Bose condensate, given in units of $\hbar \omega / \left(2|a| \sqrt{2m \omega / \hbar}\right)$, is shown as a function of $n$, for three values of the nondimensional strength $g_3$. The line linking A and B in the inset correspond to the unstable region shown in Fig. 1.
In Figure 1 we present $\beta$ as function of $n$ for $g_3$ equal to 0, 0.016 and 0.03. Our calculation for $g_3 = 0$ agrees with the result presented in Ref. (5), with the maximum number of atoms limited to $n_{\text{max}} \approx 1.62$. As we can see, for $n \leq n_{\text{max}}$ two solutions are possible, the lower being unstable. For $g_3$ slightly higher than 0 a new pattern appears, as one can see for $g_3 = 0.016$ presented in the figure. We can divide the figure, for $g_3 = 0.016$ (for example), in three regions; the first, stable, goes from $\beta = 1.5$ until point A (presented in the inset); an unstable region appears from the point A till B; another stable region goes from B towards $n \to \infty$.

Figure 2 shows the collective frequencies $\omega_{\text{col}}$ as function of $n$ for the first mode ($l = 0$). The solutions corresponding to $g_3 = 0$ agree well with the ones given in Ref. (14); and they lose stability as $\omega_{\text{col}} \to 0$. By this criteria, we determined the regions of stability for $g_3 = 0.016$. For $g_3 = 0.03$ all the solutions are stable. The collective frequencies are also shown as a function of $\beta$ in Figure 3. The total energy is shown in Figure 4. The case $g_3 = 0$ reproduces the results already found by Houbiers and Stoof (3), including the unstable (higher) solutions. For $g_3 = 0.016$ the part of the plot linking points A and B is unstable, corresponding to the unstable region of Figure 1. Otherwise it is stable. Finally, for $g_3 = 0.03$, the function of the energy in terms of $n$ is always single valued and stable.

The relevance of the three-body interaction was never emphasised in BEC studies. However, in 1985, it was pointed out in Ref. (15) that an easier experimental approach to probe density fluctuations is to consider an observable directly sensitive to the probability of finding three atoms near each other, which will correspond to the loss rate of atoms due to three-body recombination. Such a three-body recombination rate in BEC was considered recently in Refs. (16), (17) and (18). It was shown in Ref. (16) that the three-body recombination coefficient of ultracold atoms to a weakly bound $s$ level goes to infinity in the Efimov limit (19). The Efimov limit is a particularly interesting three-body effect, which happens when the two-body scattering length is very large (positive or negative). In this case, with the two boson energy close to zero, the three-boson system presents an increasing number of loosely bound three body states, which have large spatial extension and do not depend on the details of the interaction (19). In such limit, when the three-body binding is close to zero, the strength $\lambda_3$ can be large enough to give a sensible value for $g_3$. So, our main motivation here was to provide an extension to the GPG equation (10), which considers a three-body interaction and, in this way, provides the framework for a numerical investigation of the relevance of three-body interaction in Bose-Einstein condensation. In this letter, we presented

\[ b = |C_{nl}| \]
results for the chemical potential, $\mu$, the number of atoms in the condensed state ($N$), and frequency of the lowest collective mode for a range of values of $\lambda_3$, expressed respectively in terms of the dimensionless parameters $\beta$, $n$, $\omega_{\text{col}}/\omega_{\text{trap}}$ and $g_3$. The determination of $\lambda_3$ has to be considered in particular three-boson systems.

To summarize, our calculation presents, at the mean-field level, the consequences of a repulsive three-body effective potential added to an attractive two-body interaction for the Bose condensed atomic state. We propose a general framework for discussing such phenomenon. As we have shown with the present approach, a slightly repulsive three body interaction provides stable solutions for higher number of atoms where their existence is forbidden when considering only two body potential. This can be a signature of the presence of an effective repulsive three body interaction in Bose condensates.

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