Coherent dimer formation near Feshbach resonances in Bose-Einstein condensates

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The results of a recent experiment with \textsuperscript{85}Rb Bose-Einstein condensates are analyzed within the mean-field approximation including dissipation due to three-body recombination. The intensity of the dissipative term is chosen from the three-body theory for large positive scattering lengths. The remaining number of condensed atoms in the experiment, obtained with applied magnetic field pulses, were used to adjust the intensity of the dissipative term. We found that the three-body recombination parameter depends on the pulse rise time; i.e., for longer rise times the values found become consistent with the three-body theory, while for shorter pulses this coefficient is found to be much larger. We interpret this finding as an indication of a coherent formation of dimers.

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Bose-Einstein condensation of dilute atomic gases has been observed for the first time in \textsuperscript{87}Rb atoms \cite{1}. Since then, it has been condensed atoms of \textsuperscript{23}Na \cite{2}, \textsuperscript{7}Li \cite{3}, \textsuperscript{3}H \cite{4}, metastable \textsuperscript{8}He \cite{5}, \textsuperscript{85}Rb \cite{6}, \textsuperscript{41}K \cite{7} and, more recently, \textsuperscript{133}Cs \cite{8}. In Ref. \cite{9}, it was theoretically predicted that Feshbach resonances could vary the scattering length of atoms in systems of dilute alkali gases over a wide range of values. A Feshbach resonance occurs when the quasimolecular bound state energy is tuned to the energy of two colliding atoms, applying an external magnetic field to the system. The phenomenon was first realized in a Bose-Einstein condensate in Ref. \cite{10}. This opened the possibility of exploring new regimes of BEC, allowing changes of the two-body scattering length from negative to positive and also from zero to infinity. This technique was used for the condensation and collapse control of \textsuperscript{85}Rb atoms in the hyperfine state ($F = 2, m_F = -2$) \cite{6,11,12}. It was also demonstrated in Ref. \cite{13} that strongly enhanced inelastic three-body collisions occurs near Feshbach resonances. In a more recent experiment, in Ref. \cite{14}, it was explored the region of very large scattering lengths (up to \textasciitilde{} 4000 Bohr radius).

The scattering length $a$ has been observed to vary as a function of the magnetic field $B$, according to the theoretical prediction \cite{15},

\begin{equation}
a = a_b \times \left(1 - \frac{\Delta}{B - B_r}\right),
\end{equation}

where $a$ is the scattering length, $a_b$ is the background scattering length, $B_r$ is the resonance magnetic field of \textsuperscript{85}Rb, and $\Delta$ is the resonance width.

In the case of \textsuperscript{85}Rb, one has resonance width $\Delta \equiv 11.0$ G, resonance field $B_r \equiv 154.9$ G and background scattering length $a_b \equiv -450\mu a$ \cite{14}, where $a_0$ is the Bohr radius. So, given the experimental functional dependence $B = B(t)$, one can determine $a = a(t)$ and, consequently, the dynamics of the system in such physical conditions. Further, mainly in strong interaction regime, a Bose-Einstein condensate shows inelastic loss processes that cause its depletion. The dominant process of losses has been verified to be the three-body recombination \cite{14,16}, with a time dependence concerning a simple constant rate equation. All earlier observations in BEC experiments were consistent with a description of mean field including such a loss process. But, in experiments with \textsuperscript{85}Rb realized in the strong interaction regime \cite{14}, this picture indicates model breakdown. Bose-Einstein condensates initially stable were submitted to magnetic field pulses carefully contolled in the vicinity of \textsuperscript{85}Rb Feshbach resonance, aiming to test the strongly interacting regime for diluteness parameter $\chi = n a^3$ varying from $\chi = 0.01$ to $\chi = 0.5$. The loss of atoms from BEC occurred in impressively short time scales (up to two hundreds of $\mu$s) and disagrees with previous theoretical predictions \cite{17}. Such experiments reveal higher loss of atoms in shorter magnetic field pulses applied on BEC and, previously, one knew that as longer is the time spent near a Feshbach resonance as higher is the loss of atoms from BEC \cite{6} (consistent with a mean field approach where the inelastic loss term has a constant dissipative rate). According to Ref. \cite{14}, the results could indicate the existence of a new physics, that cannot be described by the Gross-Pitaevskii (GP) formalism. Motivated by this observed discrepancy, we investigate the dynamics of \textsuperscript{85}Rb Bose-Einstein condensates submitted to such external conditions and time scales, when we vary the $s$-wave two-body scattering length in the region of strong interaction. So, we consider a generalized mean field approach that includes the time dependence for both mean field coupling and three-body recombination parameter. Previous results considered a mean field approach with constant mean rate for the three-body recombination and constant value for the mean field coupling \cite{14,18}. In the present work, our first task is to reproduce the experimental data with time dependent parameters or at least verify possible limitations of the time dependent mean field approach. Next, we consider the magnitude of the recombination rate as described in literature \cite{15,19,20,21,22,23,24,25,26}, but with time functional dependence.

For describing a BEC in the framework of the mean
field approximation, we remind that such an approach is valid for very dilute systems when the average inter particle distances $d$ are much larger than $|a|$ and the particle wavelengths are much larger than $d$. Besides, it is important to pay attention to the time scales present in the system: the physical conditions must not change fast enough in order to allow the replacement of a true interatomic potential by the contact interaction. It is possible in principle for the rate of change to be larger than $\hbar/ma^2$ for extremely very short changes in the interactions $|\dot{a}|$, but it is reasonable to assume valid this time dependent approach at least for longer pulses.

We begin our description from an effective Lagrangian of the nonconservative system as in Ref. [14], in which one describes the dynamics of a trapped Bose-Einstein condensate in spherical symmetry with such a GPE generalization, in which one also considered losses from BEC by three-body recombination. This Lagrangian leads to the following equation of the system:

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ \frac{\hbar^2}{2m} \nabla^2 + \frac{m \omega^2 r^2}{2} + U_0 |\Psi|^2 - i\hbar \frac{K_3}{4} |\Psi|^4 \right] \Psi,$$

where $\omega$ is the geometric mean trapping frequency, $U_0 = U_0(t) = 4\pi \hbar^2 a(t)/m$ and $K_3 = K_3(t)$ is the recombination loss parameter. The wave-function $\Psi = \Psi(\vec{r}, t)$ is normalized to the number of atoms $N$. The three-body recombination rate $K_3$ is here introduced for describing atomic losses from the condensate when three atoms scatter to form a molecular bound state (dimer) and a third atom; so, the kinetic energy of the final state particles allows them to escape from the trap. Other nonconservative processes as amplification from thermal cloud and dipolar relaxation are neglected, since the latter has a much smaller effect than three-body recombination [14, 16] and in JILA experiments [14] the thermal cloud is negligible (only 1000 atoms in a sample of 17500).

A theoretical prediction of $K_3$ is a hard task since it is sensitive to the detailed behavior of the interaction potential $\propto \mu$. However, such a calculation becomes simpler if we consider that $\alpha$ is the only important length scale (reasonable in the weakly bound s-wave state limit) and this has been considered in many works [14, 24, 21, 22, 23, 24, 25, 26]. Following Ref. [14], the recombination rate is written as

$$K_3(t) \approx \kappa \frac{\hbar}{m} |a(t)|^4,$$

where $\kappa$ should correspond to the universal value $\kappa = 3.9$. But in Ref. [21] and in Ref. [24], it was found $0 \leq \kappa \leq 65$ and in Ref. [22], $0 \leq \kappa \leq 67.9$, that is, $\kappa$ is not universal (in general $K_3$ depends on a three-atom scale [23]).

In Fig. 1, we schematically give two characteristic pulses employed in JILA, in which $B_0$, $B_h$, $B_m$, $t_r$ and $t_h$, correspond to the initial field, the hold field, the final field, the rise time and the hold time of the pulse, respectively. For describing the dynamics of condensates subjected to these experiments, we consider in our calculations the same experimental parameters and conditions used in Ref. [14]: as $\alpha$ is known to be a function of the magnetic field $B$ by means of Eq. (1), we only use time dependent shapes of experimental magnetic field pulses employed in JILA (triangular and trapezoidal pulses). The hold field is $B_h = 156.7 \text{ G}$, and the end field in which one measures the remaining number of particles $N_r$ of the system is $B_m = 164.5 \text{ G}$ at $t = 700 \mu s$. Further, we put initial field $B_0 \equiv 166 \text{ G}$, corresponding to a harmonic oscillator state of the system ($a \sim 0$), applied to an initial sample of $N_0=16500$ condensed atoms of $^{85}\text{Rb}$. Further, in our approach we have used spherical symmetry with mean geometric frequency $\bar{\omega} = (\bar{\omega}_r^2 \bar{\omega}_z^2)^{1/3}$, for simulating the cylindrical geometry of JILA (radial: $\bar{\omega}_r = 2\pi \times 17.5$ Hz and axial: $\bar{\omega}_z = 2\pi \times 6.8$ Hz). Our time dependent calculations started with a Gaussian shape wave-function which we numerically evolve by means of Eq. (2), using the Crank-Nicolson algorithm, as in Refs. [31, 32]. We analyzed the loss of condensed atoms like in Ref. [14], by considering hold times from $t_h = 0$ (triangular) or units of $\mu s$ (shorter trapezoidal pulses) to nearly hundreds of $\mu s$ (longer trapezoidal pulses). The behavior of the scattering length, as a function of total time of the pulse, in the region of strong interaction atom-atom, follows similarly the behavior of the employed field pulses given in Fig. 1. In triangular pulses, there is a sharp peak in the resonance region; and a plateau with maximum value for $a$ and $\xi$ (minimum value of the field), when $B = B_h$ is kept constant during the time $t_h$.

In the upper frame of Fig. 2 we used symmetric rise and fall times ($t_r = 12.5 \mu s$, $t_r \equiv 25 \mu s$ and $t_r \equiv 75 \mu s$), to determine the remaining fraction of atoms $N_r/N_0$ in the $^{85}\text{Rb}$ BEC as function of the hold time, by adjusting our curve with the first point of Fig. 1 in Ref. [14]. For $t_r = 12.5 \mu s$, we found $\kappa \approx 1800$, very far away of the values described earlier in the literature [14, 21, 24, 25, 26, 27, 28, 29]. The results show the same exponential decay and good concordance with experimental data, mainly for short $t_h$ (circles in upper frame of Fig. 2). However, as one can realize, for longer
hold times, experimental data point out a higher dissipation when compared with our simulations. For other short rise times in this frame or longer rise times (lower frame), we have similar behavior, but we have to decrease $\kappa$ for better adjusting to experimental data. So, the comparison with experiments show that $\kappa$ depends significantly on values of $t_r$ and $t_h$. As we know \[ 33 \], the mean field approach should make more adequately if we were in a slower process. So, we also tried to verify if our results would give a lower value of $\kappa$ (inside interval described in literature) if we calibrated our calculation with the last point of the long pulse of JILA \[ 14 \] ($t_r \approx 252.6 \mu s$). Really, we found $\kappa \approx 100$ for this case (closer to values described in literature \[ 14, 21, 22, 23, 24, 25, 26 \]) and the results reproduce the experimental data for longer rise time but they do not make very well for shorter rise time, as we can observe in lower frame of Fig. 2. The very large value of $\kappa$ leads us to conclude that there is a coherent formation of dimers, that occurs up to nearly $t_r \sim 100 \mu s$, as one can realize observing the lower frame of Fig. 2 for shorter rise times. It is physically sensible that, for shorter pulses, the presence of coherence in the formation of dimers would be more plausible than for longer pulses. So, the present calculation included the variation of $\kappa$ with the time parameters of the pulse and the amplification of the three-body recombination rate can be associated with the coherent formation of dimers in the inelastic collisions. Together with the significant loss from the coherent formation of dimers, one should also observe a burst of atoms carrying the excess of energy, which for $^{85}\text{Rb}$ with the maximum value of $a = 4000 a_0$, would be above 70nK. Indeed, in the JILA experiment, it was seen a significant number loss from the BEC for pulses lasting only few tens of microseconds, which were accompanied by a burst of few thousand relatively hot ($\sim 150\text{nK}$) atoms that remained in the trap \[ 14 \]. In our description, for each hot atom one dimer is also formed. Therefore, the burst of atoms should be accompanied by a burst of weakly bound dimers. Using the observed temperature and momentum conservation of the recombination process, we predict that the dimers are also relatively hot ($\sim 75\text{nK}$).

We note that, if we consider a constant value of $\kappa$, in all the cases (for any choices of $t_h$) we obtain a decreasing behavior of $N_r$, as we increase the rise time $t_r$. This is in contrast with the experimental results. So, we consider to adjust the values of $\kappa$ that approximately better describe the experimental data for each given rise time $t_r$; i.e., $\kappa$ is taken as a function of the rise time ($\kappa = \kappa(t_r)$). Our results are shown in Table I. There is an obvious uncertainty in the given numbers of Table I, that are related to our approximate theoretical fitting and experimental data fluctuations. However, based on such results, the behavior of $\kappa(t_r)$ can be approximately described by a linear or exponential decreasing function. Here we consider the following simple functional time-rise dependences of $\kappa$:

\[
\kappa(t_r) = 2300 \exp (-0.01 \times \omega t_r) \quad \text{or} \quad (4)
\]
\[
\kappa(t_r) = 1900 - 7 \omega t_r \quad . \quad (5)
\]

With such decreasing functional time-rise dependence of $\kappa$, we have verified, as shown in Fig. 3 that we have the qualitative behavior observed in the experimental results given in Ref. \[ 14 \] of the remaining number of atoms $N_r$ versus $t_r$. We have considered several values of the hold time $t_h$. For very small hold time, we can also verify the same experimental results that presents a minimum of $N_r$ as a function of $t_r$. With a linear functional $t_r$ dependence of $\kappa$, the same qualitative behavior can also be reproduced; which differs quantitatively from the exponential behavior that we show. So, we conclude that the time dependent mean field approach can describe all the experimental data, if the three-body recombination coefficient depends on the rise time in this short time scale. Such dependence on the rise time can be explored, once

\begin{table}[H]
\centering
\caption{Numerical values of three-body recombination coefficient $\kappa$ as function of the rise time $t_r$ of the magnetic field pulses applied to the $^{85}\text{Rb}$ BEC.}
\begin{tabular}{ccc}
\hline
$t_r$ (µs) & $\kappa$ (shorter) & $\kappa$ (longer) \\
\hline
12.5 & 1800 & 151.6 \\
25.3 & 1700 & 202.1 \\
75.8 & 1600 & 252.6 \\
\hline
\end{tabular}
\end{table}
the uncertainties in the experimental results are reduced and by considering a better fitting of data (improving the values given in Table I). In our interpretation, the higher values of $\kappa$ for smaller values of $t_r$ are indicating the coherent formation of another species (dimers) in the condensate. In summary, we report in this work indications based on our calculations that a similar experiment realized in JILA [14] is evidencing the coherent formation of dimers from inelastic collisions in $^{85}$Rb Bose-Einstein condensates (BEC). We have solved numerically the non-conservative Gross-Pitaevskii equation in spherical symmetry, for condensed systems with very large repulsive two-body interaction, varying in time, due to application of magnetic field pulses, according to Eq. (4). According to the theoretical predictions of three-body recombination rates, we used a dissipation parameter proportional to the quartic power of the scattering length $a(t)$ and the observed experimental pulse shapes to calculate the time evolution of the remaining number of atoms in the condensate. We studied this observable as a function of the hold and rise times. The experimental results of $N_t$ versus $t_h$ can be described in the mean-field approach only with very large $\kappa$, when the rise time is small. This indicates a coherent formation of dimers in BEC. For longer pulses, when the coherent dimer formation tends to disappear, we found that $\kappa$ approaches the maximum value given by the theoretical predictions for large scattering lengths, $\kappa \sim 70$ [20, 22]. We parameterize this surprising behavior of the three-body recombination rate considering $\kappa = \kappa(t_r)$ and so it was possible to describe the property of a lower dissipation for longer pulses. Finally, it is natural to see a burst of relatively hot atoms and dimers (carrying the excess of dimer binding energy) accompanying a significant loss from the condensate for short pulses when the coherent dimer formation occurs.

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