Atom loss from the $^{85}$Rb Bose-Einstein condensate by a Feshbach resonance

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Abstract.
Loss of atoms from a $^{85}$Rb condensate on passage through a Feshbach resonance is analyzed using the generalized parametric approximation that takes into account quantum many-body effects. These effects lead to a substantial increase of the losses. A better agreement with experiments is achieved, compared to predictions of mean-field theories. The method provides much insight into the quantum effects involved, and on the nature of entangled atom pairs produced by the loss.

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The presence of a Feshbach resonance is supposed to provide a tool for controlling the interatomic interactions determining the properties of a Bose-Einstein condensate (BEC) (see [1] and references therein). A Feshbach resonance occurs when the energy of a pair of atoms in the condensate is close to that of a metastable molecular state. The scattering length, as a measure of the mean interatomic interaction, varies strongly as a function of the energy mismatch between the two states. This mismatch can be controlled by applying a varying magnetic field. The energies of the two states can be brought closer to each other, as the two states have different Zeeman shifts.

The effect was studied first in the MIT experiment on Na [2], by applying a time-varying magnetic field $B = B(t)$. The experiment resulted in a large condensate population loss. In order to provide a theoretical explanation of these experimental results, two mechanisms have been suggested. The first one is a collisional deactivation process [1, 3], relating the loss to atom-molecule and molecule-molecule inelastic collisions. This mechanism has been analyzed in [1, 3] using coupled mean-field (MF) equations for the atomic and molecular condensates. The second mechanism is an excitation process [4], involving a crossing of the resonant molecular state into non-condensate atomic states. It has been analyzed at first in [4] as a dissociation of single molecules, without taking into account many-body effects. The combined effect of both mechanisms was studied in [5], where the crossing mechanism has been incorporated into MF equations by introducing a width to the molecular condensate state. It has been shown that in the case of the MIT experiment both mechanisms contribute to the loss comparably and non-additively. The crossing loss mechanism and non-condensate states are especially important in the case of the extremely strong Feshbach resonance in $^{85}$Rb studied in the more recent JILA experiments [6].
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The non-condensate atoms are formed as entangled pairs in two-mode squeezed states [7]. Several methods have been suggested earlier, allowing a correct treatment of such essentially quantum states. A numerical solution of stochastic differential equations in the positive-$P$ representation has been used for this purpose in [8]. In the Hartree-Fock-Bogoliubov formalism (HFB) [9] [10] the MF equations were complemented by equations for the normal and the anomalous densities, describing the second-order correlations of the non-condensate atomic fields. These correlations are taken into account to the same accuracy in the parametric approximation [7] [11] [12] and in the microscopic quantum dynamics approach [13] [14]. Some qualitative results have been also presented in [15]. A modified version of the MF theory [16] differs from the HFB method by neglecting the normal density, which actually reduces the problem to a two-body one (see [10] [17]), removing quantum many-body effects. An attempt to describe the JILA $^{85}$Rb experiments using this theory in [18] has therefore met with little success.

The present work uses the parametric approximation [7] in order to describe the JILA experiments [6]. The incorporation of the quantum effects leads to a much better agreement with the experimental results compared to MF theories. The results have been preliminarily reported in [19]. A more recent work [20], performed independently, uses the microscopic quantum-field-theoretic approach of [14], in order to obtain the same goal. The approach of [20] takes account of the spatial inhomogeneity of the condensate, and therefore yields a better agreement with the experimental data, compared to the one presented here.

The approach of [14] used by [20], based on the numerical solution of a nonlinear partial-integro-differential equation, may provide the ultimate word concerning accuracy. But it lacks the transparency of the parametric approximation as used here. At the cost of avoiding inhomogeneities, the present method provides a greater qualitative insight, such as the occupation of the various non-condensate states, from which useful information can be derived regarding the profile of the entangled atom pair production. Also one can easily trace causal effects, such as the relation between the excessive condensate loss and the effects of quantum Bose enhancement on the curve-crossing process (see [12]).

Following the generalized parametric approximation [7], let us consider a system of coupled atomic and molecular fields described by annihilation operators in the momentum representation $\hat{\Psi}_a (p, t)$ and $\hat{\Psi}_m (p, t)$, respectively. The coupling of the atomic and molecular fields contains a product of two atomic creation operators and therefore describes the formation of entangled atomic pairs. Spatial inhomogeneity due to the trapping potential and the effects of elastic collisions are neglected here.

Let the initial state of the atomic field at $t = t_0$ be a coherent state of zero kinetic energy

$$\hat{\Psi}_a (p, t_0) |\text{in}\rangle = (2\pi)^{3/2} \varphi_a (t_0) \delta (p) |\text{in}\rangle,$$

where $|\varphi_a (t_0)|^2 = n_0 (t_0)$ is the initial atomic condensate density and $|\text{in}\rangle$ is the time-independent state vector in the Heisenberg representation. A pair of condensate atoms forms a molecule of zero kinetic energy. Therefore the resonant molecules can be represented by a mean field $\varphi_m (t)$ as

$$|\text{in}\rangle \hat{\Psi}_m (p, t) |\text{in}\rangle = (2\pi)^{3/2} \varphi_m (t) \delta (p),$$

where $|\varphi_m (t)|^2 = n_m (t)$ is the molecular condensate density. Fluctuations of the molecular field due to collisions involving non-condensate atoms are neglected.
The outcome of atom-molecule and molecule-molecule deactivating collisions is introduced by adding molecular “dump” states. The elimination of these states in a second-quantized description leads to the equation of motion for the atomic field \(^\dddot{\Psi}_a(p,t)\),

\[
i\dot{\Psi}_a(p,t) = \left[ \frac{p^2}{2m} + \epsilon_a(t) - i\gamma|\varphi_m(t)|^2 \right] \Psi_a(p,t) + 2g^*\varphi_m(t)\Psi_a^\dagger(-p,t) + i\hat{F}(p,t),
\]

where \(m\) is the atomic mass, \(\epsilon_a(t) = -\frac{1}{2}\mu(B(t) - B_0)\) is the time-dependent Zeeman shift of the atom in an external magnetic field \(B(t)\), relative to half the energy of the molecular state, \(\mu\) is the difference in magnetic momenta of an atomic pair and a molecule, and \(B_0\) is the resonance value of \(B\). The coupling \(g\) of the atomic and the molecular fields is related to the phenomenological resonance strength \(\Delta\) as \(|g|^2 = 2\pi|\alpha_a|\Delta/m\) \(\ddagger\), where \(\alpha_a\) is the background elastic scattering length. The quantum noise source \(\hat{F}(p,t)\) and the parameter \(\gamma\) describe the effect of deactivating collisions. The deactivation plays important role in general case \([7]\) and is included in the present calculations. However for the conditions of experiments \([9]\) the results of calculations are insensitive to these processes (a variation of the deactivation rate coefficients from 0 to \(10^{-9}\) cm\(^3\)/s change the results by less than 1%). The contribution of deactivating collisions is therefore neglected in following analysis. The atomic field operator can then be written in the form

\[
\hat{\Psi}_a(p,t) = \hat{\Psi}_a(p,t_0)\psi_c(p,t) + \hat{\Psi}_a^\dagger(p,t_0)\psi_s(p,t).
\]

The \(c\)-number functions \(\psi_{c,s}(p,t)\) are solutions of the equations

\[
i\dot{\psi}_{c,s}(p,t) = \left[ \frac{p^2}{2m} + \epsilon_a(t) \right] \psi_{c,s}(p,t) + 2g^*\varphi_m(t)\psi_{s,c}^\dagger(p,t),
\]

given the initial conditions \(\psi_c(p,t_0) = 1\), \(\psi_s(p,t_0) = 0\), and the constraint

\[
|\psi_c(p,t)|^2 - |\psi_s(p,t)|^2 = 1.
\]

The two-atom correlation functions are expressed in terms of these solutions as

\[
\langle \psi_c(p,t)\psi_{s,c}^\dagger(p',t)\rangle = (2\pi)^3\delta(p - p')\delta(s - c) + \delta(p + p'),
\]

\[
\langle \psi_s(p,t)\psi_{c,s}^\dagger(p',t)\rangle = (2\pi)^3\delta(p - p')\delta(c - s) + \delta(p + p'),
\]

where

\[
n_0(t) = |\varphi_a(t)|^2
\]

is the condensate density,

\[
\varphi_a(t) = \langle 0|\hat{\Psi}_a(0,t)|\langle\rangle = \psi_c(0,t)\varphi_s(t_0) + \psi_s(0,t)\varphi_a^\dagger(t_0)
\]

is the atomic mean field,

\[
n_s(p,t) = |\psi_s(p,t)|^2
\]

is the momentum spectrum of the non-condensate atoms, and

\[
m_0(t) = \varphi_a^2(t), \quad m_s(p,t) = \psi_s(p,t)\varphi_c(p,t)
\]

are the anomalous densities of the condensate and non-condensate atoms, respectively. The atomic density

\[
n_a(t) = (2\pi)^{-3} \int d^3p_1d^3p_2 \exp[i\cdot r] \langle \psi_c(p_1,t)\psi_{s,c}^\dagger(p_2,t)\rangle
\]

\(\ddagger\) A system of units in which Planck’s constant is \(\hbar = 1\) is used below.
then appears to be $r$-independent, and comprises the sum $n_a(t) = n_0(t) + \int d^3p n_s(p,t)$ of the densities of condensate atoms and of non-condensate (entangled) atoms in a wide spectrum of kinetic energies.

The equation of motion for the molecular mean field $\varphi_m(t)$, obtained by the removal of the effects of deactivating collisions, followed by a mean-field averaging, is

$$i \dot{\varphi}_m(t) = gm_0(t) + \frac{g}{2\pi^2} \int_0^{p_c} p^2 dp n_s(p,t), \quad (14)$$

where the cutoff $p_c$ in momentum space is necessary in order to avoid divergences. The final results, after a renormalization of the detuning $\epsilon_a(t)$ in a manner similar to the one used in [9], are insensitive to the value of the cutoff momentum if it is large enough, so that $p_c^2/(2m) > \max(-\epsilon_a(t))$.

Equations (5), (6), (10), (11), and (12) lead to the following equations of motion for the atomic mean field, and the normal and anomalous densities of the non-condensate atoms,

$$i \dot{\varphi}_a(t) = \epsilon_a(t) \varphi_a(t) + 2g^* \varphi^*_a(t) \varphi_m(t) \quad (15)$$
$$i \dot{n}_s(p,t) = 2g^* \varphi_m(t) m^*_s(p,t) - 2g \varphi^*_m(t) m_s(p,t) \quad (16)$$
$$i \dot{m}_s(p,t) = \left[ \frac{\mu^2}{m} + 2\epsilon_a(t) \right] m_s(p,t) + 2g^* \varphi_m(t) \left[ 1 + 2n_s(p,t) \right]. \quad (17)$$

These equations, in combination with (14) are the momentum representation of the HFB equations used in [9]. Therefore the present approach becomes mathematically equivalent to the HFB one having, however, some advantages in simplifying the numerical calculations.

The results presented here were obtained by a numerical solution of Eqs. (5) on a grid of values of $p$, combined with Eq. (14). The values of $\Delta = 11$ G, $B_0 = 154.9$ G, and $|a_a| = 450$ (in atomic units) are taken from [21], and the value of $\mu = -2.23$ (in Bohr magnetons) is taken from [10]. The dynamics is calculated for a linear variation of the magnetic field $B = B_0 - \dot{B}t$ from 162.3 G to 132 G with various sweep rates $\dot{B}$, chosen in accordance with the experiments [6].

The results are sensitive to the initial value of the magnetic field. This sensitivity can be attributed to the large crossing width $\Gamma_{cr}$ [5], which substantially exceeds the range of the detuning $\epsilon_a(t)$ along the full sweep. Therefore, in some sense, the system is always within the resonance. As the initial values of $\varphi_m$, $\psi_c$, and $\psi_s$ were substituted the steady-state values calculated using the initial magnetic field as a constant. The calculations were performed for a homogeneous BEC with the initial density $10^{12}$ cm$^{-3}$.

An example of the resulting dynamics is presented in figure 1. It demonstrates that the main mechanism of the condensate loss is a conversion to non-condensate atoms by the crossing mechanism, while the molecular occupation, and hence the deactivation losses, are negligibly small. The effect of Bose enhancement on the crossing from the molecular state to non-condensate modes is proportional to the mode occupation presented in figure 1b.

Figure 2a compares the results of calculations to the experimental data [6]. The results of mean-field calculations using the method [5] are presented as well. It demonstrates the better agreement with the experimental data attained by the parametric approximation, compared to the MF results. The drastic increase of loss at the slower sweeps is actually related to the effect of Bose enhancement, as
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Figure 1. (a) Time dependence of the densities of the atomic condensate (—), the molecular condensate (— — —), non-condensate atoms (— · —) and of the mean squeezing parameter $\bar{r}$ (· · · · · ·), calculated for the ramp speed $\dot{B} = 5$ G/ms. (b) The occupation $n_s(p,t)$ of several non-condensate modes with energies $p^2/(2m) = 1.1$ nK (— — —), 4.4 nK (——), 9.8 nK (— — —), and 17.5 nK (· · · · · ·).

Figure 2. (a) Ratio of the surviving atomic condensate density $n_0(t)$ to the initial one $n_0(t_0)$ (——), and the maximal non-condensate state occupation (— — —), as functions of the inverse ramp speed, calculated using the generalized parametric approximation, in comparison with the experimental data by Cornish et al. [6] (● ● ●), and the results of mean-field calculations based on [5] (— — —). (b) Energy spectra of non-condensate atoms $\tilde{n}_s(E,t)$ (· · · · · ·) and the squeezing parameter $r(E,t)$ (· · · · · ·), calculated for the ramp speed $\dot{B} = 5$ G/ms at the time $t = 1$ ms.

The non-condensate atoms are formed in two-mode squeezed states, which are entangled [7]. Entangled atoms can have many applications in quantum measurements, calculations, and communications (see [7] and references therein). The amount of entanglement can be measured by the energy-dependent squeezing parameter $r(E,t)$ and a mean squeezing parameter $\bar{r}(t)$ [7],

\[
 r(E,t) = \frac{1}{4} \ln \left| \frac{1 + 2n_s(p,t) + 2|m_s(p,t)|}{1 + 2n_s(p,t) - 2|m_s(p,t)|} \right|,
 \quad \bar{r}(t) = \frac{\int d^3p n_s(p,t)r(p^2/(2m),t)}{\int d^3p n_s(p,t)} \tag{18}
\]

where $E = p^2/(2m)$ is a kinetic energy of non-condensate atoms. In our calculations demonstrated by the plot for the maximal value of the non-condensate state occupation $n_s$ in figure 2b. The disagreement between the parametric approximation and the experimental data at intermediate sweep rates is related to the effects of spatial inhomogeneity neglected in both theories, but taken account of in the calculations [20].
the maximal squeezing takes place at the slowest sweep. Even in this case the mean squeezing does not exceed the value of 1.1 (see figure 1), and the energy-dependent squeezing does not exceed the value of 1.4 (see figure 2). These values are substantially less than max $\bar{r}(t) \approx 3.1$ and max $r(E,t) \approx 3.6$ calculated for the weak resonance ($\Delta \approx 9.5 \text{ mG}$) in Na [7]. This result justifies the conclusion of [7] that a weak resonance is preferable for formation of entangled atoms. The energy spectrum of non-condensate atoms

$$\tilde{n}_s(E,t) = \frac{mp_s(p,t)}{(2\pi^2)},$$

presented in figure 2p, is rather narrow, just as in the case of Na [7].

In conclusion, this letter presents an application of the parametric approximation [7] to a description of BEC losses in the JILA $^{85}$Rb experiments [6]. The method, while disregarding inhomogeneities, offers a rather transparent demonstration of the relation of the excessive losses observed to the quantum many-body effects of Bose enhancement, and provides detailed information on the nature of the entangled atom pairs produced in the process.

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