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Atom loss from Bose-Einstein condensates due to Feshbach resonance

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In recent experiments on Na Bose-Einstein condensates [S. Inouye *et al.*, Nature **392**, 151 (1998); J. Stenger *et al.*, Phys. Rev. Lett. **82**, 2422 (1999)], large loss rates were observed when a time-varying magnetic field was used to tune a molecular Feshbach resonance state near the state of atom pairs that belong to the condensate many-body wave function. A mechanism is offered here to account for the observed losses. It is based on the deactivation of the resonant molecular state by interaction with a third condensate atom, with a deactivation rate coefficient of magnitude $\sim 10^{-10}$ cm^3/s. [S1050-2947(99)50508-8]

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Experiments have been carried out recently [1,2] (see also the review [3]), in order to control the interatomic interaction underlying the properties of a Bose-Einstein condensate (BEC). One way to achieve this [1,2] is by tuning a magnetic field B into the vicinity of a Feshbach resonance, with the resulting modification of the atom-atom scattering length as predicted [4,5]. The experiments carried out with Na in an optical trap measured two distinct features: (a) the change in scattering length and large collisional atom losses obtained with a slow sweep of B that stopped short of the resonant field B_0, and (b) a near-catastrophic loss of atom density obtained with a fast sweep of B through the B_0 region. Two groups of investigators [6,7] have recently proposed a unimolecular mechanism relating the latter feature to a fast sweep-induced transfer of atoms out of the condensate to become hot atoms in the trap.

We present here another possible mechanism of atom loss that can account for the slow-sweep results, and that may also play a role in the fast-sweep case. The temporary occupation of the vibrationally excited molecular state m, coupled by the resonance to atom pairs in the condensate, is converted to a stable molecular dimer d by a deactivating inelastic collision with a third atom from the condensate:

$$\mathrm{Na}+\mathrm{Na}\rightleftharpoons \mathrm{Na}_2(m), \tag{1}$$

$$\mathrm{Na}_2(m)+\mathrm{Na}\rightarrow \mathrm{Na}_2(d)+\mathrm{Na}+\Delta E, \tag{2}$$

where ΔE is the excess kinetic energy released in the inelastic process. The deactivation states can be lower-lying rovibrational levels in the same spin state as the resonant level, or levels belonging to another spin state. While step (1) is completely reversible, step (2) is irreversible, since the energy release provides the products with sufficient kinetic energy to escape the trap. This latter step is characterized by a deactivation rate coefficient 2γ (in units of cm^3/s). The two steps described above may be followed by a third one — secondary collisions of the products with condensate atoms.

Except for the magnitude of γ, which we extract by fitting the experimental data, all expressions below can be derived analytically, using previously determined parameters. We begin by using a variational method to derive a set of three coupled Gross-Pitaevskii equations for the atomic condensate state $\varphi_a(\mathbf{r},t)$, the resonant molecular state $\varphi_m(\mathbf{r},t)$, and a representative deactivation state d. Because the deactivation state d never accrues a significant population, it can be eliminated from the two remaining equations, leaving terms dependent on γ,

$$i\hbar\dot{\varphi}_a=\left(\frac{1}{2m}\hat{\mathbf{p}}^2+V_a(\mathbf{r})+\mu_a B(t)+U_a|\varphi_a|^2\right)\varphi_a + U_{am}|\varphi_m|^2\varphi_a+2g^*\varphi_a^*\varphi_m-i\hbar\gamma|\varphi_m|^2\varphi_a, \tag{3}$$

$$i\hbar\dot{\varphi}_m=\left(\frac{1}{4m}\hat{\mathbf{p}}^2+V_m(\mathbf{r})+\mu_m B(t)+U_m|\varphi_m|^2\right)\varphi_m + U_{am}|\varphi_a|^2\varphi_m+g\varphi_a^2-i\hbar\gamma|\varphi_a|^2\varphi_m. \tag{4}$$

These equations are similar to those recently derived by Timmermans *et al.* [3,8]. Here m is the mass of the Na atom; $V_a(\mathbf{r})$ and $V_m(\mathbf{r})$ are the atomic and molecular optical trapping potentials (V_m includes the resonance detuning for zero magnetic field); $\mathbf{r}$ is the position in the trap; $B(t)$ is the applied homogeneous magnetic field; μ_a and μ_m are the atomic and molecular magnetic moments, respectively; and U_a, U_m, and U_{am} are, respectively, zero-momentum atom-atom, molecule-molecule, and atom-molecule interactions, proportional to the corresponding elastic scattering lengths. Although U_m and U_{am} are not known, the results of our analysis are practically insensitive to their values.

The constant g in Eqs. (3) and (4) responsible for the atom-Feshbach coupling is closely related to the empirical parameter Δ used in Refs. [1,2] to describe the strength of the resonance as a function of the field B:

$$|g|^2=2\pi\hbar^2|a_a|\mu\Delta/m, \tag{5}$$

where a_a is the off-resonance scattering length. Calculations [6,9] give $a_a=3.4$ nm, $\mu=\mu_m-2\mu_a=3.3\mu_B$ (where $\mu_B=9.27\times10^{-24}$ J/T is the Bohr magneton), and $\Delta=0.001$ mT and 0.1 mT, respectively, for the two resonances observed at 85.3 mT (853 G) and 90.7 mT (907 G)

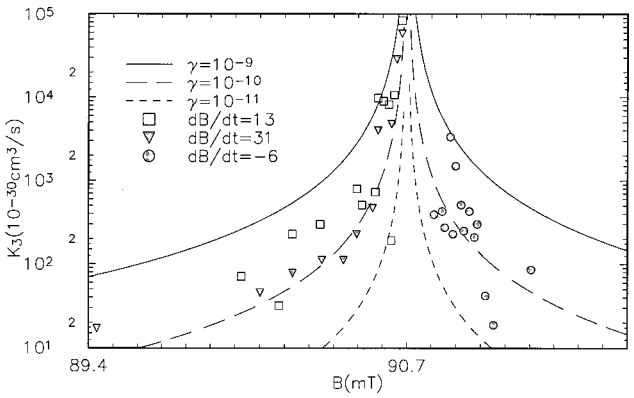

FIG. 1. Three-body rate coefficient (K_3) vs the stopping value of the magnetic field, calculated with three different values of the deactivation rate γ (in units of cm^3/s), on approaching the resonance from below or above. These are compared with the experimental results [2] (squares, triangles, and circles) for several values of the ramp speed dB/dt (in mT/s).

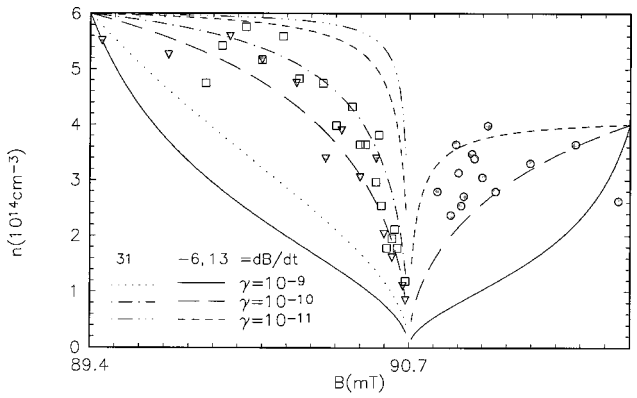

FIG. 2. Surviving mean density vs the stopping value of the magnetic field, calculated with three different values of the ramp speed dB/dt (in mT/s). The resonance was approached from below with two ramp speeds, 13 mT/s and 31 mT/s, or from above, with the ramp speed -6 mT/s. Other notations as in Fig. 1.

[1,2]. These values of Δ agree with the measured value for the 90.7-mT resonance, and with the indirectly inferred order of magnitude for the 85.3-mT resonance.

The analysis below neglects the kinetic-energy terms in Eqs. (3) and (4), in accord with the Thomas-Fermi approximation. This procedure reduces Eqs. (3) and (4) to a system of ordinary differential equations for *complex* $\varphi_a(\mathbf{r},t)$ and $\varphi_m(\mathbf{r},t)$ that depend parametrically on $\mathbf{r}$. The end result is a set of *four real* equations that can then be solved numerically, for a given value of γ. As initial conditions one can use either a Thomas-Fermi distribution or a homogeneous ($\mathbf{r}$-independent) distribution equal to the mean trap density.

The numerical solutions presented below, for both the fast and slow sweep experiments [1,2], were carried out using homogeneous initial conditions. However, as we show below, all significant results concerning the slow-sweep experiment can be derived analytically from Eqs. (3) and (4) without recourse to numerical solutions. In this experiment the time-dependent magnetic field was linearly changed from an initial value of B to a final value closer to resonance, and then the density was measured by shutting off the trap field and letting the condensate expand. The experiment was repeated using various final values of the magnetic field, and the loss was plotted as a function of this final value. It was noted [2] that the results fit a three-body rate equation for the atomic density $n(\mathbf{r},t)=|\varphi_a(\mathbf{r},t)|^2$ of the type $\dot{n}\approx -K_3 n^3$.

Analysis of Eqs. (3) and (4) shows that, out of the four real coupled equations for φ_a and φ_m, a single rate equation for the atomic density $n(\mathbf{r},t)$ can be extracted whenever the following ''*fast decay*'' approximation holds:

$$|g|^2 \ll \hbar^2 \gamma^2 n(\mathbf{r},t). \tag{6}$$

Given condition (6), the population of the molecular condensate is depleted fast enough to keep $n_m(\mathbf{r},t)=|\varphi_m(\mathbf{r},t)|^2 \ll n(\mathbf{r},t)$ at all times. The resulting rate equation attains the nonlinear form

$$\dot{n}(\mathbf{r},t) = -\frac{6|g|^2 \gamma n^3(\mathbf{r},t)}{[V(\mathbf{r})-\mu B(t)]^2+[\hbar \gamma n(\mathbf{r},t)]^2}, \tag{7}$$

where $V(\mathbf{r})=2V_a(\mathbf{r})-V_m(\mathbf{r})$. Equation (7) has a form analogous to a Breit-Wigner resonant scattering expression adapted for zero-momentum collisions. In the Breit-Wigner form one interprets $2\gamma n$ as the width of the decay channel, and the width of the input channel is proportional to $|g|^2$. This observation establishes a link between the macroscopic approach used here and microscopic approaches that treat the loss rate as a collision process.

Very close to resonance [where $B(t)$ is within 1 μT of resonance] the behavior of Eq. (7) effectively attains a one-body form. But as long as we stay out of this narrow region, by obeying the ''*off-resonance*'' condition

$$\hbar \gamma n(\mathbf{r},t) \ll |V(\mathbf{r})-\mu B(t)|, \tag{8}$$

we can write Eq. (7) (to a very good approximation) in the three-body form $\dot{n}=-K_3(\mathbf{r},t)n^3$, with

$$K_3(\mathbf{r},t) = \frac{12\pi\hbar^2|a_a|\gamma\Delta}{m\mu[B(t)-V(\mathbf{r})/\mu]^2}. \tag{9}$$

The dependence on the scattering length a_a follows from Eq. (5). Equation (9) is similar to an expression derived earlier [3,8] up to a factor 3/2, which reflects the fact that three atoms are lost per one deactivating collision.

If a magnetic-field ramp is assumed to start at time t_0 and end at time t, while Eq. (8) applies throughout the ramp, then the rate equation may be solved analytically, using K_3 of Eq. (9), to give

$$n(\mathbf{r},t) = n(\mathbf{r},t_0)[1+24\pi\hbar^2|a_a|\Delta\gamma n^2(\mathbf{r},t_0) \times (t-t_0)/(m\mu\dot{B}^2 t t_0)]^{-1/2}, \tag{10}$$

where $\dot{B}$ is the magnetic-field ramp speed and the extrapolated time of exact resonance is chosen to be $t=0$. We shall refer to the combination of Eqs. (6) and (8) that leads to Eq. (9) as the ''three-body'' approximation.

The graphs shown in Figs. 1 and 2 pertain to the slow-sweep MIT experiment for the strong 90.7-mT resonance. This resonance has been approached from below with two ramp speeds, and from above with one. Figure 1 shows K_3

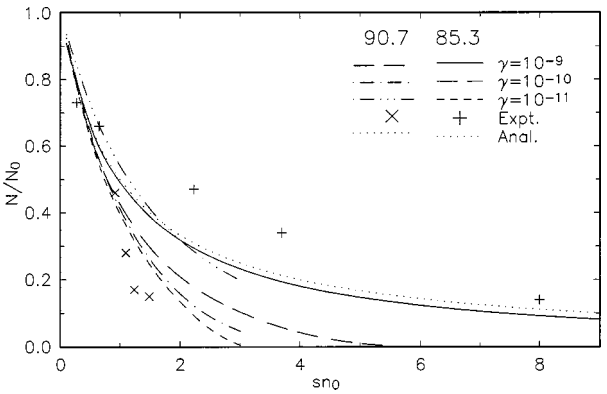

FIG. 3. Ratio of surviving trap population N to the initial one N_0 for the 85.3-mT (853-G) and 90.7-mT (907-G) resonances in the homogeneous-density approximation vs sn_0 [where the parameter s is defined by Eq. (12) and n_0 is the initial density]. The curves show results of calculations carried out for different magnitudes of the coefficient γ (in units of cm^3/s). The asymptotic analytical result Eq. (12) for both resonances is given by the dotted line. The plots for the 90.7-mT resonance with $\gamma=10^{-9}$ cm^3/s and for the 85.3-mT resonance with $\gamma=10^{-10}$ cm^3/s are practically indistinguishable. The results of the MIT fast-sweep experiment [2] are shown for comparison.

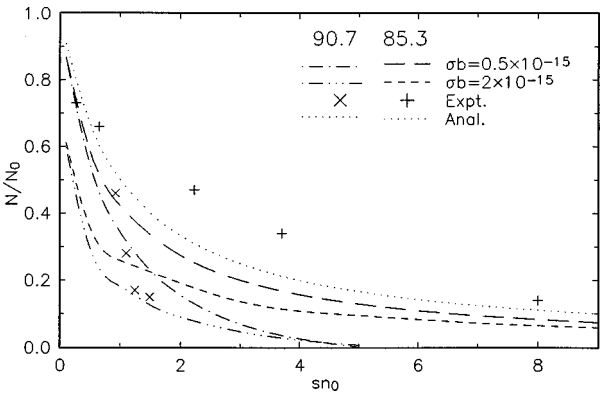

FIG. 4. Same as Fig. 3 with $\gamma=10^{-9}$ cm^3/s only, but taking account of secondary collisions using two values of the parameter σb (in units of cm^3). The asymptotic result, Eq. (12) (without taking account of secondary collisions), is shown as a dotted line for comparison.

vs the stopping value of B. The difference between Eqs. (9) and (10) and the results of a direct numerical solution of Eqs. (3) and (4) for all ramp speeds is so small that the corresponding plots are indistinguishable. The remaining atomic density, at the moment t of stopping the ramp, is shown in Fig. 2. The calculated plots were obtained using homogeneous-density initial conditions, starting from a B value of 89.4 mT on approach from below and 91.6 mT from above. The corresponding initial mean densities were extracted from the experimental data [2]. The graphs clearly show a best fit with γ of the order of 10^{-10} cm^3/s, which (given a density of about 10^{15} cm^{-3}) implies a deactivation time of $\sim 10^{-5}$ s.

An inelastic rate coefficient 2γ with a magnitude of 10^{-10} cm^3/s appears to be very reasonable. First, this value is two orders of magnitude smaller than the upper bound set by the unitarity constraint on the S matrix [10]. In the limit of small momentum, unitarity provides $2\gamma \leqslant \hbar\lambda/m$, where λ (the de Broglie wavelength) in the current situation is limited by the experimental trap dimensions. This constraint sets an upper bound of 2.5×10^{-8} cm^3/s to 2γ. Second, our estimate of 10^{-10} cm^3/s for γ is consistent with the order of magnitude of recently calculated [11] vibrational deactivation rate coefficients due to ultracold collisions of He with H_2 in highly excited vibrational levels.

The three-body approximation does not hold very close to resonance, and is therefore inapplicable to a description of the fast-sweep experiment, in which the Zeeman shift was swept rapidly through the resonance, causing dramatic losses (see Refs. [1,2]). Nevertheless, the fast decay approximation (6) may still be valid. A simple analytical expression can then be derived for the fast-sweep experiment if, in addition, the magnetic-field variation lasts long enough to reach the ''*asymptotic*'' condition

$$\mu\,\delta B \gg \hbar\,\gamma n, \tag{11}$$

where δB is the range of variation of B on both sides of the resonance. The ramp starting and stopping times can then be approximately extended to $\pm\infty$, obtaining (for all positions $\mathbf{r}$)

$$n(\mathbf{r},\infty)=\frac{n(\mathbf{r},-\infty)}{1+sn(\mathbf{r},-\infty)}, \qquad s=\frac{12\pi^2\hbar|a_a|}{m}\frac{\Delta}{|\dot{B}|}. \tag{12}$$

This asymptotic result reproduces a characteristic dependence on the ramp speed, and is independent of γ. Assuming, as before, a homogeneous initial density within the trap, Eq. (12) also describes the loss of the total population $N(t)=\int n(\mathbf{r},t)d^3r$.

An asymptotic expression for the total population can also be found when the homogeneous distribution is replaced by the Thomas-Fermi one (see Ref. [12]). In this case, given n_0 is the maximum initial density in the center of the trap,

$$\frac{N(\infty)}{N_0(-\infty)}=\frac{15}{2sn_0}\left\{\frac{1}{3}+\frac{1}{sn_0}-\frac{1}{2sn_0}\sqrt{1+\frac{1}{sn_0}}\times\ln\left[\left(\sqrt{1+\frac{1}{sn_0}}+1\right)\Big/\left(\sqrt{1+\frac{1}{sn_0}}-1\right)\right]\right\}. \tag{13}$$

The analytical results of Eq. (12), together with the direct numerical solutions of Eqs. (3) and (4) for the homogeneous initial distribution, are compared in Fig. 3 with the results of the fast-sweep experiment [1,2]. The numerical solutions clearly show a dependence on γ, as assumptions (6) and (11) underlying the asymptotic result do not hold in this case. The loss reaches a maximum at a value of γ, dependent on the various parameters (e.g., $\gamma\approx 10^{-10}$ cm^3/s for the 90.7-mT resonance when $sn_0\approx 2$), as a result of the conflicting asymptotic and fast-decay conditions (6) and (11). These solutions are, however, not as sensitive to the value of γ as were the fits to the slow-sweep experiments discussed above. Although one may claim a ''best'' fit of γ to each of the two resonances, an agreement with the results of the fast-sweep experiment is not conclusive. Thus other proposed mechanisms [6,7] may also contribute to the loss.

Additional atom loss may be provided by secondary collisions. A qualitative idea concerning their effect can be obtained by the following arguments. The deactivation reaction Eq. (2) produces $4\gamma n n_m$ ''hot'' particles (atoms and molecules) in a unit volume per unit time. Traversing a distance b at a speed v, these particles create new hot particles in a cascading process. The density of hot particles may then be estimated as $n_h \approx 4\gamma n n_m (b/v)\exp[b\sigma(n+n_m)]$, where σ is the elastic collision cross section, considered here to be identical for atom-atom and atom-molecule collisions. The additional loss rate due to these secondary collisions is estimated as $v\sigma n n_h$ for the atomic condensate and $v\sigma n_m n_h$ for the molecular condensate. An account of these losses can be taken by adding the term $1/2 v\sigma n_h$ to γn_m in Eq. (3) and to γn_a in Eq. (4). This loss rate depends essentially on the product σb. A conservative estimate of this product is obtained by taking $\sigma = 0.5\times 10^{-12}$ cm^2 (the elastic Na-Na cross section at 0.1 K [13], a typical vibrational deactivation energy), and $b = 10^{-3}$ cm (the condensate-cloud radius). A more realistic estimate may reach a higher value on account of the larger axial condensate length, the rise of the elastic cross section at energies below ~ 10 mK [13], and the added contribution of inelastic collisions. Two values of σb are therefore used in Fig. 4. This figure shows that the secondary collisions may appreciably increase the condensate loss. The effects of secondary collisions on the slow-sweep results are generally less prominent, adding up an insignificant correction to the estimated value of γ.

Another mechanism that may contribute appreciably to the loss rate in the fast-sweep case is the unimolecular process discussed in Refs. [6,7]. This treatment also takes into account the effect of the kinetic-energy terms neglected here.

In conclusion, the mechanism proposed here (based on the deactivation of the molecular Feshbach resonance state by an inelastic collision with a third atom) provides a reasonable explanation of the slow-sweep experiments. It also offers an effect competing with other mechanisms in the fast-sweep case.

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