Mean-Field Theory of Feshbach-Resonant Interactions in $^{85}$Rb Condensates

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Recent Feshbach-resonance experiments with $^{85}$Rb Bose-Einstein condensates have led to a host of unexplained results: dramatic losses of condensate atoms for an across-resonance sweep of the magnetic field, a collapsing condensate with a burst of atoms emanating from the remnant condensate, increased losses for decreasing interaction times—until very short times are reached, and coherent oscillations between remnant and burst atoms. Using a simple yet realistic mean-field model, we find that rogue dissociation, molecular dissociation to noncondensate atom pairs, is strongly implicated as the physical mechanism responsible for these observations.

Introduction—The process known as the Feshbach resonance occurs when two ultracold atoms collide in the presence of a magnetic field, whereby a spin flip of one atom can induce the pair to jump from the two-atom continuum to a quasibound molecular state. If the initial atoms are Bose condensed, the so-formed molecules will also comprise a Bose-Einstein condensate (BEC) [1]. Since the Feshbach resonance is mathematically identical to photoassociation [2,3], the process that occurs when two ultracold atoms form a molecule by absorbing a photon, insight gathered in either case is applicable to the other. In particular, the most recent results from photoassociation predict that rogue dissociation, molecular dissociation to noncondensate atom pairs, imposes a maximum achievable rate on atom-molecule conversion, as well as the possibility of coherent Rabi oscillations between the BEC and the dissociated atom pairs [3].

As predicted [4], the Feshbach resonance was used to enable Bose condensation in $^{85}$Rb by tuning the natively negative atom-atom scattering length into the positive regime [5]. Part of this experiment involved a sweep of the magnetic field across the Feshbach resonance, resulting in heavy condensate losses (∼80% for the slowest sweep rates). Additional experiments led to the observation of collapsing condensates, an event characterized by bursts of atoms emanating from a remnant BEC, and coined “bosenova” for the analogy with a supernova explosion [8]. More recently, experiments with pulsed magnetic fields that come close to, but do not cross, the Feshbach-resonance [1] and photoassociation [2,3] lie in both processes being described, in terms of second quantization, as destroying two atoms and creating a molecule. We therefore model a quantum degenerate gas of atoms coupled via a Feshbach resonance to a condensate of quasibound molecules based on Refs. [3,3]. The initial atoms are denoted by the boson field $\phi(r,t)$, and the quasibound molecules by the field $\psi(r,t)$. The Hamiltonian density for this system is

$$\frac{\mathcal{H}}{\hbar} = \phi^\dagger \left( \frac{-\hbar^2}{2m} \nabla^2 + \delta_0 \right) \phi + \psi^\dagger \left( \frac{-\hbar^2}{4m} \nabla^2 + \delta_0 \right) \psi - \frac{\Omega}{2\sqrt{\rho}} [\psi^\dagger \phi \phi^\dagger + \psi^\dagger \phi \phi^\dagger \psi],$$

(1)

$$\Omega = \lim_{\epsilon \to 0} \sqrt{2\pi \hbar^{3/2} \rho \Gamma(\epsilon)} \sqrt{\frac{\beta}{\epsilon}},$$

(2)

where $m = 2\mu$ is the mass of an atom, $\hbar \delta_0$ is the energy difference between a molecule and two atoms, $\rho$ is an invariant density equal to the sum of atom density and twice the molecular density, and $\Gamma(\epsilon)$ is the dissociation rate for a molecule with the energy $\epsilon$ above the threshold of the Feshbach resonance.

Switching to momentum space, only zero-momentum atomic and molecular condensate modes are retained, represented by the respective $c$-number amplitudes $\alpha$ and $\beta$. We also take into account correlated pairs of noncondensate atoms using a complex amplitude $C(\epsilon)$, which...
represent pairs of noncondensate atoms in the manner of the Heisenberg picture expectation value \( \langle a_p^\dagger a_{-p} \rangle \), with \( \hbar \) being the relative energy of the atoms. The normalization of our mean fields is such that \( |\alpha|^2 + |\beta|^2 + \int d\epsilon |C(\epsilon)|^2 = 1 \). We work from the Heisenberg equation of motion of the boson operators under the simplifying assumption that the noncondensate atoms pairs are only allowed to couple back to the molecular condensate, ignoring the possibility that noncondensate atoms associate to make noncondensate molecules. This neglect is justified to the extent that Bose enhancement favors transitions back to the molecular condensate. The final mean-field equations are

\[
i\dot{\alpha} = -\frac{\Omega}{\sqrt{2}} \alpha^* \beta, \tag{3a}\]

\[
i\dot{\beta} = \delta_0 \beta - \frac{\Omega}{\sqrt{2}} \alpha \dot{\alpha} - \frac{\xi}{\sqrt{2\pi}} \int d\epsilon \sqrt{\epsilon} C(\epsilon), \tag{3b}\]

\[
i\dot{C}(\epsilon) = \epsilon C(\epsilon) - \frac{\xi}{\sqrt{2\pi}} \sqrt{\epsilon} \beta. \tag{3c}\]

The analog of the Rabi frequency for the rogue modes \( \xi \) is inferred using Fermi Golden rule, which gives the dissociation rate for a positive-energy molecule as

\[
\Gamma(\epsilon) = \sqrt{\epsilon} \xi^2. \tag{4}\]

Next the problem is reformulated in terms of two key parameters with the dimension of frequency. The density-dependent frequency

\[
\omega_\rho = \frac{\hbar \rho^{2/3}}{m}, \tag{5}\]

has been identified before, along with the operational significance that, once \( \Omega \gtrsim \omega_\rho \), rogue dissociation is expected to be a dominant factor in the dynamics \[3\] . Here it is convenient to define another primary parameter with the dimension of frequency. Considering on-shell dissociation of molecules to atoms with the relative energy \( \epsilon \), the Wigner threshold law delivers a dissociation rate \( \Gamma(\epsilon) \) such that \( \Gamma(\epsilon)/\sqrt{\epsilon} \) converges to a finite limit for \( \epsilon \to 0 \); hence, we define

\[
\Xi = \left( \lim_{\epsilon \to 0} \frac{\Gamma(\epsilon)}{2\sqrt{\epsilon}} \right)^2, \tag{6}\]

which indeed has the dimension of frequency. Comparison of Eqs. \[3\], \[4\], \[5\] and \[6\] gives the parameters in the mean-field equations as

\[
\Omega = 2^{3/2} \sqrt{\pi} \Xi^{1/4} \omega_\rho^{3/4}, \quad \xi = \sqrt{2} \Xi^{1/4}. \tag{7}\]

**Renormalization**—When the coupling to the continuum of noncondensate atom pairs is included, the continuum shifts the molecular state \[13\]. As explained before \[3\], and will be discussed in more detail below, we have taken the dominant state pushing into account in our calculations. However, there is a relevant residual effect to consider.

To begin with, consider the equation of motion for the molecular amplitude, including the coupling to noncondensate atom pairs but not to the atomic condensate [set \( \Omega = 0 \) in Eqs. \[3\]]. Again, the particular energy dependence of the coupling comes from the Wigner threshold law, which is here assumed to be valid for all relevant energies; but, as is necessary in the numerical calculations anyway, we cut off the coupling between molecules and atom pairs at some frequency \( \epsilon_M \). The question of renormalization is the question of the dependence of the results on the cutoff \( \epsilon_M \).

Equations \[3\] (with \( \Omega = 0 \)) are easy to solve using, say, the Fourier transformation. With the initial condition that \( \beta(t = 0) = 1 \), for positive times the solution has the Fourier transform

\[
\beta(\omega) = \frac{i}{\omega + i\eta - \delta_0 - \Sigma(\omega)}, \tag{8}\]

where the self-energy is

\[
\Sigma(\omega) = \frac{\xi^2}{2\pi} \int_0^{\epsilon_M} d\epsilon \frac{\sqrt{\epsilon}}{\omega + i\eta - \epsilon}, \tag{9}\]

and \( \eta = 0^+ \). Now, a real pole of \( \beta(\omega) \) corresponds to a true stationary state of the Hamiltonian. It turns out that for suitable detunings there is a real pole \( \omega \leq 0 \), which obviously corresponds to the coupling-renormalized energy of the molecules.

Assuming that the value of \( \omega \) is negative, the integral \[8\] is carried out easily and the equation giving the pole becomes

\[
\omega - \left( \delta_0 - \frac{\sqrt{\Xi} \epsilon_M}{\pi} \right) - \frac{2}{\pi} \sqrt{-\omega} \Xi \arctan \left[ \frac{\sqrt{\epsilon_M}}{\sqrt{-\omega}} \right] = 0. \tag{10}\]

The term involving the detuning is the main contribution to the renormalization. As we have done before in our numerical calculations \[3\], we choose the bare detuning \( \delta_0 \) so that, for the given energy cutoff \( \epsilon_M \), the renormalized detuning \( \delta_0 - \sqrt{\Xi} \epsilon_M/\pi \) attains the desired value. Hereafter we use the symbol \( \delta \) for the renormalized detuning. This is the parameter that is varied by changing the laser frequency in photoassociation, or the magnetic field in the Feshbach resonance. We carry out the rest of the renormalization by setting \( \epsilon_M \to \infty \). We find the equation giving the characteristic frequency corresponding to the molecules as \( \omega - \delta - \sqrt{-\omega} \Xi = 0 \). The proper solution is

\[
\omega = \delta + \frac{1}{2} \sqrt{\Xi} \left( \sqrt{-\delta - 4\epsilon_M} - \sqrt{\Xi} \right), \tag{11}\]

which is valid for all negative detunings and gives the characteristic frequency of the molecule. Nevertheless, complete diagonalization of the problem (with \( \Omega = 0 \)) shows that the mode evolving at this frequency is not the original or “bare” molecules, but a coherent superposition of molecules and noncondensate atoms pairs.
Numerical procedures– The mean-field equations are integrated using the norm-preserving predictor-corrector algorithm described in Ref. Magnetic fields are converted to detunings according to \( \hbar \delta = 2 \mu_B (B_0 - B) \), where the position of the Feshbach resonance is \( B_0 = 154.9 \) G, and where the difference in magnetic moments between bound molecules and free atom pairs, \( \Delta \mu \approx 2 \mu_B \) (where \( \mu_B \) is the Bohr magneton), is borrowed from \(^{87}\text{Rb}\). Compared to the ensuing detunings \( \delta \), the interactions energies between the atoms due to the background scattering length \( a = 23.8 \) nm are immaterial. We therefore ignore atom-atom interactions unrelated to the Feshbach resonance, as well as the (unknown) atom-molecule and molecule-molecule interactions.

We have used a number of different methods to estimate the parameter \( \Xi \), all giving similar values. The present argument goes as follows. One of the experiments in Ref. gives the characteristic frequency (presumably) of molecules, \( \omega = -2.07 \times 10^5 \) s\(^{-1}\), at the magnetic field \( B = 159.69 \) G corresponding to the detuning \( \delta = -8.42 \times 10^7 \) s\(^{-1}\). Solving from Eq. (1), we have \( \Xi = 5.29 \times 10^8 \) s\(^{-1}\), and thus \( \zeta = 381 \) s\(^{-1}\). It should be noted that, while our rogue-dissociation coupling can be shown to give the correct atom-atom scattering theory close to the resonance (\( \delta \to 0 \)), Eq. (1) will not correctly reproduce the molecular energy on the side of large magnetic fields in Fig. 5 of Ref. (1). Passable agreement could be reached by treating the energy cutoff \( \epsilon_M \) as a variable finite parameter; unfortunately, the abrupt cutoff at \( \epsilon_M \) introduces physical and numerical artifacts, which need to be cleaned up via a judicious energy dependence of the coupling. For example, the entire experimental range of magnetic fields can be fit by multiplying the original coupling by an exponential [\( e^{-\epsilon/\epsilon_M} \)] or rational [\( e^{2\epsilon_M/\epsilon + \epsilon_M^2} \)] cutoff. As our aims are strictly qualitative, we discuss these details elsewhere.

Results– We begin with the Cornish et al. experiments implementing a sweep of the magnetic field across the Feshbach resonance, which is of course a version of the age-old Landau-Zener problem. Although a sweep of the detuning \( \delta \) from above to below threshold at a rate slow compared to the condensate coupling \( \Omega \) will move the system adiabatically from all atoms to all molecules, rogue dissociation will override coherent atom-molecule conversion when \( \Omega \lesssim \omega_{\rho} \). Nevertheless, the JILA experiments sweep from below to above threshold, for a density \( \rho = 1 \times 10^{12} \) cm\(^{-3}\) the condensate coupling is \( \Omega = 1.93 \times 10^5 \) s\(^{-1}\) \( \approx 250 \omega_{\rho} \), and so rogue dissociation should seriously dominate. This is indeed the case (see Fig. 4). Apparently, coherent conversion occurs not between atomic and molecular BEC, but between atomic BEC and dissociated atom pairs. Holding this thought, we conclude that mean-field theory indicates rogue dissociation as a primary sink of atoms in the Ref. sweeps across the Feshbach resonance.

Next we consider the experiments of Claussen et al., for which nontrivial electromagnetic coil technology was developed to create trapezoidal magnetic field pulses that bring the system near— but not across— resonance, hold for a given amount of time, and return to the original field value. Neglecting the burst, these remnant-focused experiments revealed a contradiction with the conventional understanding of condensate loss: rather than a loss that increased monotonically with increasing interaction time, the results indicated a loss that increased with decreasing interaction time, until very short times were reached. The present mean-field approach works similarly, as shown in Fig. 2. Our interpretation is that adiabaticity is again at play. At very short pulse durations, increasing interaction time leads to increasing condensate loss, as expected. In contrast, as the time dependence of the pulse gets slower, the system eventually follows the pulse adiabatically, and returns close to the initial condensate state when the pulse has passed.

Finally, we turn to the experiments performed by Donley et al., in which two trapezoidal pulses were applied to a \(^{85}\text{Rb}\) condensate, and the fraction of remnant and burst atoms measured for a variable between-pulse time and magnetic-field amplitude. These experiments revealed coherent remnant-burst oscillations with amplitudes of up to \( \sim 25\% \). As it happens, we have recently predicted coherent oscillations between atoms and dissociated atom pairs in a rogue-dominated system, although we harbored doubts regarding any practical realization. Casting these doubts aside, we consider a time dependent detuning (magnetic field) in essence lifted from Fig. 2 of Ref. [Fig. 3(a)], and determine the fraction of remnant condensate atoms, noncondensate atoms, and molecules at the end of the pulse sequence as a function of the holding time between the two pulses [Fig. 3(b)]. Oscillations are seen with the amplitude of about \( 15\% \) between condensate and noncondensate atoms at the frequency of the molecular state corresponding to the magnetic field during the holding period. The molecular fraction appears too small to account for the amplitude of the oscillations. In fact, what we termed molecular frequency is the characteristic frequency of a coherent superposition of molecules and noncondensate atom pair. Here the oscillations, directly comparable to Fig. 4(a) in Ref. , are Ramsey fringes in the evolution between an atomic condensate and a molecular condensate dressed with noncondensate atom pairs.

Although our rogue-dissociation ideas provide a neat qualitative explanation for the three experiments we have discussed, in all fairness it must be noted that we have fallen short of a full quantitative agreement. It appears that our model is missing a so far unidentified additional loss mechanism for the condensate atoms.

Conclusions– We have demonstrated that a minimal mean-field model is sufficient to qualitatively explain a number of puzzling results in Feshbach-resonant systems. On the whole, collapsing-condensate physics is therefore understood as a matter of rogue dissociation, which leads to strong losses in the threshold neighborhood, decreased remnant fraction for decreasing interaction time—until
very short times are reached, and coherent remnant-burst oscillations. Furthermore, although atom-molecule coherence has no doubt been achieved [1], the amplitude of the remnant-burst oscillations need not be indicative of the number of condensate molecules present. Ironically, the strength of the Feshbach resonance has led to a regime dominated by rogue dissociation, which tends to counteract the production of a molecular condensate.

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FIG. 1. (a) Experimental ( ) and theoretical ( o) atom loss incurred in sweeping an \(^{85}\text{Rb}\) BEC across the Feshbach resonance, where the magnetic field is swept in a linear fashion from \(B_i = 162\) G to \(B_f = 132\) G. In each numerical run, the fraction of molecular condensate is \(\sim 10^{-6}\). (b) Results for \(\dot{B}^{-1} = 100\ \mu s/G\) are typical, and suggest that the system undergoes collective adiabatic following from BEC to dissociated atom pairs.

FIG. 2. Theory of a magnetic field pulse applied to a \(^{85}\text{Rb}\) condensate for \(\rho = 1.9 \times 10^{13}\ \text{cm}^{-3}\) and \(\Omega = 8.42 \times 10^3\ \text{s}^{-1}\). (a) Remnant fraction versus detuning (magnetic field) rise time. (b-d) Results for a pulse with 150 \(\mu s\) rise time indicate adiabatic passage of BEC atoms to and from dissociated atom pairs. The minimum in panel (a), similar to Ref. [4], occurs at the onset of adiabaticity.
FIG. 3. Simulation of the Ref. [10] experiments for a density \( \rho = 5.4 \times 10^{13} \text{ cm}^{-3} \) and \( \Omega = 1.42 \times 10^6 \text{ s}^{-1} \). (a) Time dependence of the detuning, and (b) the fraction of atoms in the remnant condensate (solid line), in noncondensate atoms pairs (dashed line) and in the molecular condensate (short-dashed line) after the pulse sequence as a function of the hold time \( t_h \) between the two trapezoidal pulses. The frequency of the oscillations is compatible with the prediction from Eq. (11), identifying these oscillations as Ramsey fringes in the transition between the atomic condensate and a molecular condensate dressed by noncondensate atom pairs.