

Will be published:
Phys. Rev. A 71, 063603 (2005)

Sweeping a molecular Bose-Einstein condensate across a Feshbach resonance.

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(Dated: November 7, 2007)

We consider the dissociation of a molecular Bose-Einstein condensate during a magnetic-field sweep through a Feshbach resonance that starts on the molecular side of the resonance and ends on the atomic side. In particular, we determine the energy distribution of the atoms produced after the sweep. We find that the shape of the energy distribution strongly depends on the rate of the magnetic-field sweep, in a manner that is in good agreement with recent experiments.

Introduction. — Feshbach resonances have established themselves as one of the most important tools in the area of ultracold atomic gases [1]. These resonances provide the opportunity to make use of an applied magnetic field to tune the interactions between the atoms, essentially by changing the energy of a diatomic molecular state from a region where the molecules are more stable to a region where the atoms are more stable. For bosonic atoms, Feshbach resonances allow for coherent oscillations between atomic and molecular Bose-Einstein condensates [2]. Moreover, in a Fermi gas these Feshbach resonances recently have made a novel BCS-BEC crossover phenomenon accessible to experiments [3–7].

In this Letter, we study the response of a spatially uniform molecular condensate to a magnetic-field sweep across a Feshbach resonance. The essential physics of the nonequilibrium dissociation of the molecules is the same for bosonic and fermionic atoms, except for the feedback effects arising from the atomic statistics. We show that under appropriate conditions these feedback effects can be neglected, and in that case our results are equally valid for fermionic and bosonic atoms.

We focus in particular on two quantities. First, we develop a method for determining the decay of the molecular condensate during the sweep. Second, we investigate for different kinds of sweeps the resulting energy spectrum of the dissociated atoms, which turns out to be closely related to the time evolution of the molecular condensate. Our approach to the time evolution is based on the equation of motion for the molecular condensate wave function $\phi_m(t)$, developed by Duine and Stoof [1, 8]. While no experiment has yet probed the molecular dissociation as a function of time, the decay of the molecular condensate density is in principle experimentally accessible by a series of destructive measurements.

Measurements of atomic energies after a dissociation ramp have been performed recently by Mukaiyama *et al.* [9] and by Dürr *et al.* [10]. The ramps of Ref. [9] are restricted to cases where all the molecules dissociate during the sweep. The shape of the dissociation spectrum for this type of sweep is well described by an analytical expression, derived by Mukaiyama *et al.* [9] and also by Göral *et al.* [11]. For such a relatively slow type of ramp, our calculated spectra agree with this analytical

form as well. In Ref. [10] also a different, more rapid, type of sweep experiment is reported, in which most of the dissociation occurs *after* the sweep is over. As a result there is now a sharp peak in the atomic energy distribution corresponding to half the molecular energy at the end of the sweep. These spectra are not described by the above mentioned analytical result. Our approach, however, allows us to calculate also the spectra for such fast sweeps.

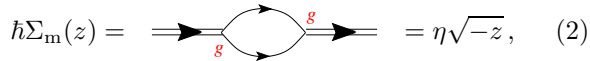
Both these sweep experiments involve bosonic atoms, in particular ^{23}Na and ^{87}Rb , respectively. An additional motivation for investigating sweeps in the molecule-to-atom direction comes from considerations related to the cooling of fermionic atoms such as ^6Li and ^{40}K . To avoid the problems due to Fermi statistics, one proposal is to first cool diatomic molecules to Bose-Einstein condensation, and then to slowly sweep the system across the resonance to the atomic side. However, the effect of the sweep rate on the resulting temperature of the atomic gas is not well-understood at present. It is, therefore, important to study the dissociation process and the spectrum during a sweep across a Feshbach resonance in some detail.

Generalized Gross-Pitaevskii equation. — A Feshbach resonance is characterized by its magnetic field location B_0 , its width ΔB , the background scattering length a_{bg} , and the magnetic-moment difference $\Delta\mu$ between two atoms and the bare molecule associated with the Feshbach resonance. Assuming that these quantities are for the atomic gas of interest known from experiment, the equation of motion for the bare molecular condensate wave function $\phi_m(t)$ becomes [1]

$$i\hbar\partial_t\phi_m(t) = \left[\delta(t) - i\eta\sqrt{i\hbar\partial_t}\right]\phi_m(t), \quad (1)$$

where $\delta(t) = \Delta\mu(B(t) - B_0)$ is the so-called detuning that is time dependent during the sweep. The imaginary term in this equation of motion describes the decay of molecules into pairs of atoms and is determined in the Bose case by the quantity $\eta = m^{1/2}a_{\text{bg}}\Delta B\Delta\mu/\hbar = m^{3/2}g^2/2\pi\hbar^3$, where g is the atom-molecule coupling. When the atoms are fermionic, the right-hand side is a factor of two smaller. Note that η^2 has the units of energy and physically quantifies the width of the resonance.

The imaginary term arises from the molecular self energy



$$\hbar\Sigma_m(z) = \text{diagram} = \eta\sqrt{-z}, \quad (2)$$

where the single and double lines represent atomic and molecular propagators, respectively. The square root of energy reflects the three-dimensional final density of states expected from a Fermi's Golden Rule calculation of the dissociation process. The $\sqrt{i\hbar\partial_t}$ form in Eq. (1) arises from evaluating the complex self energy in Eq. (2) from above on the real axis.

The above self energy leads physically to a dressing of the molecules and as a result to a molecular density of states that for negative detuning contains a delta function with weight $Z = (1 + \eta/2\sqrt{|\epsilon_m|})^{-1}$ at the dressed molecular binding energy $\epsilon_m(\delta) = \delta - \eta^2/2 + \eta\sqrt{\eta^2/4 - \delta}$ [1]. Since the wave function ϕ_m appearing in Eq. (1) represents the condensate wave function for bare molecules, the dressed molecular density is a factor Z^{-1} larger than the bare molecular density and equal to $|\phi_m|^2/Z$. Moreover, the bare molecular density can now change in two ways. Coherent changes involve a shift in the linear superposition making up the dressed molecular wave function, i.e., a change of the bare molecular fraction Z , while the dressed molecular density remains constant [1, 2]. Incoherent changes are associated with the break-up of the dressed molecule itself.

The generalized Gross-Pitaevskii equation in Eq. (1) involves some approximations. First, we are considering sufficiently low molecular densities that the molecule-molecule interactions can be neglected for most of the sweep duration, which is justified for the experiments of interest to us. Second, we are not including the effect of the thermal part of the molecular gas. This is justified for sufficiently low temperatures. Most importantly, we are neglecting feedback effects, i.e., the dynamics and statistics of the atoms that are formed during and after the sweep. In particular, we do not allow for their re-association. The neglect of atomic statistics, i.e., Bose enhancement or Pauli blocking, is reasonable for monotonic sweeps, because the dissociation then always occurs at different energies. In that case we can estimate that the atomic statistics can be absolutely neglected if the molecular density obeys $n_m < \hbar\dot{\delta}/\sqrt{2}\pi^2g^2$. Not surprisingly, this approximation is better for faster ramps, and worst for a constant positive detuning.

We now outline the method of solving Eq. (1), given a particular time-dependent detuning $\delta(t)$. We are especially interested in magnetic-field sweeps across the resonance that take the detuning δ from some negative value δ_i at $t = 0$ to the final positive value δ_f at time $t = T$. Introducing an auxiliary constant detuning δ_c , we can write

$$[i\hbar\partial_t + i\eta\sqrt{i\hbar\partial_t} - \delta_c] \phi_m(t) = [\delta(t) - \delta_c] \phi_m(t). \quad (3)$$

The solution of this differential equation is the sum of a particular solution and the solution of the corresponding homogeneous equation. We thus have

$$\phi_m(t) = \psi(t) + \int_{-\infty}^t dt' G(t-t') [\delta(t') - \delta_c] \phi_m(t'). \quad (4)$$

Here $G(t)$ is the Green's function for the operator acting on $\phi_m(t)$ in the left-hand side of Eq. (3), i.e.,

$$G(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\hbar\omega^+ - \eta\sqrt{-\hbar\omega^+} - \delta_c}, \quad (5)$$

where $\hbar\omega^+ = \hbar\omega + i0$. The real part of the pole in $G(\omega)$ gives the molecular energy and the imaginary part gives the dissociation rate, both at the detuning δ_c . Moreover, $\psi(t)$ is the solution of the homogeneous equation of Eq. (3). For $\delta_c < 0$, the solution is an oscillatory function, $\psi(t) \propto e^{-i\omega_c t/\hbar}$, with a frequency determined by the molecular binding energy corresponding to the detuning δ_c , i.e., $\hbar\omega_c = \epsilon_m(\delta_c)$. In the following we use $\delta_c = \delta_i$, because the integral in Eq. (4) then has a lower limit of 0 instead of $-\infty$.

The retarded Green's function $G(t)$ is calculated by closing the contour in the negative half-plane. The integrand has a branch cut because of the square root in the energy denominator. For $\delta_c < 0$, there is also a pole at ϵ_m . Taking these into account we obtain

$$G(t) = \theta(t) \left[-\frac{i\eta}{\pi} \int_0^{\infty} d\omega \frac{\sqrt{\hbar\omega} e^{-i\omega t}}{(\hbar\omega - \delta_c)^2 + \eta^2\hbar\omega} - \frac{i}{\hbar} e^{-i\omega_c t/\hbar} \frac{2\sqrt{-\hbar\omega_c}}{\eta + 2\sqrt{-\hbar\omega_c}} \right].$$

Having calculated the Green's function $G(t)$ and the wave function $\psi(t)$ corresponding to δ_c , we can numerically solve Eq. (4) for $\phi_m(t)$.

Magnetic field sweeps. — In Fig. 1 we show the decay of the bare molecular wave function $\phi_m(t)$ for a particular ramp that is also shown in the top panel. The center panel shows the oscillatory decay of the real part of $\phi_m(t)$. The imaginary part yields similar qualitative information and is not shown. The dotted background is the nondecaying oscillatory $\phi_m(t)$ for a negative detuning that is held fixed at δ_i . We see that $\phi_m(t)$ for the ramp has a gradually decreasing oscillation frequency, corresponding to the decreasing magnitude of the binding energy $\epsilon_m(\delta)$ as δ approaches zero from the negative side. The bottom panel shows the decay of the bare density $n_m(t) = |\phi_m(t)|^2$. The decay for $\delta(t) < 0$ is mostly coherent, so that the dressed molecule density remains almost fixed. On the other hand, the decay at positive detuning is incoherent, and the decay of the bare density $n_m(t)$ corresponds to the decay of dressed molecules.

The ramp in the experiment of Mukaiyama *et al.* [9] involves an initial and final detuning $\delta_{i,f}$ of about $\mp 50\eta^2$,

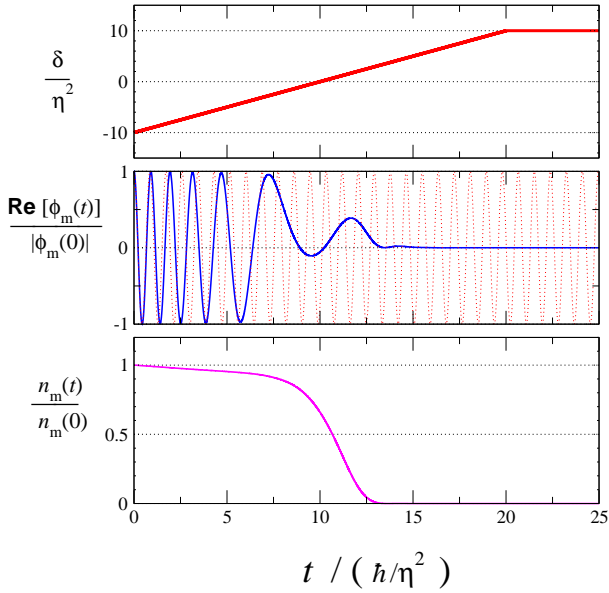


FIG. 1: Decay of the molecular wave function $\phi_m(t)/|\phi_m(0)|$ with time, when the detuning changes linearly with time from $\delta_i = -10\eta^2$ to $\delta_f = +10\eta^2$ as shown in the top panel. The center panel shows the real part of $\phi_m(t)$. The bottom panel shows the decay of the molecular density, $n_m(t)/n_m(0) = |\phi_m(t)|^2/|\phi_m(0)|^2$.

and ramp times of $T \gtrsim 100\hbar/\eta^2$. For the results shown in Fig. 1, we used smaller values for both, so as to have fewer oscillations to visualize.

We now outline how the incoherent dissociation spectrum is obtained, once $\phi_m(t)$ has been calculated. We calculate the time derivative of the molecular density from the equation of motion in Eq. (1). Not surprisingly, only positive frequencies contribute, because the molecules are stable for negative energies. We obtain

$$\int_{-\infty}^{\infty} dt \dot{n}_m \Big|_{\text{incoh}} = -\frac{\eta}{\pi\hbar} \int_0^{\infty} d\omega \sqrt{\hbar\omega} |\phi_m(\omega)|^2, \quad (6)$$

where $\phi_m(\omega)$ is the Fourier transform of $\phi_m(t)$. The integrand in the right-hand side is interpreted as the molecular dissociation spectrum $f_{\text{mol}}(\epsilon) = \eta\sqrt{\epsilon} |\phi_m(\epsilon)|^2 / \pi\hbar$. Since each atom has half the energy of the dissociating molecule, $f_{\text{mol}}(\epsilon)$ corresponds to the atomic spectrum at $\epsilon/2$, i.e., $f_{\text{at}}(\epsilon) = 4f_{\text{mol}}(2\epsilon)$. The additional factor of 2 is because each molecule gives rise to two atoms.

Before presenting results for the spectrum, we briefly discuss the analytical result mentioned previously [9, 11]. This result can be derived by assuming that for a particular detuning, each decaying molecule has a sharply defined energy. This means that the width of the molecular spectral function is neglected. Moreover, it is implicitly assumed that all the molecules are dissociated before the sweep is over. If we denote by $n_m(\epsilon)$ the density of molecules at energy ϵ and use $dt = d\epsilon/\dot{\epsilon} \simeq d\epsilon/\dot{\delta}$, we have

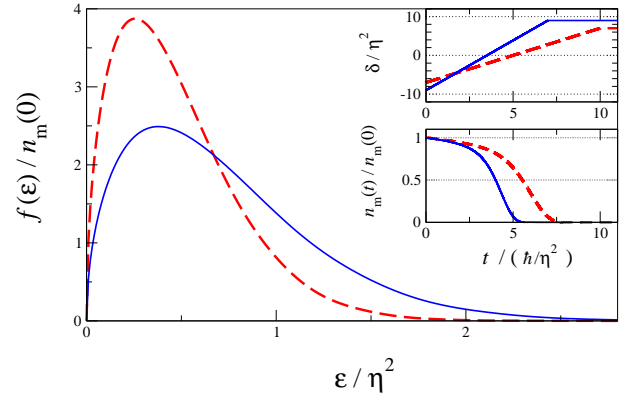


FIG. 2: Spectra for cases where the analytic derivation is valid, because the molecules decay almost completely before the sweep is over. Insets show the detuning ramps with different ramp rates, and the bare molecular condensate densities.

$n_m(\epsilon + d\epsilon) - n_m(\epsilon) = -(2\eta\sqrt{\epsilon}/\hbar\dot{\delta})n_m(\epsilon)d\epsilon$. Solving for $n_m(\epsilon)$, the molecular dissociation spectrum follows then from $f_{\text{mol}} = dn_m(\epsilon)/d\epsilon$. The atomic energy spectrum f_{at} can be deduced from f_{mol} as before with the result

$$f_{\text{at}}(\epsilon) = n_m(0) \frac{8\eta\sqrt{2\epsilon}}{\hbar\dot{\delta}} \exp\left[-\frac{4\eta(2\epsilon)^{3/2}}{3\hbar\dot{\delta}}\right]. \quad (7)$$

We stress that this expression is not a Landau-Zener or adiabatic result. Its derivation does not require the sweep to be slow, although it is required that the sweep continues until all the molecules have dissociated. Moreover, the derivation relies on the approximation $\epsilon \simeq \delta$, which is not accurate at small energies $\epsilon \ll \eta^2$, for which we have that $\epsilon \simeq \delta^2/\eta^2$. In Fig. 2 we show calculated spectra for two cases where the above mentioned conditions holds. The spectra indeed have the exponential form of Eq. (7), however they are in general normalized according to the initial dressed molecular density $n_m(0)/Z_i$ instead of the initial bare molecular density $n_m(0)$. The ramp represented by the solid curves has a higher ramp rate and hence the resulting spectrum is tilted to higher energies. Note that experimentally, only the total atomic energy has been measured as a function of ramp speeds [9, 10]. These measured total energies are fit well by the total energies calculated analytically as $\int d\epsilon \epsilon f_{\text{at}}(\epsilon)$. Since our spectra match the analytic result for the experimentally relevant case of $Z_i \simeq 1$, agreement with the measured total energies follows, and is not shown here.

In Fig. 3 we show spectra calculated for two cases where Eq. (7) does not hold because the sweep is over before all the molecules have decayed. This type of sweep has been employed in a recent experiment [10]. The density images in that experiment indicate that the spectrum is peaked at the energy corresponding to the final detuning. This feature is clear in Fig. 3. The dashed curves represent an infinitely fast ramp. The spectrum shows a

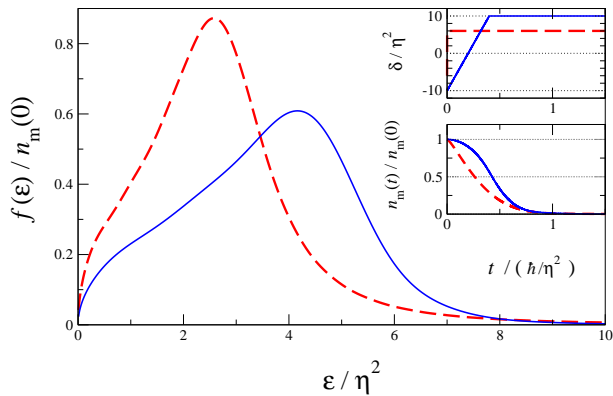


FIG. 3: Spectra for cases where the analytic form is not valid. Dashed curves: Infinitely fast ramp at which the detuning switched from $\delta_i = -6\eta^2$ to $\delta_f = +6\eta^2$ at $t = 0$. Full curves: Fast ramp that is over before all the molecules can decay.

peak around $\delta_f/2$, but is spread over a relatively large range of energies. The spread demonstrates that our method takes into account the distribution of molecular energies, i.e., the width of the molecular density of states at a fixed positive detuning. The solid curves in Fig. 3 represents a ramp that is over before all the molecules have decayed. A significant fraction decays while the detuning is constant at its final value. The atomic spectrum here also shows a peak at an energy around half the final detuning.

In order to demonstrate mainly coherent loss of bare molecules, we display in Fig. 4 a sweep that ends at negative detuning, i.e., before reaching the resonance. The density of bare molecules decreases, but most of this decrease is due to the coherent change of the dressed molecular wave function. The final density n_f is slightly smaller than $(Z_f/Z_i)n_m(0)$, where Z_i and Z_f are the weight of the delta function in the molecular density of states at the initial and the final detuning, respectively. The difference between n_f and $(Z_f/Z_i)n_m(0)$ appears as the total weight of the incoherent spectrum. Note also that the density undergoes some coherent oscillations before settling at its final value. These are internal Josephson oscillations of the dressed molecular condensate.

Conclusions. — We have shown how to calculate the time evolution of the molecular condensate wave function $\phi_m(t)$ during sweeps across a Feshbach resonance. We have also shown how the time dependence of this wave function leads to the dissociation spectrum. Our calculation for the atomic energy spectrum is more general than the result obtained by Mukaiyama *et al.* [9] and by Göral *et al.* [11]. The theory presented here is applicable for ramps of essentially arbitrary shape and initial conditions. This has been demonstrated with the fast ramps, in Fig. 3. Moreover, we have obtained the, in first instance surprising, result that a nonzero dissociation spec-

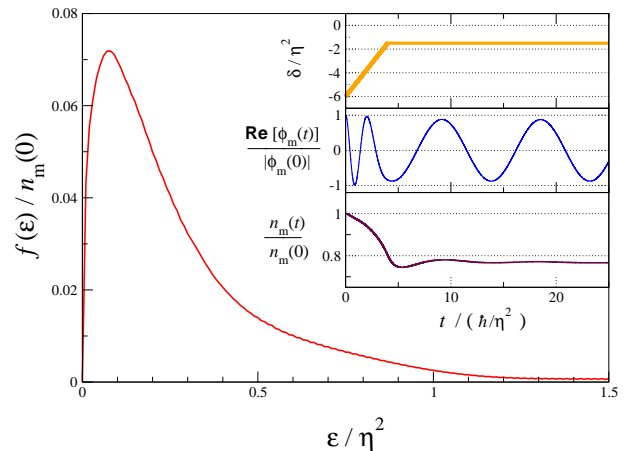


FIG. 4: A sweep that starts and ends at negative detuning. In this case, the final density is expected to be $(Z_f/Z_i)n_m(0) \simeq 0.7775n_m(0)$. The actual final density, $n_f \simeq 0.735n_m(0)$, is smaller, in agreement with the nonzero atomic spectrum.

trum can also be obtained by a changing magnetic field that always remains below the Feshbach resonance.

Finally, we point out two important issues that remain unsolved. First is the problem of incorporating the effect of the atomic statistics. In principle, this can be achieved by coupling the generalized Gross-Pitaevskii equation for the molecular condensate to a quantum Boltzmann equation for the atoms. It remains to be seen, however, if this leads to a feasible approach. Second, our calculation is based on the approximation for the molecular self energy given in Eq. (2). For broad Feshbach resonances, such as the one in ${}^6\text{Li}$ that is widely used at present for the study of the BCS-BEC crossover [4–7], the molecular self energy can no longer be expressed in terms of the η parameter alone, and depends also on the background scattering length a_{bg} [1]. Incorporating this improvement is also left for future work.

We thank Randy Hulet for helpful comments. This work is supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

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