Molecular Bose-Einstein condensates (BEC) have been recently formed in experiments on atomic BEC and on quantum-degenerate Fermi gases. These experiments exploited the effect of Feshbach resonance, present when the energy of an atomic pair is close to the energy of a bound molecular state. The energy mismatch can be controlled by applying an external magnetic field, thanks to the difference between the magnetic momenta of the molecule and of the atomic pair. By varying the magnetic field the energy of the molecular state is forced to cross different states of the atomic pairs, belonging to a discrete spectrum in the case of a trapped gas, or to a continuum otherwise. The resonance value of the magnetic field strength \( B_0 \) corresponds to the crossing of the lowest discrete state, or the lower boundary of the continuum, respectively.

In the experiments the resonances were mostly swept in a backward direction, so that the molecular state crossed the atomic ones downwards. This led to the transfer of population from the lowest atomic state in the case of BEC, or from an energy band in the case of a Fermi gas, to the molecular state, as had been proposed in Ref. 6. Assuming all the atomic population is initially in the BEC state, the backward sweep would have been ideally suitable for forming molecules, were it not for two destabilizing mechanisms. The resonant molecule is generally populated in an excited rovibrational and electronic state, and therefore can be deactivated by inelastic collisions with atoms and other molecules (see Refs. 6, 8, 9). In addition, during the backward sweep some higher-lying non-condensate atomic states can be populated temporarily (by counterintuitive transitions — see Ref. 10), most notably in a strong resonance or at low densities (see Ref. 6). These two effects restrict the efficiency of conversion from the atomic condensate to the molecular one. The non-condensate atoms produced by molecular dissociation are formed as entangled atomic pairs (see Ref. 11). This process cannot be described by mean field (MF) theories. Therefore the analysis of formation of a molecular BEC incorporating both effects requires a non-MF approach in which the damping due to deactivating collisions is incorporated. Such an approach — a generalized parametric approximation (PA) — has been described in Ref. 11, and applied to a Na BEC. The non-MF effects become even more important in forward sweeps. An alternative study of molecular formation described in Ref. 12, using the macroscopic quantum-dynamics approach of Ref. 13, takes into account non-MF effects but not inelastic collisions.

In the \(^{87}\text{Rb} \) experiments a BEC of \( 10^5 \) atoms has been kept initially in a harmonic trap with frequencies \( 2\pi \times (50, 120, 170) \) Hz. The magnetic field ramp was started, following the switching off of the trap, after a pre-expansion interval \( t_p \geq 2 \) ms. This measure allows the reduction of condensate density, and thus improves conversion efficiency (see Ref. 11). The field has been ramped from 1008 G to 1005.2 G with various speeds, passing the 1007.4 G resonance of strength \( \Delta = 0.2 \) G (see Ref. 14), and held for 3 ms. During this time a gradient magnetic field has been applied, leading to a relative motion of the atoms and the molecules due to the difference of magnetic momenta between the molecule and an atomic pair, \( \mu \approx 2.8\mu_B \) (see Ref. 15). Next, the magnetic field was ramped up to 1008 G (in a forward sweep), converting the molecules back to atoms. The reconverted atoms inherit the velocity of the molecules, and thus form a second condensate cloud.

**Association of atoms in an expanding BEC.** The PA approach as used in 11 for a homogeneous gas is inapplicable directly to experiments on traps. However, the MF approach of 8, 9 (which can be easily extended to traps) should suffice for the description of association in the case concerned. This is shown by Fig. 4. It compares the atomic and molecular densities calculated with the PA approach 11 and the MF approach of 8, 9, for an initial atomic density corresponding to the peak density reached at the expansion time of 2.3 ms. The values used for the deactivation rate coefficients are \( k_a = 7 \times 10^{-11} \) cm\(^3\)/s (see Ref. 16) and \( k_m = 5 \times 10^{-11} \) cm\(^3\)/s for atom-molecule and molecule-molecule collisions, respectively. The elastic scattering length is \( a_e = 99 \) atomic units (see Ref. 16). As one can see, already when the magnetic field is 0.3 G below the resonance (in a sweep totaling 2.2 G) the temporary occupation of non-condensate atom states practically vanishes, and the results of the two kinds of calculations coincide. For faster sweeps or...
molecules are formed after the expansion starts when the trap is switched off and the densities decrease substantially.

The expansion of a pure atomic condensate cloud has been considered in Ref. [17]. We generalize this theory here to the case of a hybrid atom-molecule condensate. Let us consider an initial atomic field with a Thomas-Fermi distribution, and a zero molecular field, at \( t < t_0 - t_p \). We can represent the two mean fields in the following form,

\[
\varphi_a (r, t) = A(t) \Phi_a (\rho, t) e^{iS},
\]

\[
\varphi_m (r, t) = A(t) \Phi_m (\rho, t) e^{2iS},
\]

using the scaled coordinates \( \rho_j = r_j/b_j (t) \), \( 1 \leq j \leq 3 \), and a scaling factor \( A(t) = (b_1 (t)b_2 (t)b_3 (t))^{-1/2} \). The scales \( b_j \) obey the set of equations

\[
\dot{b}_j (t) = \omega_j^2 A^2 (t) / b_j (t), b_j (t_0 - t_p) = 1.
\]

The phase in Eq. (2),

\[
S(t) = \frac{m}{\hbar} \sum_{j=1}^{3} |\dot{b}_j (t) - \frac{\epsilon_0}{\hbar} \int_{t_0-t_p}^{t} dt' A^2 (t')|
\]

accumulates most of the contributions of the kinetic energy. Here \( \epsilon_0 = 4\pi\hbar^2 a _a n_0 / m \) is a chemical potential of the atomic BEC and \( n_0 \) is its peak density while the trap is on.

Substitution of Eq. (2) into (1) leads to the following set of coupled equations for the transformed mean fields,

\[
i\dot{\Phi}_a (\rho, t) = \left[ \epsilon_a (t) - i A^2 (t) k_a |\Phi_m (\rho, t)|^2 \right] \Phi_a (\rho, t) + 2A(t) g^* \Phi_m (\rho, t) \Phi_m (\rho, t),
\]

\[
i\dot{\Phi}_m (\rho, t) = -i A^2 (t) \left[ \frac{1}{2} k_m |\Phi_m (\rho, t)|^2 + k_m |\Phi_m (\rho, t)|^2 \right] \Phi_m (\rho, t) + A(t) g \Phi_a^2 (\rho, t).
\]

The residual kinetic energy terms are neglected here for the same reasons as in Ref. [17]. The loss processes and atom-molecule transitions distort \( \Phi_a (\rho, t) \) and \( \Phi_m (\rho, t) \) from the Thomas-Fermi shapes, leading to additional energy shifts compared to the pure atomic case. These shifts, however, are of the order of \( A^2 (t) \epsilon_0 \), and can only lead to a negligible small shift of the resonance (of less than \( 10^{-4} \text{ G} \) in the present case).

Equations (5) have a rather clear physical sense. They describe a ballistic expansion of the atomic and molecular BEC with the same velocity distribution, reducing the densities by the factor \( A^2 (t) \), and leading to a rescaling of the coupling and deactivation parameters. This reflects...
the fact that the acceleration predates the formation of molecules that inherit the velocity of the atoms they are formed from.

The results of a numerical solution of Eq. (5) are shown in Fig. 1. The inhomogeneity and the expansion reduce the atomic density, leading to a slower loss of atoms and molecules. The dependence on the sweep rate is presented in Fig. 2 for two values of $k_a$ (the best fit and upper limit taken from Ref. [16]). The results are in agreement with the experimental data of Ref. [2] reporting that $\sim 7\%$ of atoms are converted to molecules and $\sim 30\%$ remain in the atomic BEC for ramp speeds less than 2 G/ms.

Dissociation of molecules on a forward sweep. Consider now the dissociation of molecules on a forward sweep, when the molecular state crosses the atomic ones upwards. Such a sweep has been used in experiments for detection of molecules. The experiments demonstrate no significant dependence of the reconversion efficiency on the ramp speed. Our calculations using the PA [11] demonstrate that under the experimental conditions all molecules are dissociated except for a small part lost due to deactivating collisions during the sweep. The molecules dissociate to entangled atomic pairs in a wide energy spectrum (see Ref. [11]) characterized by the peak energy $E_{\text{peak}}$. The calculations demonstrate that $E_{\text{peak}}$ increases with the ramp speed (see Fig. 3). The results show no significant dependence on the molecular density, justifying the applicability of the homogeneous density approximation to real inhomogeneous situations. Although the ramp-speed dependence of $E_{\text{peak}}$ is clearly nonlinear, within the interval 0.2 G/ms $< B < 5$ G/ms it can be approximated by a straight line with the slope of 70 nK ms/G, which is close to the experimental value of 60 nK ms/G reported in Ref. [18].

In the present case the dissociation can be described by a simple analytical curve-crossing model based on the approach of Ref. [8]. A molecule dissociates into two entangled atoms, each with an energy $E$, by a crossing occurring at $\mu (B (t) - B_0) = 2E$. In the weak-resonance case, the quantum curve-crossing theory [19] and the semiclassical Landau-Zener theory yield approximately the same result for the crossing probability, i.e., $e^{2\pi \lambda} - 1 \approx 1 - e^{-2\pi \lambda} \approx 2\pi \lambda$, where $\lambda = 8\pi h a_n n_m (t) \Delta / (m|\dot{B}|)$ (see Ref. [11]). Neglecting deactivating collisions the molecular density $n_m (t) = |\gamma_m (t)|^2$ is given by the solution of Eq. (50) in Ref. [9],

$$ n_m (t) = n_m (t_d) \exp \left[ -2a_n \mu \Delta / h^2 \right] \int_{t_d}^{t} dt' \sqrt{m\mu (B (t') - B_0)} , $$

where $t_d$ is the starting time of the dissociation ramp. The resulting energy distribution of the produced atoms is given by

$$ f (E) = \frac{1}{2} \sqrt{E} E_{\text{peak}}^{-3/2} \exp \left[ -\frac{1}{3} (E/E_{\text{peak}})^{3/2} \right] , \quad (6) $$

with

$$ E_{\text{peak}} = \frac{1}{2m} \left( \frac{h^2 m|\dot{B}|}{4a_n \Delta} \right)^{2/3} . \quad (7) $$

This model is in good agreement with the numerical results (see Fig. 4). Similar models have been independently developed in Refs. [4, 12].

Optimized molecular formation on a backward sweep. Figure 1 demonstrates that the molecular population reaches a maximum, corresponding to a conversion efficiency $\sim 50\%$, about 0.1 G below the resonance, and falls by half about 0.5 G below the resonance. The low conversion efficiency observed in experiments 2 is due to collision loss during the long sweep to 2.2 G below the resonance. Although the PA results of Fig. 1 overestimate the loss by neglecting the expansion, the molecular
FIG. 4: Conversion efficiency (a) and the lifetime of the molecular BEC $\tau_n$ (b) at the optimal ramp speed $\langle dB/dt \rangle_{\text{opt}}$, all plotted as functions of the initial atomic density $n_0$, calculated for the resonances at 1007 G (circles) and 685 G (triangles), using the rates of molecule-molecule deactivation $10^{-10}$ for the two rates, respectively. The dotted lines in part (b) demonstrate $\langle dB/dt \rangle_{\text{opt}}$ for the two rates, respectively.

population of the expanding gas falls by half on reaching 2.2 G. Under the conditions of the experiments the lifetime of the molecules formed is about 0.5 ms, too short for an effective detection. As in the case of Na (see Ref. [11]), the lifetime and conversion efficiency increase on reducing the initial condensate density. This is demonstrated in Fig. 4 showing results of calculations using the PA density and the resonance strength (see Fig. 4). The optimal ramp speed $\langle dB/dt \rangle_{\text{opt}}$ for the two rates, respectively.

As in the case of Na studied in Ref. [11], the conversion efficiency is determined by a concurrence of three processes: the association of the atomic BEC and the two loss processes — the dissociation of the molecular BEC onto non-condensate atoms and the deactivation by inelastic collisions. A reduction of the ramp speed enhances all three processes. The calculations of Ref. [12], taking no account of the inelastic collisions, result in a monotonic increase of the conversion efficiency with a decrease of the ramp speed. The inelastic collisions, however, tend to reduce the conversion efficiency at slow ramp speeds (see Fig. 4), as has also been demonstrated in Ref. [11]. The optimal ramp speed increases with the density and the resonance strength (see Fig. 4).

Conclusions. The experiments on formation of molecules from a $^{87}$Rb BEC due to a Feshbach resonance can be described by a MF theory of expanding atom-molecule BEC. Non-MF calculations using the PA describe the energy of non-condensate atoms formed by molecular dissociation in a forward sweep and can predict optimal conditions for the formation of a molecular BEC in a backward sweep.

[1] J. Herbig et al., Science 301, 1510 (2003).
[2] S. Dürr, T. Volz, A. Marte, and G. Rempe, Phys. Rev. Lett. 92, 020406 (2004).
[3] K. Xu et al., Phys. Rev. Lett. 91, 210402 (2003).
[4] T. Mukaiyama et al., cond-mat/0311558 (2003).
[5] C. A. Regal, C. Ticknor, J. L. Bohn, and D. S. Jin, Nature 424, 47 (2003); K. E. Strecker, G. B. Partridge, and R. G. Hulet, Phys. Rev. Lett. 91, 080406 (2003); J. Cubizolles et al., Phys. Rev. Lett. 91, 240401 (2003); S. Jochim et al., Phys. Rev. Lett. 91, 240402 (2003); M. W. Zwierlein et al., Phys. Rev. Lett. 91, 250401 (2003).
[6] E. Timmermans, P. Tommasini, M. Hussein, and A. Kerman, Phys. Rep. 315, 199 (1999).
[7] F. H. Mies, E. Tiesinga, and P. S. Julienne, Phys. Rev. A 61, 022721 (2000).
[8] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne and C. J. Williams, Phys. Rev. A 60, R765 (1999).
[9] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne and C. J. Williams, Phys. Rev. A 62, 043605 (2000).
[10] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne, and Y. B. Band, J. Phys. B 32, 1845 (1999); V. A. Yurovsky and A. Ben-Reuven, Phys. Rev. A 63, 043404 (2001).
[11] V. A. Yurovsky and A. Ben-Reuven, Phys. Rev. A 67, 043611 (2003).
[12] K. Góral et al., cond-mat/0312178.
[13] T. Köhler, T. Gasenzer and K. Burnett, Phys. Rev. A 67, 013601 (2003).
[14] T. Volz et al., Phys. Rev. A 68, 010702(R) (2003).
[15] A. Marte et al., Phys. Rev. Lett. 89, 283202 (2002).
[16] V. A. Yurovsky and A. Ben-Reuven, Phys. Rev. A 67, 050701(R) (2003).

[17] Yu. Kagan, E. L. Surkov and G. V. Shlyapnikov, Phys. Rev. A 54, R1753 (1996); Y. Castin and R. Dum, Phys. Rev. Lett. 77, 5315 (1996).

[18] S. Dürr, presentation at EURESCO conference on BEC (Spain, 2003).

[19] V. A. Yurovsky, A. Ben-Reuven, and P. S. Julienne, Phys. Rev. A 65, 043607 (2002).