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Ultracold Polar Molecules

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This work focused primarily on formation of ultracold 87RbCs molecules in their rovibrational ground state by magnetoassociation followed by STIRAP, resulting in 14 papers acknowledging EOARD/AFOSR support (4 in PRL). RbCs was only the second ultracold polar molecule to be produced worldwide. Production of 87RbCs is difficult because large positive scattering lengths make clouds difficult to overlap (but 85RbCs looked promising), but 85RbCs is difficult because 85Rb is hard to produce at high densities. We revealed broad Feshbach resonances that we hope will allow production of higher-density 85Rb clouds. We are now attempting to achieve the next step, formation of 85RbCs molecules.

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Final Report on Grant FA8655-10-1-3033 on Ultracold Polar Molecules

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The EOARD grant to the University of Durham supported work associated with the AFOSR MURI on *Ultracold polar molecules: new phases of matter for quantum information and quantum control.* The Durham grant paid the salary of a half-time postdoctoral researcher, Dr. Ruth LeSueur, and associated consumables costs. It also provided travel costs for collaboration with other members of the MURI team, notably the PI, Prof. Paul S. Julienne.

Our work under this project focussed mostly on the formation of ultracold RbCs molecules in their rovibrational ground state from their constituent atoms, by magnetoassociation followed by STIRAP. At the start of the project, all that had been done was that the Innsbruck experimental group (under Hanns-Christoph Nägerl and Rudi Grimm) had measured a Feshbach resonance spectrum for ^{87}Rb + Cs mixtures, identifying a set of magnetic fields at which resonances occurred. However, the spectrum was completely unassigned. Over the course of the project we provided the theoretical work that enabled both the Innsbruck group and the Durham experimental group (under Simon Cornish) to produce and manipulate RbCs Feshbach molecules and to transfer them to their absolute ground state. RbCs was only the second ultracold polar molecule to be produced.

Overall, the project resulted in 14 papers that acknowledged EOARD/AFOSR support, including 4 in Physical Review Letters.

Early in the project, we obtained a preliminary assignment of the Feshbach resonance spectrum for ^{87}RbCs. We then used this assignment to refine the interaction potential. In collaboration with the group of Eberhard Tiemann (Hannover), we used an iterative procedure to obtain a potential that reproduces both the high-lying states responsible for Feshbach resonances and the deeply-lying states measured by Fourier Transform spectroscopy. This allowed the Innsbruck group to carry out further measurements of the near-threshold levels, which in turn allowed further refinement of the interaction potential. The resulting agreement between experiment and theory is shown in Figure 1. The theoretical results were published in a landmark paper together with the corresponding experiments [1].

We also collaborated extensively with the Durham experimental group, who were also able to produce ^{87}RbCs Feshbach molecules, using a rather different setup. This was again published jointly [2].

The potential model and understanding of the bound states that we obtained allowed both the Innsbruck and Durham group to control the molecules produced by magnetoassociation. In separate collaborations with the two groups, we achieved a major success in producing ultracold ^{87}RbCs molecules in their rovibrational ground state. This was the culmination of a 5-year quest, and RbCs was only the second ultracold polar molecule to be produced worldwide. These results were published in two high-profile joint papers in 2014 [3, 4].

One difficulty that limits the efficiency of ^{87}RbCs molecule formation is that the interspecies scattering length is large and positive, and this makes clouds of ^{87}Rb and Cs hard to overlap. We therefore investigated ^{85}RbCs, using the potentials we had developed for ^{85}RbCs, and showed that it would not suffer from this problem. The Durham experimental group of Simon Cornish therefore began work on ^{85}RbCs: their results showed Feshbach resonances very close to the magnetic field values we predicted, confirming the accuracy of our potential model. We published a joint experiment/theory paper with them on these results [5]. The key results are shown in Figure 2.

One issue with ^{85}RbCs is that ^{85}Rb is hard to produce at densities high enough for efficient molecule formation. The difficulty is that ^{85}Rb has a large negative scattering length at most magnetic fields, which leads to condensate collapse. However, our studies of ^{85}RbCs also revealed new resonances in ^{85}Rb itself and it turned out that no systematic study of the resonances had been published. We therefore undertook such a study and have published another joint experiment/theory paper on it [6]. This revealed some additional broad Feshbach resonances that we hope will allow the production of higher-density ^{85}Rb clouds.

We are now applying for funding to achieve the next step, which is formation of ultracold ^{85}RbCs molecules by tuning across the Feshbach resonances.

We also collaborated with Prof. Paul Julienne in several other projects that produced high-profile publications:

1. We worked with Selim Jochim's experimental group in Heidelberg [7] to understand high-precision trap-sideband-resolved measurements of the bound states of $^6Li_2$, and used them to produce new potential curves and an improved position for the broad Feshbach resonance in this key benchmark system.

2. We collaborated with the Innsbruck group on a study of Efimov states of the Cs trimer, which reached the startling conclusion that these states exist at energies that are "universal" in the sense that their positions are almost independent of the short-range properties of the system [8]. Chris Greene (Purdue) refers to this as "the bombshell paper" in the field of Efimov physics.

3. We collaborated with the Innsbruck group on a detailed study of the Feshbach resonances and weakly

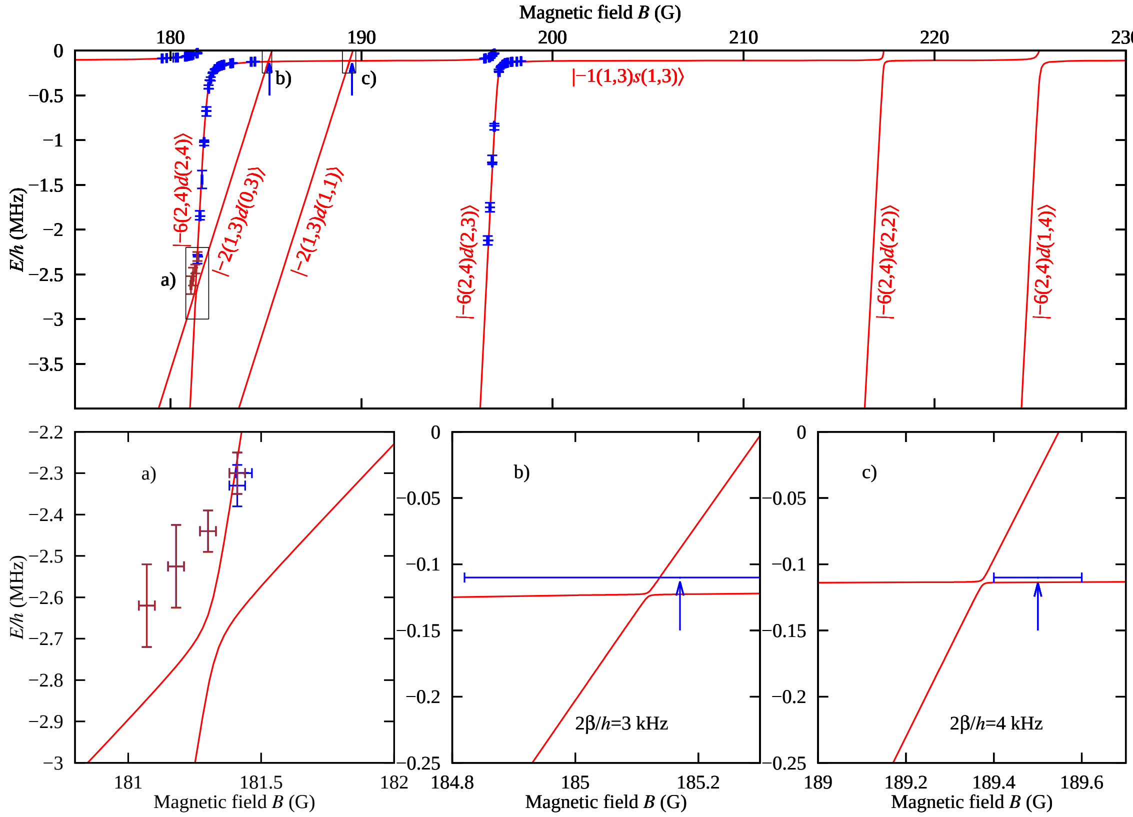

FIG. 1. Bound states of ^{87}RbCs Feshbach molecules in the vicinity of the resonances currently used to produce molecules, with quantum numbers $v(f_{\rm Rb}, f_{\rm Cs})L(m_{\rm Rb}, m_{\rm Cs})$. Calculated energies are shown in red and Innsbruck experiments in blue. The lower three panels show the behavior at avoided crossings. From ref. [1].

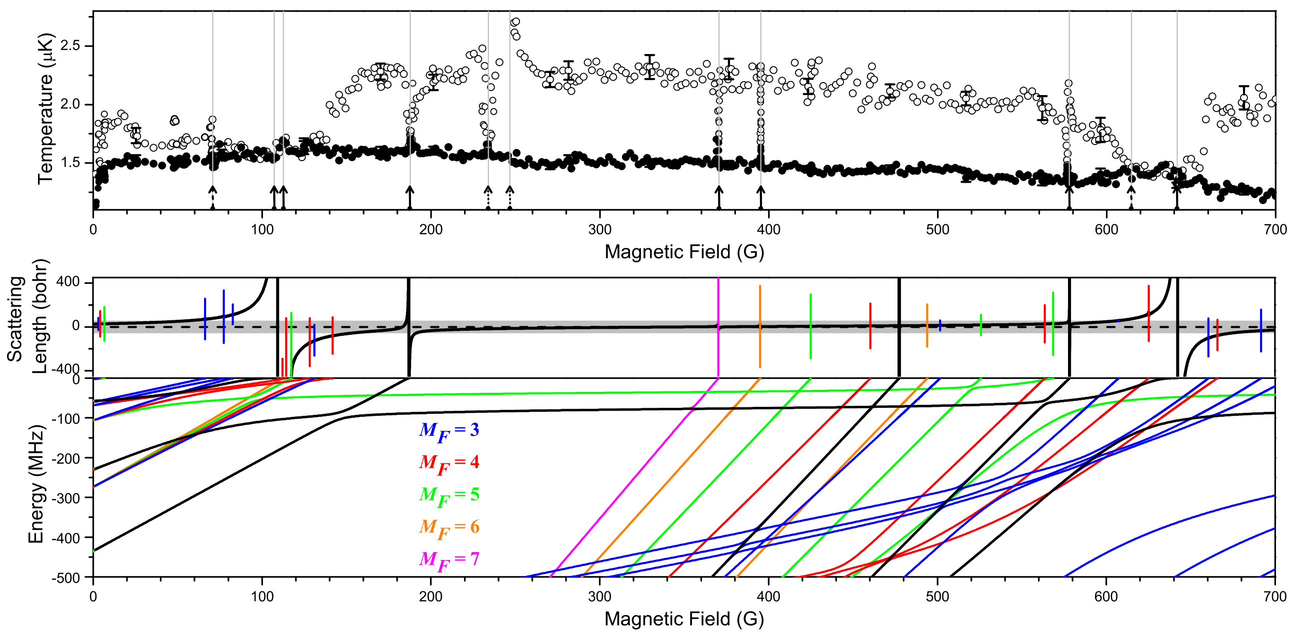

FIG. 2. Top panel: observation of interspecies Feshbach molecules in ^{85}RbCs. Center and bottom panels: calculated scattering length, showing poles at resonance, together with the near-dissociation bound states that cause the resonances and may be used in future for molecule formation. From ref. [5].

bound states of Cs_2 [9], and again used them to produce new potential curves that are a great improvement over existing ones, particularly in the important high magnetic field region.

4. We worked to develop multichannel quantum defect theory (MQDT) as an efficient computational tool for cold molecular collisions [10, 11]. We showed that with MQDT we can produce a complete contour plot of elastic/inelastic rations for sympathetic cooling in the strongly coupled system Li+NH using coupled-channel calculations at just 5 combinations of energy and field. Previous methods required over 200 such calculations, so this saving brings many more systems within reach of calculations.

5. We investigated the behaviour of the effective range, which determines the energy-dependence of cross sections and is very important in studies of few-body and many-body physics with ultracold atoms. This work led to development of new closed-form expressions for the effective range in the vicinity of a Feshbach resonance [12].

6. We compared and contrasted the wide resonances in ^{6}Li and ^{7}Li, and investigated the extent to which mass-scaling applies between these two systems [13].

7. We investigated the way in which loss cross sections in real inelastic/reactive approach the "universal" regime previously described by Idziaszek and Julienne. We compared the results of a single-channel loss model with full close-coupling calculations in a real system. The results suggest a remarkable conclusion: that coupled-channel calculations at very low energy (in the s-wave regime) could be used to estimate a loss parameter and then to predict the range of possible loss rates at higher energy, without the need for explicit coupled-channel calculations for higher partial waves [14].

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