Postdoc position on the theory of ultracold atoms and molecules

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A postdoctoral position is available to work on the theory of cold and ultracold molecules, starting as soon as possible after July 2017. The main topics we work on are:

1. Collisions of ultracold atoms
2. Formation of ultracold molecules from ultracold atoms
3. Properties of ultracold molecules in electric, magnetic, microwave and laser fields
4. Collisions of ultracold molecules with atoms and molecules

The group has substantial funding from the Engineering and Physical Sciences Research Council (EPSRC). Recently awarded grants are:

1. *A Stable Quantum Gas of Fermionic Polar Molecules* (2016-19), joint with the experimental group of Simon Cornish at Durham.
2. *Understanding Collisions of Ultracold Polar Molecules* (2017-20), also joint with the Cornish group
3. *QSUM: Quantum Science with Ultracold Molecules* (2017-22), joint with the Cornish group, the experimental group at Imperial College London (Ed Hinks, Mike Tarbutt and Ben Sauer), and the theory group of Dieter Jaksch at Oxford.

Jeremy Hutson is a member of both the Physics and Chemistry Departments at Durham. This position will be based in the Chemistry Department, but with membership of the Joint Quantum Centre (JQC) Durham/Newcastle and the Atomic and Molecular Physics grouping in the Physics Department. We also have a wide network of collaborative links to experimental and theoretical groups around the world, including Innsbruck, Boulder, Maryland and elsewhere.

General

The study of cold molecules (below 1 K) and ultracold molecules (below 1 mK and as low as 100 nK) is a "hot topic" in modern physics and chemistry [1]. The potential applications of such molecules include

- precision measurement (applications such as detecting the electric dipole of the electron, which is important for physics beyond the Standard Model of particle physics, or detecting the time-variation of fundamental "constants" such as the fine-structure constant or the electron-to-proton mass ratio)
- quantum simulators, in which cold molecules are used to create "designer Hamiltonians" and can be used to solve problems in quantum condensed matter physics that are completely unapproachable with conventional computers
- quantum information manipulation and storage ("quantum computing")
- development of a controlled ultracold chemistry, in which chemical transformations are carried out on a complete ensemble of molecules simultaneously and preserving quantum-mechanically coherence.

Ultracold molecules may turn out to be a transformational technology for the middle of the 21st century. It is not inconceivable that your iPhone will contain arrays of ultracold molecules in 25 years time, and even if it does not we will have learned a great deal of new physics and explored new phases of matter using the quantum playground that ultracold molecules provide.

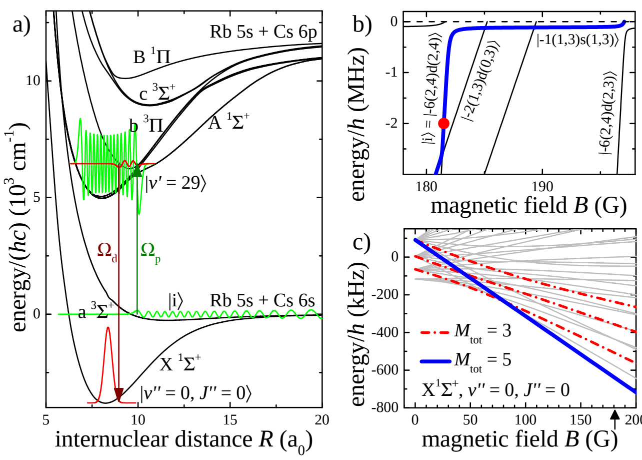

FIG. 1: Production of ground-state RbCs from ultracold Rb and Cs atoms. Top right: the way that magnetic fields are used to form "Feshbach" molecules very near dissociation and then navigate to a state suitable for ground-state transfer. Left: the 2-photon STIRAP scheme used to transfer Feshbach molecules to the ground state. Bottom right: the pattern of hyperfine levels in the ground state, showing that the state formed becomes the absolute ground state at fields above 90 G. None of this would have been possible without guidance from theory: see ref. [2] for more details.

Recent achievements

In collaboration with experimental groups in Durham and Innsbruck, we have recently succeeded in producing ultracold RbCs molecules at a temperature around 1 μK. The molecules are formed from ultracold atoms by magnetoassociation [2, 3], and then transferred to their absolute ground state by Stimulated Raman Adiabatic Pumping (STIRAP) [4, 5]. The procedure is illustrated schematically in Figure 1. RbCs was only the second polar molecule to be formed in this way, though it has been followed by NaK at MIT [6] and NaRb in Hong Kong [7]. There have also been major advances in laser cooling of molecules such as SrF and CaF, and the group at Imperial College has recently succeeded in cooling CaF to around 50 μK in a 3-dimensional magneto-optical trap (MOT) [8].
We have used our gas of ultracold RbCs to measure the binding energy of RbCs more precisely than has been possible for any other molecule [9]. We have also carried out detailed microwave spectroscopy of the hyperfine structure and demonstrated coherent control of the rotational, hyperfine and Zeeman levels [10]. We are currently investigating the interplay between the hyperfine levels and the AC Stark effect due to a trapping laser, and the Cornish group is carrying out measurements of collisional loss rates for molecules in different states.
There are also fascinating problems in the physics of three-body systems that can be probed with ultracold atoms. We have recently collaborated with the experimental group in Innsbruck group to study Efimov states, which are exotic states of three-body systems that can exist when the dimer has a bound state very close to dissociation. We discovered a new form of universality for such states that is currently causing much excitement among few-body physicists [11] and carried out the first measurements of an excited Efimov state in ultracold cesium [12].
We have also done extensive work on sympathetic cooling of cold molecules with ultracold atoms (see, for example, refs. [13, 14]) and on precise interaction potentials for atomic interactions (see, for example, refs. [15–18]).

Current Projects

The study of cold molecules is an extremely fast-moving field. We have specialist conferences once or twice a year at which people from the world's leading groups meet to discuss recent progress and future directions. Almost every one of these meetings turns up major new experimental directions that require theoretical input and new theory that proposes new experiments. It is therefore quite hard to predict exactly what will be of most interest in a year's time. The project ideas below are based on the current state of the art, but that will change, and the projects will adapt too.

Project 1: Extending molecule formation to other species: KCs and CsYb

Our gas of ultracold RbCs opens up many new possibilities, but it has fairly low density. Its density is limited by an unlucky coincidence: the interspecies scattering length for ^{87}Rb + Cs is large and positive, so that clouds of the two atoms are hard to overlap (and a mixed BEC phase-separates). We are therefore working to extend molecule formation to KCs, which does not have this problem. In an initial theoretical study, we predicted Feshbach resonances in all three isotopic combinations (^{39}KCs, ^{40}KCs and ^{41}KCs) and studied the miscibility of the atomic mixtures [19]. Very recently, the Innsbruck group measured the first Feshbach resonances in ^{39}KCs, and we adjusted the KCs interaction potentials to make improved predictions of other resonances and miscibility [20]. The new predictions for resonance positions and bound-state energy levels of ^{41}KCs are shown in Figure 2. Simon Cornish's experimental group in Durham is currently constructing a KCs apparatus; we will collaborate with them and with the Innsbruck group to form ultracold KCs molecules, transfer them to their absolute ground state, and explore their properties. ^{40}KCs has the particular advantage that the molecules are *fermionic*, and gases of dipolar fermions have many potential applications.

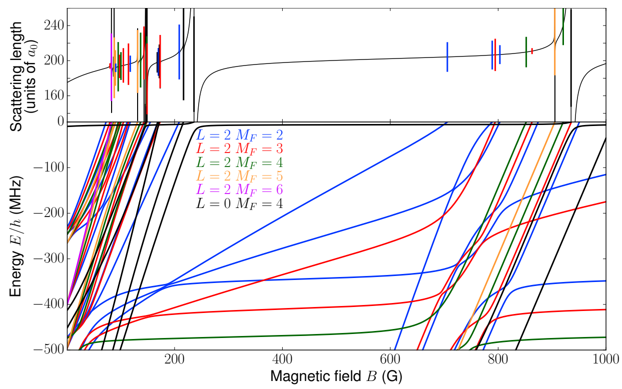

FIG. 2: Scattering length and energies of near-threshold bound states for ^{41}KCs. Resonance widths greater than 1 μG are shown as vertical bars with lengths proportional to $\log(\Delta/\mu G)$

Molecules formed from pairs of alkali-metal atoms have singlet ground states, with no net electron spin and no significant magnetic moment. We would like to form molecules with both an electric and a magnetic dipole moment, which offer important possibilities for quantum simulation and quantum computing. We are therefore working to form CsYb molecules, which have a $^2\Sigma$ ground state (with electron spin $S = \frac{1}{2}$). We predicted some years ago that such systems will have magnetically tunable Feshbach resonances [21], and carried out a detailed theoretical study of all the alkali-Yb combinations that suggested that CsYb is a particularly good choice for experiments [22]. Very recently, Simon Cornish's group has succeeded in making mixtures of ultracold Cs and Yb, and we have interpreted their thermalisation measurements to learn about the scattering lengths [23]. The next stage is for the Cornish group to measure photoassociation spectra, which we will use to refine interaction potentials and predict the positions and widths of Feshbach resonances for molecule formation.

Project 2: Collisions of RbCs with ultracold atoms and molecules

Some time ago, we showed that RbCs is one of a small family of alkali dimers that is stable to all 2-body collision processes [24]; other molecules such as KRb can be destroyed by reaction to form K_2+Rb_2 [25, 26].

There are nevertheless key unanswered questions about the collisions of ultracold molecules such as RbCs. In particular, John Bohn's group [27, 28] has developed a statistical model that suggests that ultracold molecules will undergo "sticky" 2-body collisions"; such collisions, even if nonreactive, may last long enough that a third molecule will encounter the 2-body collision complex, and the resulting 3-body collision would then probably cause recombination and eject the molecules from the trap.

The "sticky collisions" model is by no means established as physical reality. The statistical model assumes that energy is completely redistributed between vibrational modes during a collision, and this may not happen. The proposal that it *may* happen is related to ideas of quantum chaos and the randomness of energy levels in complex systems. However, it is well known that approximate quantum numbers often persist in molecules even when the density of states is very high.

We have therefore begun a combined experimental and theoretical programme to explore the collisions of ultracold RbCs, both with other RbCs molecules and with ultracold Rb and Cs atoms. Simon Cornish's group has begun experiments on collisions of RbCs molecules in different hyperfine and Zeeman states. They will extend these to study atom-molecule collisions, and will also explore collisions in confined geometries (with molecules confined in "pancakes" and "tubes" in optical lattices). We have started to explore signatures of quantum chaos in ultracold collisions, initially for simple systems such as Yb+Yb* [29] and Li+CaH and Li+CaF [30]. Surprisingly, Li+CaF shows evidence of persistent quantum numbers, while Li+CaH shows strong signatures of quantum chaos.

On the theory side, the next step is to develop more accurate models for atom-molecule collisions involving heavy molecules such as RbCs and understand the extent to which energy is randomised during collision (or, alternatively, is restricted to a subset of the phase-space available, resulting in an effective density of states much smaller than the full density.

Future Projects under QSUM

Our recently awarded grant *QSUM: Quantum Science with Ultracold Molecules* will fund a 5-year project with a broad remit to develop ultracold molecules as a platform for quantum science. It draws in the projects described above, but goes much further. We plan to create "designer arrays" of ultracold molecules using optical tweezers and study their few-body interactions. We plan to load ultracold molecules into 1-d, 2-d and 3-d lattices and study their many-body interactions and correlations. All this will require detailed collaboration between experiment and theory, with many new challenges to overcome.

Tools

We use a wide range of theoretical methods, ranging from molecular electronic structure theory to simulations of atomic and molecular clouds. Our greatest expertise is in *quantum calculations of atomic and molecular collisions* and the weakly bound states that are formed between pairs of atoms and molecules. Jeremy Hutson is the principal author of the MOLSCAT, BOUND and FIELD packages, which are powerful general-purpose programs for carrying out quantum-mechanical bound-state and scattering calculations using coupled-channel methods. The packages are very versatile, and we can often fit new types of bound-state and scattering calculations into their framework. In recent years we have adapted them to handle interactions and collisions in electric, magnetic and radiofrequency fields, and to handle atomic and molecular species of many different types.

We have a long-standing interest in *interaction potentials.* We often start with interaction potentials from the literature, or calculate our own using advance molecular electronic structure methods. The systems of interest for ultracold atoms and molecules are particularly challenging for such calculations, because they usually involve multiple electronic states and heavy, highly polarisable collision partners. Nevertheless, once high-precision experimental results become available, we usually need to refine the potentials to fit the experiments and to predict new ones. Such refinement has been crucial in many of the advances described above, including molecule formation in RbCs and the discovery of universality in Efimov physics.

Tools

We are in a world-leading position in the theory of both ultracold molecule formation and cold molecular collisions, and there are many leading experimental labs around the world who are keen to collaborate with us. There is much to explore in the quantum playground provided by ultracold atoms and molecules.

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