ESF POLATOM Final Report

November 23, 2012

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Contents

1 Purpose of the visit

Motivated by the successes of discovering Bose-Einstein condensates (BECs) in the 20^{th} century, research into a fermionic counterpart has advanced greatly in recent years after the successful creation of an ultracold fermionic gas by the group of D. Jin in 2003 [1], with the confirmed observation of fermionic superfluidity by the group of Nobel Laureate Prof. W. Ketterle at MIT in 2004 [2]. The physics of ultracold Fermi gases is dominated by the inter-particle interactions, from which large-scale order emerges. This long-range order is responsible for the exciting new phases of matter that arise in these systems and the rich physics they display. If the interactions are small and attractive then the fermions form Cooper pairs, a regime described by Bardeen-Cooper-Schrieffer (BCS) theory which describes the ultracold fermionic quantum gases created by Jin and Ketterle. If the interactions are repulsive then the fermions form bound dimers which behave like a Bose-Einstein condensate (BEC). Interestingly, there is a smooth crossover between these two very different regimes where the inter-particle interactions become extremely strong and the gas exhibits universal behaviour, yet neither theory by itself can sufficiently explain this behaviour [3, 4].

My current research as part of my PhD thesis at the University of Melbourne is investigating the properties of few interacting fermionic atoms in a harmonic trap at ultracold temperatures, particularly focusing on the strongly-interacting regime. These results can then be used to construct a many-body theory of a trapped ultracold fermionic gas. The first step is the solution of the two- and three-body problems, that is, finding the energy eigenspectrum of two interacting opposite-spin fermions by themselves and then with the addition of a third fermion which may interact with the pair. These solutions can be immediately applied to a quantum virial expansion of the thermodynamic equation of state of the strongly interacting fermionic gas or alternatively, they can be used to construct a microscopic theory of the many-body unpolarised fermionic gas at low temperatures.

This focus on the physics of few-body interactions between particles can also be applied to excited Rydberg atoms. Specifically, a gas of Rydberg atoms is of interest since the dipolar interactions are controllable and can be tuned to a strongly interacting regime. Rydberg atoms are a particular type of dipolar atom caused by excitation of the atom into a high-energy state that possesses a large dipole moment. The level of excitation, determined by the principal quantum number n, controls the range of the interaction as well as the crossover into a regime where the gas is a plasma and the interactions become strong. In such a regime the emergence of long ranged order gives rise to new phases of matter such as Wigner crystals and phases with metallic properties. The group led by Dr. Servaas Kokkelmans at the Eindhoven University of Technology is a leading contributor to research into ultracold dipolar gases, particularly those involving Rydberg atoms.

His group has expertise in both the creation and understanding of Rydberg systems. Dr. Kokkelmans has already demonstrated that the strongly interacting case of this long-ranged interaction exhibits rich physics in ultracold systems [7].

The purpose of the visit was to develop a theoretical framework with which to better understand the properties of Rydberg systems as interest in them grows. As in the case of neutral atoms the first step is to seek solutions to the problem of two Rydberg atoms. There has been little work done in this particular area. The aim is to investigate the interactions between Rydberg atoms, particularly in strongly-interacting or other regimes where long-range is possible.

The secondary purpose of the visit was to see these systems realised in an experimental setup. Such experiments are not being performed at the University of Melbourne until very recently and an understanding of the experimental work which complements the theoretical approach is vital to understanding the problem.

2 Description of the work

Interest in Rydberg atoms has recently arisen within the context of ultracold atomic gases, which are the subject of a lot of research in their own right, including my own research at the University of Melbourne. The application to Rydberg physics is as follows: ultracold gases are by definition at very low temperature where the average speed of individual atoms is comparatively slow. Specifically, the heavy mass of atomic species used for Rydberg physics (eg. Rubidium) and the low temperature of the gas means that over the timescale of the excitation of the atoms to the highly excited Rydberg state and their subsequent decay the atoms themselves can be considered to have not moved significantly (less than one wavelength of the excitation laser field). This regime is referred to as the frozen gas limit [6].

The properties of Rydberg atoms are usually characterised by scaling laws dependent on the principal quantum number n. In particular, the strength of the interaction between two Rydberg atoms scales with $n^1 1$ leading to very strong interactions. This quantity is usually derived by viewing the two Rydberg atoms as two dipoles, where the highly excited electron of each atom is separated enough from the nucleus so that each atom can be viewed as a dipole, yet the two atoms are further separated so that the interaction can be treated as two dipoles affecting each other.

The other remarkable feature of Rydberg atoms is that the strong interaction between atoms means that excitation of one atom to a Rydberg state greatly affects its neighbours to the point where excitation of nearby atoms is prevented. This is known as the 'Rydberg blockade effect.' Within a small region, the single excitation can then be shared amongst several

atoms. The single excitation can be viewed as a superposition of several different excitation, a uniquely quantum phenomenon.

The other approach is to consider that in the frozen gas limit the atom-atom interaction can be viewed as two stationary nuclei creating a Coulombic double-well potential in which the two excited electrons move. This is a move away from the dipole approximation which is usually used to model the interaction to a picture which views the electrons as separate particles to the nuclei they are normally attached to. When the two nuclei are far apart the potential behaves as two independent Coulomb wells, and the Rydberg electron can occupy the usual single atom Rydberg states. As the two atoms come together the central barrier between the wells is lowered below the ionization limit; the electrons feel an interaction with both nuclei and with each other. At some point it is expected that there is a transition from two independent atoms to a regime where the electrons are more free to move and the shared excitation within a blockade radius may have similarities to the physics of a neutral plasma.

To treat the system in this way we borrow from quantum chemistry and employ the linear combination of atomic orbitals as molecular orbitals (LCAO-MO) technique. The LCAO-MO is a well-established technique from molecular physics used for example to show that ionic hydrogen has a stable bound state. It works by using single-particle states to build an electronic wavefunction when several single-particles are combined into a molecule. The resulting molecular wavefunction depends on the separation of the atoms within the molecule. Variational methods are then used to find the separation distance which minimises the energy. This is the groundstate of the molecule.

For the Rydberg system the atoms will not enter a bound state, so there is no minimum to find but the interaction energy still depends on the separation distance, and the mathematical method is still valid. There are however several differences: molecular states are built using groundstate wavefunctions of the individual atoms, but Rydberg states are highly excited. This not only affects the numerical methods required to compute the wavefunction, but also means that the relevant length-scales of the system are different. Molecule formation can be treated purely as two atoms, but Rydberg atom formation in an ultracold atomic gas is constrained by the properties of the gas, particularly average interparticle separation, and the Rydberg blockade radius.

The difference with applying this technique to Rydberg atoms is that we are not using the well-known hydrogen wavefunctions but a set of wavefunctions modified for Rydberg physics. The modifications are intended to incorporate the effects of penetration of the core by the excited electron and subsequent polarisation of the other electrons. These Rydberg states can be found numerically but in this project I elected to use the wavefunctions of Kostelecky & Nieto [10] which are slightly modified hydrogen-like wavefunc-

tions with the benefit being that they are analytic. This allowed me to use the techniques developed in my work on ultracold Fermi gases to apply the LCAO-MO method to Rydberg atoms. The calculations focus on finding not a ground state but the general interaction energy as a function of the separation of the two atoms, constrained by the properties of the ultracold atomic gas being excited to Rydberg levels.

3 Description of main results

The main difficulty in this project was overcoming the numerical instabilities and inaccuracies which arose in the calculations. In principle, the fact that the wavefunctions are analytic should mean that these inaccuracies are less significant and one can use analytic techniques for some of the calculation before employing numerical techniques. In this case however, the high-energy Rydberg states mean that the wavefunctions are highly oscillatory and the modifications made to turn hydrogen states into more general Rydberg states greatly impinge on their convergence and accuracy. The result is that we were not able to achieve accurate results for the highly-excited regime of Rydberg atoms, typically $n > 40$. The alternative approach was to consider the restriction of the problem to one-dimension as a toy-model for the full three-dimensional system. However, even in one-dimension the non-convergence of the wavefunctions prevented accurate results beyond $n > 15$. Below this threshold, the method produced a model of the interaction energy between two atoms, but this is not the regime of interest. In particular, atoms that are excited only to $n \approx 15$ are not strongly interacting enough to display interesting physics when separated by distances typical to the interparticle distance of an ultracold atomic gas. As a rough guide, a typical interparticle distance of an ultracold atomic gas is $100nm$ while the average size of an $n = 15$ Rydberg atom is only $\approx 11nm$. The model is not yet accurate for the energies that are considered to be in the regime of Rydberg physics.

4 Future collaborations

The science goals of the project have not been fully met and as such future collaboration with Dr. Kokkelmans will be required to finalise the results. In particular, the accuracy issues need to be resolved in order to produce a model of the interaction energy for the regime of highly-excited Rydberg atoms. An intended result of this project is the preparation of a paper for publication (see below). This will be in cooperation with Dr. Kokkelmans and my own supervisor at the University of Melbourne Dr. Andrew Martin. Future projects would then focus on extending the results of the two-atom model to exploring the physics of Rydberg excitations in a gas of ultracold

atoms. Lastly, just as my visit to the CQT group at Eindhoven University of Technology followed on from the visit of Dr. Kokkelmans' student Rick van Bijnen in 2006, this collaboration can potentially lead to future visits between the members of the two groups.

5 Projected publications

Although the model is currently incomplete, the outline of the project is clear. The application of the LCAO-MO method to Rydberg atoms is straight forward and the main difficulty of numerical inaccuracy is mostly a technical one. The steps to be completed are: (a) produce a one-dimensional 'toy-model' to serve as a road map for fine-tuning the method to the relevant regime of interest; (b) extend the method to the three-dimensional problem; (c) compare the model to other known results about Rydberg atoms, in particular those derived using the dipole-dipole approximation, and look for a transition from two separated and independent atoms to a shared excitation regime. These steps will form the outline of a publication.

6 Other comments

I am grateful to the European Science Foundation for the funds provided for the 'Common perspectives for cold atoms, semiconductor polaritons and nanoscience (POLATOM)' activity via the Exchange Visit Grant programme.

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