

ATOMIC $2S_{1/2}$ TO $3P_{3/2}$ TRANSITION FOR
PRODUCTION AND INVESTIGATION OF A FERMIONIC
LITHIUM QUANTUM GAS

CHRISTIAN GROSS

Master of Science ETH in Physics

A THESIS SUBMITTED FOR THE DEGREE OF DOCTOR
OF PHILOSOPHY

CENTRE FOR QUANTUM TECHNOLOGIES
NATIONAL UNIVERSITY OF SINGAPORE

2016

Declaration

I hereby declare that this thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has also not been submitted for any degree in any university previously.

A handwritten signature in black ink, appearing to read 'Ch. Gross', is positioned above a horizontal line.

CHRISTIAN GROSS

August, 2016

Acknowledgments

I would like to thank everyone who contributed in one or the other way to the work that is presented in this thesis. The buildup phase of a cold atom experiment is an interesting, sometimes challenging and often a surprisingly multifaceted process and so are the contributions of my colleagues over the past few years. It is probably wishful thinking but I do hope that I have expressed my gratitude to the relevant people in a more timely and more appropriate fashion than it can be done here with a few lines.

However, in particular I would like to thank my supervisor Kai Dieckmann, the principal investigator Wenhui Li, the postdocs Saptarishi Chaudhuri, Li Ke, and Jimmy Sebastian, and my PhD colleague Jaren Gan. I would also like to thank the colleagues from the LiK-mixture lab, Mark Lam, Sambit Bikas Pal, Markus Debatin and Kanhaiya Pandey, for all their contributions on countless occasions.

A special thank goes to the experimental support team of CQT, not only for their great work but, in particular, for treating me as a colleague. It was a pleasure to work with you!

Contents

Summary	ix
List of Tables	xi
List of Figures	xiii
1. Introduction	1
2. Ultracold atoms	8
2.1. Ultracold atoms in the classical limit	8
2.2. Interactions and collisions	10
2.2.1. Collisions at low temperatures	11
2.2.2. Scattering cross section	12
2.3. Ideal quantum gas in a harmonic trap	14
2.3.1. Feshbach resonances and BEC-BCS crossover	18
3. Experimental setup and techniques	22
3.1. Production of a quantum degenerate Fermi gas	22
3.2. Vacuum chamber and magnetic field coils	27
3.2.1. Atomic ^6Li source	27
3.2.2. MOT Chamber	29
3.2.3. Science chamber	30
3.3. Laser system for the red MOT	32
3.3.1. Laser setup	32
3.4. Laser system for the UV MOT	36
3.5. Imaging	38
3.6. Optical dipole trap and transport to the science chamber	41
3.6.1. Optical dipole trap	41
3.6.2. Crossed ODT for optical transport	43
3.7. Ion detection	46
3.7.1. Ion detection with channel electron multiplier	47
3.7.2. Integration of ion detection in the MOT chamber	48
4. Two-stage laser cooling to high phase-space density	50
4.1. Laser cooling and trapping	50
4.1.1. Doppler cooling	51
4.1.2. Magneto-optical trap	53

4.1.3.	Capture velocity	54
4.1.4.	Laser cooling of ${}^6\text{Li}$	54
4.2.	Magneto-optical trap on the D_2 transition	56
4.2.1.	Loading phase	56
4.2.2.	Compressed MOT phase	57
4.3.	UV cooling to high phase-space densities	59
4.3.1.	Optimization of phase-space density	60
4.3.2.	UV and red repumping light	62
4.3.3.	Temporal evolution	64
4.3.4.	Lifetime and 2-body loss rate of the UV MOT	65
4.4.	Summary	67
5.	Optical transport in a crossed ODT and cooling to quantum degeneracy	68
5.1.	Experimental approach	68
5.2.	Optical dipole trap	70
5.2.1.	Characterization of the trapping potential	71
5.2.2.	Loading of the ODT	74
5.3.	Near-adiabatic and loss-free optical transport	78
5.3.1.	Trajectory for optical transport	79
5.3.2.	Characterization of the optical transport	80
5.4.	Evaporative cooling to quantum degeneracy	81
5.4.1.	Weakly interacting Fermi gas	82
5.4.2.	Evaporation near the Feshbach resonance	84
5.5.	Summary	88
6.	Photoassociation spectroscopy (attempt) below the $2S$-$3P$ asymptote	89
6.1.	Photoassociation spectroscopy	89
6.1.1.	Principle of photoassociation spectroscopy	90
6.1.2.	Decay and detection of photoassociated molecules	90
6.1.3.	Structure of diatomic molecules	92
6.1.4.	Significance of PA spectroscopy	94
6.1.5.	PA spectroscopy of lithium below the $2S$ - $2P$ asymptote	95
6.1.6.	PA spectroscopy of lithium below the $2S$ - $3P$ asymptote	96
6.2.	Experimental approach	97
6.2.1.	Photoionization of ${}^6\text{Li}$	97
6.2.2.	Reduction of ionization background	100
6.2.3.	Experimental sequence for spectroscopy measurement	101
6.3.	Ionization detection on atomic transition	103
6.3.1.	Atomic transition frequency and fine structure splitting of the $3P$ state of ${}^6\text{Li}$	104
6.3.2.	Detection and suppression of ASE	104

6.4. PA scan below $2S-3P$ asymptote	107
6.4.1. Frequency range between -140 GHz to -35 GHz	107
6.5. Summary	109
7. Photoassociation rate	111
7.1. Photoassociation transition strength	111
7.1.1. Transition dipole moment	112
7.1.2. Calculation of transition rates	114
7.2. Numerical calculation of continuum states	115
7.2.1. Radial Schrödinger equation and Numerov algorithm	116
7.2.2. Ground-state potentials of ${}^6\text{Li}$	117
7.2.3. Scattering cross section	118
7.3. Numerical calculation of bound states	119
7.3.1. Excited-state potentials	121
7.3.2. Bound states of $2S-3P$ potential	122
7.4. Calculation of dipole matrix elements and transition rates	123
7.5. Summary and outlook	129
8. Conclusion and outlook	130
 A. Atomic properties of ${}^6\text{Li}$	 147
A.1. Derived quantities for the cooling transitions of ${}^6\text{Li}$	147
A.2. Zeeman shift of $2^2S_{1/2}$ and $2^2P_{3/2}$ levels	147
A.3. s-wave scattering length of $ 1\rangle$ - $ 2\rangle$ mixture	149
 B. Photoassociation	 150
B.1. Atomic units	150
B.2. Selected dipole matrix elements for ${}^6\text{Li}_2$ and ${}^7\text{Li}_2$	150
B.3. $2S-2P$ photoassociation transitions of ${}^6\text{Li}_2$	151

Summary

In this thesis we describe our apparatus and approach for the production of a fermionic lithium quantum gas. Laser cooling on the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition is employed and investigated to produce an atomic cloud with an improved, high phase-space density. This is achieved because of the lower Doppler limit as compared to the one of the conventional D_2 line and the compression dynamics of the magneto-optical trap. Following an all-optical scheme, we then directly load the atoms into a small-angle crossed optical dipole trap, which simultaneously offers two important features. It provides a large volume, which is advantageous for the loading process, and a sufficient axial confinement such that this optical potential can be used to transport the atoms. With this configuration, intermediate trapping potentials can be avoided, resulting in a simplified experimental sequence. We subsequently move the atoms into a glass cell in order to facilitate a good optical access for manipulating and probing the atomic cloud. Evaporative cooling is performed to produce a quantum degenerate Fermi gas and the production of a large molecular BEC near a Feshbach resonance demonstrates the overall efficiency of our scheme.

We have implemented an ion detection system based on a channel electron multiplier. The prime motivation for this was the investigation of long-range bound states of the $2S$ - $3P$ internuclear potential, which can be probed by photoassociation spectroscopy. The transition frequencies to these molecular states are related to atomic properties, but have not been investigated so far. However, in a preliminary measurement that was performed in a magneto-optical trap, no spectroscopic features were observed. Based on available *ab initio* potential energy curves, a calculation of the free-to-bound transition strength was carried out to analyze the negative result and to evaluate the prospect for future investigations.

List of Tables

4.1. Parameters for calculation of capture velocity	54
5.1. ODT parameters	72
6.1. Photoionization with single photon	99
7.1. Long-range dispersion coefficients for lithium interaction potentials	117
7.2. Photoassociation rate coefficient to states of $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ potentials . . .	128
7.3. Photoassociation rate coefficient to states of $A^1\Sigma_u^+$ and $1^3\Sigma_g^+$ potentials . . .	128
A.1. Atomic properties and derived quantities of ^6Li	147
B.1. Atomic units	150

List of Figures

3.1. Top view of the experimental setup.	23
3.2. Partial level structure of ${}^6\text{Li}$	24
3.3. Modular design of experimental apparatus	25
3.4. Atom source of the experiment	27
3.5. Glass cell	30
3.6. Simplified level scheme of the D_2 transition	32
3.7. Illustration of the laser system for D_2 transition	33
3.8. Simplified level scheme of the UV transition	36
3.9. Illustration of the laser system for UV transition	38
3.10. Axial ODT trap frequency versus crossing angle of ODT beams	45
3.11. Schematic laser setup for the crossed optical dipole trap	46
3.12. Schematic illustration of the CEM setup	48
3.13. 3D model of the CEM in the MOT chamber	49
4.1. Magneto-optical trap	53
4.2. Capture velocity	55
4.3. Loading of red MOT	58
4.4. Characterization of red CMOT	59
4.5. Experimental sequence for UV MOT	60
4.6. TOF measurement after laser cooling	61
4.7. Performance of the UV MOT	63
4.8. Atom number and density of UV MOT as function of repumping power	64
4.9. Transient dynamics of the UV MOT after compression	65
4.10. Trap loss measurement for the UV MOT	66
5.1. Trap frequencies of ODT	73
5.2. Number of atoms in ODT as function of UV detuning	75
5.3. Loading dynamics of ODT	76
5.4. ODT loading as function of optical power	77
5.5. Velocity profile of optical transport	80
5.6. Evaporative cooling at 330 G	83
5.7. Evaporative cooling of strongly interacting Fermi gas	86
5.8. Observation of molecular BEC	87
6.1. Photoassociation level scheme	98
6.2. Overview of spectroscopy setup	102

6.3. Alternating probe and trapping phases for spectroscopy measurement	105
6.4. Ion signal due to ASE light	106
6.5. Photoassociation frequency scan	109
7.1. Molecular transition dipole moment	114
7.2. Ground-state potential energy curves of lithium dimer	118
7.3. Elastic scattering of lithium atoms	120
7.4. Molecular potentials and bound states of ${}^6\text{Li}$ dimer	124
7.5. Dipole matrix elements for PA transitions to $3\,{}^1\Sigma_u^+$ and $3\,{}^3\Sigma_g^+$ states	125
7.6. Transition dipole matrix elements to different vibrational states	126
A.1. Zeeman energy shifts for $2\,{}^2S_{1/2}$ states of ${}^6\text{Li}$ (0 to 400 G)	148
A.2. Zeeman energy shifts for $2\,{}^2P_{3/2}$ states of ${}^6\text{Li}$ (0 to 400 G)	148
A.3. Zeeman energy shifts for $2\,{}^2P_{3/2}$ states of ${}^6\text{Li}$ (0 to 5 G)	149
A.4. Magnetic field dependence of s -wave scattering length for $ 1\rangle$ - $ 2\rangle$ of ${}^6\text{Li}$. . .	149
B.1. Dipole matrix element for PA transitions to $2S$ - $2P$ asymptote of lithium . . .	150
B.2. Transition dipole matrix elements to bound states of the $A\,{}^1\Sigma_u^+$ potential . .	151
B.3. Transition dipole matrix elements to bound states of the $1\,{}^3\Sigma_g^+$ potential . . .	151

1. Introduction

Quantum degenerate Fermi gas A driving force for the investigation of ultracold atoms is the possibility to investigate quantum many-body physics in a controllable environment. The system under investigation offers an exceptional purity and can be engineered using tools that were developed over the past three decades in the field of atomic physics. This allows reducing the dimensionality of the configuration and to tune the mutual interaction strength between the particles over a wide range (Bloch et al., 2008). An often referenced outstanding question is high-temperature superconductivity, which is predicted to be correlated to the antiferromagnetic state of a Mott insulator (Anderson, 1993). While the Fermi-Hubbard model, which describes interacting fermions in a lattice structure, might not be sufficient for a full description of a real high-temperature superconductor (Lee et al., 2006), such a model can be vital for the physical understanding of the underlying problem. While the model itself is rather simple, full numerical simulations are elusive because quantum correlations of the many-body state result in an enormous number of degrees of freedom. Using ultracold atoms in optical lattices can be seen as an implementation of a quantum simulator targeting a specific physical model, as exemplarily demonstrated by the observation of antiferromagnetic correlations (Hart et al., 2015).

Laser cooling and the first realization of a magneto-optical trap can be regarded as the starting point of the rapidly evolving research field of ultracold atoms (Chu et al., 1985; Raab et al., 1987). Soon it was found that the atomic clouds could be cooled below the limit imposed by the Doppler cooling theory for a two-level system (Lett et al., 1988). Rather surprisingly, interference effects between the trapping lasers in combination with the multilevel structure of the atoms was found to provide an additional cooling mechanism, which was first described by Dalibard and Cohen-Tannoudji (1989) and Ungar et al. (1989). The motivation for investigating new regimes of the physical system of ultracold atoms often motivated and triggered the development of new experimental and scientific methods. Evaporative cooling

of the atoms, which relies on elastic collisions in the trapped ensemble, made it possible to reach a much lower temperature regime and to initiate a phase transition to a Bose-Einstein condensate (BEC) of the confined atoms ([Anderson et al., 1995](#)). The formation of a BEC below a critical temperature is a direct consequence of the quantum statistics for bosons and leads to a significant change in the appearance of the atomic density profile. On the other hand, fermionic particles obey the Fermi-Dirac statistics arising from the Pauli exclusion principle, and no phase transition occurs for an ideal Fermi gas even in the limit of zero temperature. The first quantum degenerate Fermi gases with ultracold atoms were realized by [DeMarco and Jin \(1999\)](#) with potassium and by [Truscott et al. \(2001\)](#) with lithium atoms. A major development was the observation of the collisional stability of a Fermi gas near a Feshbach resonance ([Cubizolles et al., 2003](#)), which allows tuning of the interaction strength between the atoms over a large range ([Courteille et al., 1998](#)). This led to the creation of strongly interacting Fermi gases ([Kinast et al., 2005](#); [O'Hara et al., 2002](#)) and the investigation of the corresponding thermodynamic properties ([Nascimbène et al., 2010](#)).

The introduction of an optical lattice can emulate the crystal structure in solids and can be used to create a system that is described by the Fermi-Hubbard model ([Esslinger, 2010](#)). A major achievement was the demonstration of a Mott insulating phase in a partially filled conduction band as a result of mutual interactions between atoms on the same lattice site ([Jördens et al., 2008](#); [Schneider et al., 2008](#)). At sufficiently low temperatures, the Fermi-Hubbard model predicts an antiferromagnetic phase. The transition temperature has not been reached with ultracold atoms yet, however, antiferromagnetic correlations between different spin states of the atoms have been observed ([Greif et al., 2013, 2015](#); [Hart et al., 2015](#)). With the realization of a 'quantum gas microscope' by [Bakr et al. \(2009\)](#) for bosons, a new tool was introduced to probe ultracold atoms on a microscopic level with single-site resolution. Over the past few years, the corresponding technique was developed for fermionic lithium and potassium and allowed the direct observation of local, antiferromagnetic correlations in a two-dimensional lattice ([Cheuk et al., 2016](#); [Parsons et al., 2016](#)).

A main motivation for the work presented in this thesis is the investigation of a strongly interacting fermionic quantum gas. Lithium is particularly well suited for this purpose, but the experimental realization is more involved as compared to the one for other alkali-metal atoms. The reason is that standard sub-Doppler cooling is not observed for lithium and other,

generally rather elaborate experimental schemes are required to reach quantum degenerate temperatures (Hadzibabic et al., 2003; Zimmermann et al., 2011). In order to circumvent this, we employ and further investigate a narrow laser cooling transition to the second excited state of ^6Li , which was first demonstrated by Duarte et al. (2011). The reduced natural linewidth of this transition results in a lower temperature of the laser cooled atomic cloud and a much improved phase-space density facilitates the following cooling sequence. In parallel to these efforts, there was considerable interest in improving and developing laser cooling schemes for lithium and potassium. There, the additionally employed 'gray-molasses' cooling stage significantly reduces the temperature of the atomic ensemble (Fernandes et al., 2012; Grier et al., 2013; Salomon et al., 2013) and was used for efficient all-optical production schemes for quantum gases (Burchianti et al., 2014; Salomon et al., 2014).

Atomic clouds are cooled, manipulated and probed by optical means. For optimal access to the ultracold atoms and greatest experimental flexibility, we transport the atomic ensemble into a small glass cell after laser cooling. Constraints imposed onto the optical access to the atoms by the pre-cooling stages can be avoided in this way. Such a transport scheme, in which the atoms are confined in an optical dipole trap, was pioneered by Gustavson et al. (2001) and was implemented in a number of other experiments. With a modification to the conventional method, we achieve a considerable simplification of the optical transport scheme, which allows us to reduce the number of different confinement potentials used in the experimental sequence. The overall efficiency is demonstrated with the creation of a large quantum degenerate Fermi gas and the production of a molecular BEC.

Photoassociation spectroscopy A second topic discussed in this thesis is an attempt to observe photoassociation transitions to states below the $2S-3P$ asymptote of lithium. Interactions between particles of dilute ultracold atomic ensembles predominantly occur via binary collisions and are of fundamental importance for the production of quantum degenerate gases. For sufficiently low temperatures only s -wave collisions contribute to the scattering because the centrifugal barrier for higher partial waves restricts the approaching atoms to a range of relative distances R where the internuclear interaction potential is negligible (Weiner et al., 1999). The long-range tail of these potentials, which critically influences the scattering properties at low temperatures (Gribakin and Flambaum, 1993), follow a power law in $1/R$ for ground-state alkali-metal atoms that is dominated by the $1/R^6$ term (Marinescu et al.,

1994). Further, the detailed knowledge of the interaction potentials of lithium permits highly accurate predictions on the locations of Feshbach resonances, which has direct implications on the investigation of strongly interacting Fermi gases (Julienne and Hutson, 2014; Zürn et al., 2013).

The mutual interaction between atoms depends on their electronic states. Of special interest for photoassociation (PA) spectroscopy are the internuclear potentials between a ground-state atom and an atom in the first electronically excited state. At large atomic separations, these potentials approach the nS - nP asymptote, where n is the principal quantum number and S and P indicate the atomic orbital of the free colliding atoms. The potential energy curve depends on the symmetry of the combined electronic wave function of the two atoms and multiple potentials are correlated to the same atomic asymptote. Some of these potentials are repulsive, while others provide a potential well that, if sufficiently deep, can support bound molecular states (Jones et al., 2006). If colliding ground-state atoms absorb a photon at the right frequency, they can undergo a free-bound transition to such a molecular state, which represents a PA process. While the formed molecules are short-lived and not of particular interest, the laser frequencies at which these free-bound transitions occur are extensively studied and allow for a precise characterization of the addressed internuclear potential. If the dimer is composed of two identical isotopes, then the leading contribution to the long-range part of the excited-state potential is defined by the resonant dipole-dipole interaction, which falls off as C_3/R^3 . At large separations, the two atoms seemingly ‘share’ an excitation and the strength of this interaction is related to the transition dipole matrix element between the atomic S and P state and therefore to the radiative lifetime of the nP state (Bouloufa et al., 2009).

PA measurements are performed with ultracold atomic samples, which leads to a high spectral resolution and enables the precise determination of the absolute binding energies of weakly bound states. The first PA measurements were performed with sodium and rubidium atoms (Lett et al., 1993; Miller et al., 1993) and a series of PA measurements with lithium was conducted by Abraham et al. (1995b). The dispersion coefficient C_3 can be estimated based solely on the observed binding energies (LeRoy and Bernstein, 1970), however, for an accurate calculation of the radiative lifetime of the $2P$ state of lithium also the short and intermediate range of the internuclear potential has to be considered (McAlexander et al.,

1995, 1996).

PA spectroscopy has been performed for most laser cooled atomic species (Jones et al., 2006; Stwalley and Wang, 1999; Weiner et al., 1999) and a special interest is the investigation of the PA process under the influence of a Feshbach resonance (Courteille et al., 1998; Deiglmayr et al., 2008). Both phenomena are closely related and can be described in the context of resonantly enhanced scattering. From a practical point of view, a Feshbach resonance can be used to modify the ground-state scattering wave function in order to enhance the PA rate (Krzyszewski et al., 2015; Pellegrini et al., 2008; Semczuk et al., 2013) but also to investigate fundamental physical constants (Gacesa and Côté, 2014). Conversely, the investigation of PA transitions in the vicinity of a Feshbach resonance can be employed to probe the pairing mechanism in a strongly interacting Fermi gas (Partridge et al., 2005).

The internuclear potentials approaching the $2S-2P$ asymptote of lithium are experimentally and theoretically well investigated, as discussed by LeRoy et al. (2009) and Dattani and LeRoy (2011) and references therein. However, for the $2S-3P$ asymptote, which in this work is used for laser cooling, almost no experimental data exist for deeply bound molecular states and no measurements are reported for the weakly bound states commonly observed with PA spectroscopy (Dattani, 2015; Musial and Kucharski, 2014). More generally, with the exception of cesium (Pichler et al., 2006), no experiments have been reported on the photoassociative investigation of the potentials approaching the $nS-(n+1)P$ asymptote. These potential energy curves have a qualitatively different character than the $nS-nP$ potentials, which is due to the reduced atomic transition strength to the second excited P state and was discussed by Stwalley and Wang (1999). In this work we have attempted, but not yet succeeded, to observe these PA transitions of ${}^6\text{Li}_2$. In particular for the lithium dimer, all spectroscopic investigations are of great interest for the following reason. The low complexity of the lithium system with only six electrons allows for accurate numerical calculations and precise experimental data can be used as a benchmark for the employed numerical methods (Jasik and Sienkiewicz, 2006).

This thesis

In Chapter 2, important theoretical concepts and relations are introduced that are needed for the analysis of the measurements and the experimental results discussed in later chapters.

This includes a description of the density distribution of the atomic cloud during the various experimental stages. Furthermore, binary elastic collisions are discussed, which are crucial for evaporative cooling and are relevant for the photoassociation process.

In Chapter 3, a detailed description of the apparatus and the design considerations are provided and relevant experimental methods and techniques are introduced. The implemented cooling strategy is motivated and the corresponding technical elements are discussed. We have also incorporated an ion detection setup, which can be used for spectroscopy measurements.

In Chapter 4, our measurements on laser cooling of ${}^6\text{Li}$ on the narrow $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ UV transition are presented. We start with a description of the first cooling stage on the standard D_2 line. The atoms are then transferred into a spatially smaller MOT on the UV transition. We describe our optimized experimental scheme to achieve high number and phase-space densities and discuss density limiting effects on this transition. Part of this chapter was published in *Physical Review A*, **90**, 033417 (2014).

In Chapter 5, the experimental sequence for obtaining a quantum degenerate Fermi gas is described. After laser cooling on the UV transition, the atoms are transferred into a large-volume crossed optical dipole trap. The same confinement potential is also used for transporting the atoms into a small glass cell, which provides excellent optical access. The atoms are prepared in a $|1\rangle$ - $|2\rangle$ mixture of the energetically lowest Zeeman states of the $2^2S_{1/2}$ ground state and for evaporative cooling the s -wave scattering length is tuned by applying a magnetic bias field. A strongly interacting Fermi gas or a molecular BEC is created if the evaporation is performed near the Feshbach resonance at 832 G. Part of this chapter was published in *Physical Review A*, **93**, 053424 (2016).

In Chapter 6, our experimental approach to drive photoassociation transitions to states below the $2S$ - $3P$ asymptote of ${}^6\text{Li}_2$ is described. From the beginning it is important to note that this experiment actually failed and that we were not able to identify any signature of a PA transition in the presented attempt. For this measurement we have implemented a rather sensitive ion detection scheme to compensate for the expected weak transitions and a continuous absolute frequency measurement setup. We discuss the physics of the PA process

and describe the developed experimental scheme, which was tested on the atomic transition to the $3P$ state.

In Chapter 7, the photoassociation rate to molecular states of potentials correlated to the $2S$ - $3P$ asymptote are calculated. This is a free-bound transition and the calculation of the overlap integral between the initial and final state is evaluated. The potentials that were used to determine the relevant radial wave functions and the related numerical methods are described. This calculation is performed in part to understand the unsuccessful experimental approach but also to evaluate the prospect for a future investigation of this PA transition.

2. Ultracold atoms

In this chapter, a selection of theoretical relations and principles are introduced that are important for describing the physical properties of a trapped atomic cloud. Of particular relevance for the analysis of measurements is the knowledge of the density distribution of a harmonically confined gas during the various experimental stages. Furthermore, elastic collisions between atoms are discussed, which are important for evaporative cooling of the gas and also for the photoassociation process that is described in Chapter 6.

2.1. Ultracold atoms in the classical limit

The system under investigation is a confined atomic cloud that is isolated from the environment. For the production and investigation of ultracold atoms, elastic collisions and interatomic interactions are important. However, interacting systems are inherently difficult to describe or model because of the large number of degrees of freedom for macroscopic systems. Therefore, theoretical models often rely on approximations, such as a mean-field approach. In the ideal gas limit for example, any interactions are ignored in the mathematical description but they are implicitly assumed to be present in order to establish a thermal equilibrium. While this may seem inconsistent, many properties of a trapped atomic cloud can be well characterized within this approximation, as discussed in the following.

An important condition is a sufficiently low number density of the gas. In this way, binary collisions dominate the interaction processes such that three-body collisions, and also higher orders, only have a minor effect on the properties of the system. In this regime the gas is called *dilute*. This condition can be formulated by $nr_0^3 \ll 1$, where n is the density of the gas and r_0 is the *range* of the interatomic potential $V(r)$. This potential, under which influence the atoms collide, is assumed to be short-range, which implies that interaction energy can be neglected for $r > r_0$. A comprehensive discussion of the dilute gas limit was given, for

example, by [Walraven \(2014\)](#).

Statistical description - canonical ensemble Here, the atomic cloud is confined in a conservative potential $U(r)$ and the gas is described in the classical limit, in which quantum statistical effects only have marginal implications. The atoms are viewed as distinguishable and point-like particles with a continuous energy spectrum and mutual interactions are neglected. The corresponding Hamiltonian is given by

$$H(\mathbf{r}_1, \mathbf{p}_1; \dots; \mathbf{r}_N, \mathbf{p}_N) = \sum_{n=1}^N \frac{\mathbf{p}_n^2}{2m} + U(\mathbf{r}_n) = \sum_{n=1}^N H_0(\mathbf{r}_n, \mathbf{p}_n), \quad (2.1)$$

where m is the atomic mass, $\mathbf{r}_n$ the position and $\mathbf{p}_n$ the momentum of the n^{th} atom. The system of N atoms is described by a sum of one-body Hamiltonians $H_0(\mathbf{r}_n, \mathbf{p}_n)$ because interatomic interactions are not accounted for. Thermodynamic properties of the system can be derived within the framework of the canonical ensemble and the corresponding partition function is given by ([Huang, 1987](#))

$$Z_N = \frac{1}{N!} \frac{1}{(2\pi\hbar)^{3N}} \int d\mathbf{r}^N d\mathbf{p}^N e^{-H(\mathbf{r}_1, \mathbf{p}_1; \dots; \mathbf{r}_N, \mathbf{p}_N)/k_B T}, \quad (2.2)$$

where $\hbar$ is the reduced Planck constant and k_B is the Boltzmann constant. In the canonical description of the system, a thermal contact with a large reservoir at temperature T is assumed and the microcanonical description would therefore seem more appropriate for the isolated atomic cloud. However, the equivalence between the different ensembles can be shown for macroscopic systems ([Huang, 1987](#)).

The link between the partition function and thermodynamic properties of the system is established via $F = -k_B T \text{Log}[Z_N]$, where F is identified as the free energy and $\text{Log}[\cdot]$ is the natural logarithm. This defines a thermodynamic potential and expressions for pressure p , entropy S and chemical potential μ can be derived using relations describing small, reversible transformations that are expressed by $dF = -pdV - SdT + \mu dN$ ([Huang, 1987](#)).

Density distribution in harmonic trap The confinement of the atoms can often be assumed to be provided by a harmonic potential defined by $U(\mathbf{r}) = \sum_{i=1}^3 \frac{1}{2} m \omega_i^2 r_i^2$. In this equation ω_i denotes the angular trap frequency along the spatial direction r_i , with $i = x, y$ and z . This

can be used to calculate the canonical partition function defined in Eq. (2.2) and one finds $Z_N = \frac{1}{N!} Z_1^N$ with $Z_1 = (k_B T / \hbar \bar{\omega})^3$, where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trap frequencies. This shows that for the noninteracting system the N -particle canonical partition function can be expressed by the one-particle partition Z_1 . The phase-space occupancy $f(\mathbf{r}, \mathbf{p})$ of the system can now be defined according to

$$f(\mathbf{r}, \mathbf{p}) = \frac{N}{Z_1} e^{-H_0(\mathbf{r}, \mathbf{p})/k_B T}, \quad (2.3)$$

which corresponds to the number of atoms within a box of size $2\pi\hbar$ around the point $(\mathbf{r}, \mathbf{p})$ in phase space. Integration over the momentum space results in an expression for the spatial density distribution of the form

$$n(r) = n_0 \prod_{i=1}^3 e^{-(r_i/R_i)^2}, \quad (2.4)$$

where the peak density n_0 and the radii R_i of the atomic cloud are given by

$$n_0 = N \left(\frac{m \bar{\omega}^2}{2\pi k_B T} \right)^{3/2} \text{ and } R_i = \sqrt{\frac{2k_B T}{m \omega_i^2}}. \quad (2.5)$$

Therefore, for a given atomic mass and trap frequency, the size of the confined ideal gas only depends on the ensemble temperature and R_i is often referred to as the thermal radius of the cloud. The density in phase space at the center of the trap follows from Eq. (2.3) and is given by

$$\rho_0 = N \left(\frac{\hbar \bar{\omega}}{k_B T} \right)^3 = \Lambda_T^3 n_0, \quad (2.6)$$

where $\Lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$ is identified as the thermal de Broglie wavelength (Huang, 1987). For $\rho_0 \ll 1$, the interparticle spacing is much larger than the 'size' of the atomic wave packet, which can be related to Λ_T via the Heisenberg uncertainty relation, and the gas can be described in the classical limit (Walraven, 2014).

2.2. Interactions and collisions

In the previous section the trapped atomic cloud was described in the classical limit, where quantum statistics only plays a minor role. However, the binary collisions that were assumed

to establish thermal equilibrium are treated as a quantum mechanical two-body problem.

2.2.1. Collisions at low temperatures

The collision of two atoms can formally be reduced to an effective one-body problem in the center-of-mass frame. In this frame, a single particle moves under the influence of a centrally symmetric interaction potential $V(R)$, where R is the mutual separation. This symmetry allows for the separation of the wave function into a product of a radial and angular part, represented by $\psi(R, \theta, \phi) = \Phi(R) Y(\theta, \phi)$ and is expressed in spherical coordinates. Using the substitution $u(R)/R = \Phi(R)$, the radial Schrödinger equation is given by (Landau and Lifshitz, 1977)

$$\left(\frac{d^2}{dR^2} + \frac{2\mu}{\hbar^2} (E - V(R)) - \frac{J(J+1)}{R^2} \right) u_{E,J}(R) = 0, \quad (2.7)$$

where μ is the reduced mass of the two atoms and J is the angular momentum number. The collisional energy E is often written in terms of the wave number k , defined by $k = \sqrt{2\mu E}/\hbar$. In general, this equation has to be solved numerically, as further discussed for two colliding lithium atoms in Chapter 7. However, for short-range potentials the asymptotic solution for $R \rightarrow \infty$ assumes a simple analytic form according to

$$u_{E,J}(R) = A \sin \left(kR - \frac{J\pi}{2} + \delta_J(k) \right), \quad (2.8)$$

where A is a normalization factor and δ_J is the collisional phase shift. This parameter describes the effect of the scattering event on the wave function at distances R , where the interaction potential can be neglected. For this reason, $u_{E,J}(R)$ coincides asymptotically with the shape of a free wave function, which is obtained from the Schrödinger equation 2.7 with $V(R) = 0$. For many applications the scattering wave function is normalized with respect to the energy, which is defined according to

$$\int_0^\infty u_{E',J}(R) u_{E,J}(R) dR = \delta(E' - E), \quad (2.9)$$

where δ is the Dirac delta function. For the normalization coefficient of the asymptotic wave function given in Eq. (2.8) one obtains $A = \sqrt{2\mu/\pi k \hbar^2}$ (Côté, 1995).

The angular momentum term $J(J+1)/R^2$ in the radial Schrödinger equation (2.7) adds a repulsive contribution to the effective potential. For low collisional energies E this prevents

atoms from reaching small separations where the mutual interatomic interaction potential becomes relevant. For ultracold atoms, this often restricts the scattering to occur with zero angular momentum J , which is referred to as s -wave scattering. For small k , the collisional phase shift can then be expressed according to the *effective range* expansion (Landau and Lifshitz, 1977)

$$k \cot \delta_0(k) \underset{k \rightarrow 0}{=} -\frac{1}{a} + \frac{1}{2} r_e k^2 + \dots, \quad (2.10)$$

where a is the s -wave scattering length and r_e is the effective range of the interaction potential. The scattering length follows from the limiting case and is given by $a = -\lim_{k \rightarrow 0} \tan \delta_0(k) / k$ and the asymptotic wave function assumes the simple form $u_{E,J}(R) = A \sin[k(R - a)]$. A negative (positive) scattering length corresponds to an effectively attractive (repulsive) interaction potential (Duine and Stoof, 2004).

2.2.2. Scattering cross section

The collisional properties of a trapped atomic cloud can be related to the scattering wave function given in Eq. (2.8). For this, the solution Ψ of this process is expressed by

$$\Psi \approx e^{ikz} + f(\theta) \frac{e^{ikr}}{r}, \quad (2.11)$$

where the first term represents an incoming plane wave, with wave number k , propagating along the z axis and the second term corresponds to the scattered fraction in the form of an outgoing spherical wave. Using the cylindrical symmetry of the problem, the scattering amplitude can be decomposed into a series of partial waves given by $f(\theta) = \sum_{J=0}^{\infty} (2J+1) f_J P_J(\cos\theta)$, where $P_J(\cos\theta)$ are the Legendre polynomials (Landau and Lifshitz, 1977). A relation between the total scattering cross section σ and the phase shift δ_J is established via

$$\sigma = \sum_{J=0}^{\infty} \frac{4\pi (2J+1)}{k^2 \cot^2 \delta_J + k^2}, \quad (2.12)$$

where the summands correspond to the partial-wave scattering cross sections σ_J . For s -wave scattering, the effective range expansion given in Eq. (2.10) can be used to obtain

$$\sigma_0(k) = \frac{4\pi a^2}{1 + k^2 a^2 (1 - r_e/a) + \dots}, \quad (2.13)$$

which shows that even for a diverging scattering length a , the value of the s -wave cross section remains finite and is *unitarity* limited by $4\pi/k^2$.

These relations for the scattering cross sections are valid under the assumption of distinguishable particles and have to be modified to account for the fermionic and bosonic nature of the colliding atoms. For identical fermions (bosons) in identical internal states, the spatial wave function has to be antisymmetric (symmetric) under exchange of the two atoms, which restricts them to scatter via odd (even) partial waves. For identical fermions this implies that the scattering processes are restricted to partial waves with J larger than zero, which are greatly suppressed at ultralow temperatures. However, s -wave scattering is allowed for identical fermions in different internal states and the cross section for distinguishable particles is recovered (Walraven, 2014).

Elastic scattering rate The efficiency of evaporative cooling depends on the rate at which elastic collisions occur, as they re-establish a thermal equilibrium in the trapped gas. This rate can be calculated by $\gamma_{el} = nv_{rel}\sigma$, where $v_{rel} = \sqrt{16k_B T/\pi m}$ is the average relative speed of two atoms (Luo et al., 2006). The density, and consequently also the scattering rate, depend on the position within the trap and therefore a trap-averaged value should be used. For a harmonically confined atomic cloud the averaged density can be calculated using Eq. (2.3) for the phase-space occupancy, resulting in

$$\bar{n} = \frac{1}{(2\pi\hbar)^3} \frac{1}{Z_1} \int d\mathbf{r} d\mathbf{p} n(\mathbf{r}) e^{-H_0(\mathbf{r},\mathbf{p})/k_B T} = \frac{n_0}{2\sqrt{2}}. \quad (2.14)$$

Using this result in the relation for the elastic scattering rate yields an expression for the averaged collisional rate in a harmonic trap:

$$\overline{\gamma_{el}} = \frac{Nm\bar{\omega}^3\sigma}{2\pi^2 k_B T} \quad (2.15)$$

Specifically, for a balanced mixture of two spin states of identical fermions, the elastic scattering rate is calculated with the cross section given in Eq. (2.13) and with the number of atoms N per spin state (O'Hara et al., 2001a).

2.3. Ideal quantum gas in a harmonic trap

At high temperatures with $\Lambda_T^3 n_0 \ll 1$, a trapped atomic cloud can be described in the classical limit, as shown in Section 2.1. This description is valid for various stages of our experiment, in particular when the atoms are confined in the magneto-optical trap or in the optical dipole trap before evaporative cooling. However, as the temperature is reduced the underlying quantum nature of the atoms has to be considered in order to accurately describe the properties of the physical system. Once the length scales of the thermal de Broglie wavelength Λ_T and the average atomic separation in the dilute gas become comparable, the wave functions of the atoms start to spatially overlap such that they have to be considered as being indistinguishable.

Statistical description Here, the investigated system is a harmonically trapped ideal spin-polarized Fermi gas, which implies that all atoms are in the same internal state. The statistical description of the trapped quantum gas is preferentially performed in the grand canonical ensemble with the intensive thermodynamic properties of temperature T and chemical potential μ (Schwabl, 2006). Assuming that the energy level spacing of the harmonic trap $\hbar\omega$ is much smaller than the thermal energy $k_B T$, it is permissible to use continuous variables for position and momentum ($\mathbf{r}, \mathbf{p}$) for the atoms. This is a semiclassical approximation (Thomas-Fermi approximation) which was discussed in more detail by Butts and Rokhsar (1997). The phase-space occupancy can then be expressed according to

$$f(\mathbf{r}, \mathbf{p}) = \frac{1}{e^{(\mathbf{p}^2/2m + U(\mathbf{r}) - \mu)/k_B T} + 1} , \quad (2.16)$$

where $U(\mathbf{r})$ is the harmonic potential defined in Section 2.1. For an ideal Bose gas the '+'-sign in the denominator is replaced by a '-'-sign and was, for example, discussed by Pethick and Smith (2008).

Density distribution The integration of $f(\mathbf{r}, \mathbf{p})$ over the momentum space yields the density distribution of the confined ideal gas according to

$$n(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f(\mathbf{r}, \mathbf{p}) = -\frac{1}{\Lambda_T^3} \text{Li}_{3/2} \left(-e^{(\mu - U(\mathbf{r}))/k_B T} \right) . \quad (2.17)$$

The n^{th} Polylogarithm is given by $\text{Li}_n(z) = \frac{1}{\pi^n} \int d^{2n}q \frac{1}{z^{-1}e^{\mathbf{q}^2} - 1}$, which is valid for $z < 1$ (Ketterle and Zwierlein, 2008). As a direct consequence of quantum statistics, the shape of the atomic cloud deviates from a Gaussian distribution obtained for a harmonically confined classical gas. At ultracold temperatures, bosons may undergo a phase transition and form a Bose-Einstein condensate (BEC), which is accompanied by a remarkable change in the spatial density distribution of the gas. However, the ideal Fermi gas does not undergo any phase transition even in the limit $T \rightarrow 0$ and the corresponding change in the shape of the atomic cloud is more subtle at low temperatures.

The Fermi gas is experimentally probed via absorption imaging, which is described in Section 3.5. The retrieved images show a two-dimensional profile that is related to the density distribution integrated along the line-of-sight and are used to extract thermodynamic properties. Formally, these integrated profiles can be calculated from the density distribution $n(\mathbf{r})$, where $\int_{-\infty}^{\infty} dx \text{Li}_n(ze^{-x^2}) = \sqrt{\pi} \text{Li}_{n+1/2}(z)$ proves to be a useful identity for the Polylogarithm. For the harmonically confined Fermi gas, the column density $n_{2D}(x, y)$, the projected line profile $n_{1D}(x)$ and the total number of atoms N are given by:

$$n_{2D}(x, y) = -\frac{1}{\Lambda_T^2} \frac{k_B T}{\hbar} \frac{1}{\omega_z} \text{Li}_2 \left(-e^{\mu/k_B T} e^{-\frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2)/k_B T} \right) \quad (2.18)$$

$$n_{1D}(x) = -\frac{1}{\Lambda_T} \left(\frac{k_B T}{\hbar} \right)^2 \frac{1}{\omega_y \omega_z} \text{Li}_{5/2} \left(-e^{\mu/k_B T} e^{-\frac{m}{2}\omega_x^2 x^2/k_B T} \right) \quad (2.19)$$

$$N = -\left(\frac{k_B T}{\hbar \bar{\omega}} \right)^3 \text{Li}_3 \left(-e^{\mu/k_B T} \right) \quad (2.20)$$

The last equation establishes a relation between the atom number and the chemical potential and can also be used to infer the Fermi energy E_F . In the temperature limit of $T \rightarrow 0$, states that are energetically below μ are occupied with unit probability, while states above this threshold remain empty. This follows from the distribution function $f(\mathbf{r}, \mathbf{p})$ given in Eq. (2.16) and defines the Fermi energy. For the harmonically confined spin-polarized Fermi gas, the Fermi energy is given by

$$E_F = \mu = (6N)^{1/3} \hbar \bar{\omega}, \quad (2.21)$$

where $\bar{\omega}$ is the geometric mean of the trap frequencies. This corresponds to the highest single-particle energy at zero temperature and the associated Fermi wave vector is defined by $k_F = \sqrt{2mE_F}/\hbar$.

In the experiment, the atomic density profile is generally recorded during a ballistic expansion of the gas after the trapping potential was suddenly switched off. An atom with momentum $\mathbf{p}_0$ that is originally at $\mathbf{r}_0$ in the trap propagates to $\mathbf{r} = \mathbf{r}_0 + \frac{\mathbf{p}_0}{m}t$ during the time-of-flight t . Specifically, for the projected density profile, one finds:

$$n_{1D}(x, t) = -\frac{1}{\Lambda_T} \left(\frac{k_B T}{\hbar} \right)^2 \frac{1}{\omega_y \omega_z \sqrt{1 + t^2 \omega_x^2}} \text{Li}_{5/2} \left(-e^{\left(\mu - \frac{m}{2} \frac{\omega_x^2 x^2}{1 + t^2 \omega_x^2} \right) / k_B T} \right). \quad (2.22)$$

This relation shows that the trap frequencies of the confinement potential have to be known in order to extract physical quantities from the observed density distributions.

Density profile of BEC Fermionic atoms close to a Feshbach resonance can form weakly bound bosonic molecules, as discussed in more detail in Section 2.3.1. Because these molecules obey the Bose-Einstein statistics, they can form a BEC at sufficiently low temperatures. Starting from the phase-space occupancy for a bosonic gas in a harmonic potential, one finds for the number of atoms

$$N = \left(\frac{k_B T}{\hbar \bar{\omega}} \right)^3 \text{Li}_3 \left(e^{\mu / k_B T} \right), \quad (2.23)$$

which is similar to the relation for the Fermi gas. However, for bosons the chemical potential μ is restricted to non-positive values and the polylogarithm approaches a maximum value in the limit of $T \rightarrow 0$, given by $\text{Li}_3(e^{\mu / k_B T}) \leq \text{Li}_3(1) \approx 1.202$. This limits the number of atoms that can be accounted for by the statistical description $f(\mathbf{r}, \mathbf{p})$, which does not include the occupation of the ground state. The total number of atoms is therefore expressed as a sum given by $N_{\text{tot}} = N + N_0$, where N_0 is the number of atoms occupying the ground state of the system. For a macroscopic occupation of the ground state, the chemical potential μ can be set to zero and it follows (Bagnato et al., 1987)

$$\frac{N_0}{N_{\text{tot}}} = 1 - \left(\frac{T}{T_C} \right)^3, \text{ with } T_C = \frac{\hbar \bar{\omega}}{k_B} \left(\frac{N}{1.202} \right)^{1/3}, \quad (2.24)$$

which describes the fraction of atoms occupying the ground state as a function of the temperature T below the critical temperature T_C .

For the ideal Bose gas, the density profile of the BEC is determined by the ground-state wave function of the harmonic potential. However, the interaction energy between the particles generally exceeds the kinetic energy in a BEC and therefore has to be considered in the description of the density distribution. For short-range interactions and densities with $n^{1/3}a \ll 1$, a mean-field approach can be used to determine the macroscopic wave function $\phi(\mathbf{r})$, expressed by the Gross-Pitaevskii equation (Pethick and Smith, 2008)

$$\left(U(\mathbf{r}) + g|\phi(\mathbf{r})|^2 \right) \phi(\mathbf{r}) = \mu\phi(\mathbf{r}) , \quad (2.25)$$

where the kinetic energy term is neglected according to the Thomas-Fermi approximation. The interaction energy is represented by the non-linear effective interaction term $gn(\mathbf{r}) = g|\phi(\mathbf{r})|^2$ with $g = 4\pi\hbar^2 a/m$. The solution for the density distribution is therefore given by

$$n_c(\mathbf{r}) = \text{Max} \left(\frac{\mu - U(\mathbf{r})}{g}, 0 \right) . \quad (2.26)$$

The density distribution of a weakly interacting BEC in a harmonic potential is defined by an inverted parabola for $r_i \leq R_i$ and zero outside this range, where the 'Thomas-Fermi' radius is given by $R_i = \sqrt{2\mu/m}/\omega_i$. For the molecular BEC discussed in Chapter 5, the mass m in this relation corresponds to the molecular mass, therefore twice the atomic value. While the confinement potential $U(\mathbf{r})$ is twice the value for molecules as compared to the atoms, the trap frequencies ω_i remain unchanged (Jochim et al., 2003b).

During a ballistic expansion after rapidly switching off the trapping potential, the initially condensed cloud maintains a parabolic shape with rescaled radii during a time-of-flight (TOF) measurement (Castin and Dum, 1996; Kagan et al., 1996). Generally, the atomic or molecular clouds are only partially condensed, such that also a thermal fraction is present. This fraction is often assumed to approximately follow a Gaussian distribution (Bourdel et al., 2004; Ketterle et al., 1999), which also preserves its shape during a TOF expansion (Weiss et al., 1989). The resulting fitting function for the observed density profiles can therefore be expressed as a sum of a Gaussian distribution and the Thomas-Fermi profile given in Eq. (2.26).

2.3.1. Feshbach resonances and BEC-BCS crossover

The scattering length a and the scattering cross section σ of atoms are determined by the internuclear potential under which influence they collide. It can be shown that if this potential supports a bound state with a binding energy E_B just below the collisional continuum, then the scattering length is positive and its value is given by $a^2 = -\hbar^2 / (2\mu E_B)$, where μ corresponds here to the reduced mass of the atoms (Duine and Stoof, 2004). Conversely, a negative scattering length results if the potential has a virtual bound state just above the continuum.

Feshbach resonances

The internuclear potential cannot be changed and therefore E_B and a are fixed for a given potential. However, if the colliding atoms are coupled to a bound state of another potential, the scattering length can be resonantly enhanced. For a magnetic Feshbach resonance, the principle is as follows. Alkali-metal atoms in the ground state collide either via a singlet or a triplet potential, where the symmetry refers to the combined electronic spin state of the two atoms. These potentials are generally sufficiently deep in order to support multiple bound states, and it can be shown that the hyperfine interaction can provide a weak coupling between states of the two potentials (Tiesinga et al., 1993). If the potentials have a different magnetic moment, then an applied magnetic field can shift the energy levels of the respective potential against each other. At a given magnetic field, the atoms collide via continuum states of one potential (*open channel*), while the scattering states of the other potential are energetically not accessible (*closed channel*). If the magnetic field is changed such that a bound state of the closed channel energetically aligns with the continuum state of the open channel, then the scattering can be resonantly enhanced because of the mutual coupling. A more detailed description of Feshbach resonances was given, for example, in articles by Duine and Stoof (2004), Köhler et al. (2006) and Chin et al. (2010).

At high magnetic fields, the two energetically lowest hyperfine states of ^6Li have the same electronic spin projection $m_s = -1/2$ and are labeled with $|1\rangle$ and $|2\rangle$ (see appendix A.1). Atoms of a $|1\rangle$ - $|2\rangle$ mixture therefore interact via the triplet potential (open channel) and the continuum scattering states of the singlet potential are energetically not accessible (closed channel). To access a Feshbach resonance, the magnetic field can now be varied in order

to change the relative value of the potential energy curves, which brings a bound state into resonance with the continuum triplet state (Houbiers et al., 1998; Julienne and Hutson, 2014). The resulting magnetic field dependence of the scattering length in the vicinity of the Feshbach resonance can be approximated by (Chin et al., 2010)

$$a(B) = a_{\text{bg}} \left(1 - \frac{\Delta}{B - B_0} \right), \quad (2.27)$$

where a_{bg} is the scattering length of the open channel far away from resonance, Δ is the width, and B_0 is the position of the Feshbach resonance. An incoherent mixture $|1\rangle - |2\rangle$ of ^6Li atoms has a Feshbach resonance at $B_0 = 832.2 \text{ G}$ with $\Delta = -262.3 \text{ G}$ and $a_{\text{bg}} = -1582a_0$ (Zürn et al., 2013). This Feshbach resonance is said to be *broad* and open-channel dominated, which means that the scattering properties of the atoms near the resonance can be described by a single channel interacting via an effective potential (Ketterle and Zwerlein, 2008). The admixture of the closed channel to this scattering state is small and was experimentally measured by Partridge et al. (2005). This provides ideal conditions for the investigation of the strongly interacting regime of the 'BEC-BCS' crossover physics.

BEC-BCS crossover

Close to a Feshbach resonance, an ultracold Fermi gas can enter the strongly interacting regime where quantum many-body effects play an important role (Bloch et al., 2008). This range is accessed when the scattering length between the atoms becomes comparable or exceeds the interparticle spacing. At a typical density on the order of 10^{13} cm^{-3} of a trapped atomic cloud, this corresponds to an average separation of about 9000 Bohr radii a_0 . It follows from Eq. (2.27) that the s -wave scattering length a close to a Feshbach resonance diverges, as illustrated in appendix A.4 for the $|1\rangle - |2\rangle$ mixture of ^6Li (Zürn et al., 2013).

A particular appeal of the strongly interacting Fermi gas is its stability against collisional losses near a Feshbach resonance (Bourdel et al., 2003; Cubizolles et al., 2003; Dieckmann et al., 2002), which is in strong contrast to the Bose gas (Stenger et al., 1999). An inelastic collisional loss process generally results in the formation of a deeply bound diatomic state. Because of energy and momentum conservation, at least three particles have to be present within a small volume element for this process to occur. For a Fermi gas comprising one or two spin states, this process incorporates at least two identical particles and is accordingly

suppressed because of Pauli's exclusion principle (Petrov et al., 2004).

On the side of the Feshbach resonance with a positive scattering length a , the effective interaction potential supports a two-body bound state and allows the formation of bosonic molecules. At sufficiently low temperatures, the ground state of the system is a molecular Bose-Einstein condensate (mBEC). On the other side for the resonance, with $a < 0$, an effectively attractive interaction between the atoms is realized and a pairing of the atoms occurs here because of a many-body effect. In the limit of weak attractive interactions, the ground state of the system is a superfluid of weakly bound Cooper pairs described by the Bardeen-Cooper-Schrieffer (BCS) model (Nozière and Schmitt-Rink, 1985).

BEC limit Weakly bound Feshbach molecules can be formed as follows. A Fermi gas is first evaporatively cooled on the $a < 0$ side of the resonance before a magnetic field ramp is performed to adiabatically transfer the atoms into a weakly bound molecular state on the $a > 0$ side (Cubizolles et al., 2003; Regal et al., 2003). However, the collisional properties of ^6Li allow for a shortcut to this scheme and evaporation of the atomic cloud can be performed directly on the $a > 0$ side to create a molecular sample (Chin and Grimm, 2004; Jochim et al., 2003a).

For $|k_F a| \ll 1$ the gas enters the BEC limit, where the binding energy increases and the size of the molecular atom pair becomes much smaller than the average separation between two such Feshbach molecules. The s -wave scattering length between the molecules is found to be $a_{\text{mol}} = 0.6 a_{12}$ such that the effective interaction is repulsive (Petrov et al., 2004). At sufficiently low temperature, the trapped gas can therefore undergo a phase transition to form a stable molecular BEC (Greiner et al., 2003; Jochim et al., 2003b).

BCS limit Weak attractive interactions on the $a < 0$ side of the Feshbach resonance can support bound states for fermions of opposite spin and momentum on top of a filled Fermi sea, leading to a paired ground state of the Fermi gas (Bardeen et al., 1957; Ketterle and Zwierlein, 2008). The binding energy of these pairs depends exponentially on the interaction term $1/(k_F a)$ and is related to the superfluid critical temperature given by $k_B T_c = 0.28 E_F e^{\pi/2 k_F a}$ (Giorgini et al., 2008; Nozière and Schmitt-Rink, 1985).

The experimental proof of the superfluid phase on the BCS side of the resonance is more challenging than the detection of a BEC on the $a > 0$ side. While a change in the density

profile of the atoms is predicted (Chiofalo et al., 2002), this seems difficult to suffice as a proof of superfluidity. Pioneering measurements of the heat capacity and the temporal evolution of an expanding ultracold Fermi cloud were consistent with a superfluid phase (Kinast et al., 2005; O’Hara et al., 2002), however, only the emergence of a vortex lattice in a rotating gas served as a direct proof of superfluidity (Zwierlein et al., 2005).

Crossover While the s -wave scattering length diverges close to the Feshbach resonance, the scattering cross section is unitarity-limited by $\sigma_0 = 4\pi/k^2$. In this regime, characterized by $1/k_F |a| \ll 1$, neither the BEC nor the BCS description is applicable. However, it was shown experimentally that the physical system evolves smoothly from one limit to the other (Bourdel et al., 2004).

The thermodynamic properties of the unitary Fermi gas assume universal character, which means that they are independent of the atomic species or the details of the interaction potential (Bloch et al., 2008; Ho, 2004). Interestingly, in the limit at zero temperature the chemical potential μ can be related to the Fermi energy of a noninteracting gas with a single parameter via $\mu = \xi(0)$. An experimental measurement with ^6Li resulted in a value of $\xi(0) = 0.37$ (Ku et al., 2012; Zürn et al., 2013), which agrees well with a recent theoretical calculation (Carlson et al., 2011). A comprehensive description of this smooth BEC to BCS crossover is given in review articles by Chin et al. (2010), Bloch et al. (2008), Köhler et al. (2006) and Giorgini et al. (2008).

3. Experimental setup and techniques

In this chapter the experimental apparatus for the production and investigation of a quantum degenerate ^6Li gas is described. First, an overview of the experimental sequence to reach quantum degeneracy is given, which establishes the requirements for the setup. Then, the laser systems for the atomic $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ and $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transitions are described. These transitions correspond to realizations of the magneto-optical trap with light at 671 nm and 323 nm, respectively, with a partial level scheme of ^6Li illustrated in Fig. 3.2. This is followed by a discussion of an optical dipole trap for transporting the atoms and an implemented ion detection scheme for a spectroscopy measurement.

3.1. Production of a quantum degenerate Fermi gas

Selection of ^6Li as atomic species Among the alkali-metals, only lithium and potassium offer stable fermionic isotopes. Both have accessible Feshbach resonances (Houbiers et al., 1998; Regal and Jin, 2003) and are therefore suited to investigate quantum many-body physics (Bloch et al., 2008). The BEC-BCS crossover regime has been studied with either isotope, however, ^6Li offers especially favorable properties and is chosen for our experiment. The ^6Li Feshbach resonance is exceptionally broad and strongly open channel dominated across more than half of its width ΔB (Chin et al., 2010), which is advantageous for the study of the BEC-BCS crossover. Furthermore, the lifetime of the trapped sample on the molecular side of the resonance was found to be on the order seconds (Ketterle and Zwerlein, 2008), while reported values for ^{40}K are a few tens of milliseconds (Regal et al., 2004).

Quantum degenerate Fermi gases have also been realized with strontium ^{87}Sr and ytterbium $^{173}\text{Yb}/^{171}\text{Yb}$, which are alkaline-earth metal atoms (DeSalvo et al., 2010; Fukuhara et al., 2007). The total electron spin of these atoms is zero such that they do not have magnetic Feshbach resonances. However, optical Feshbach resonances are explored for such atomic

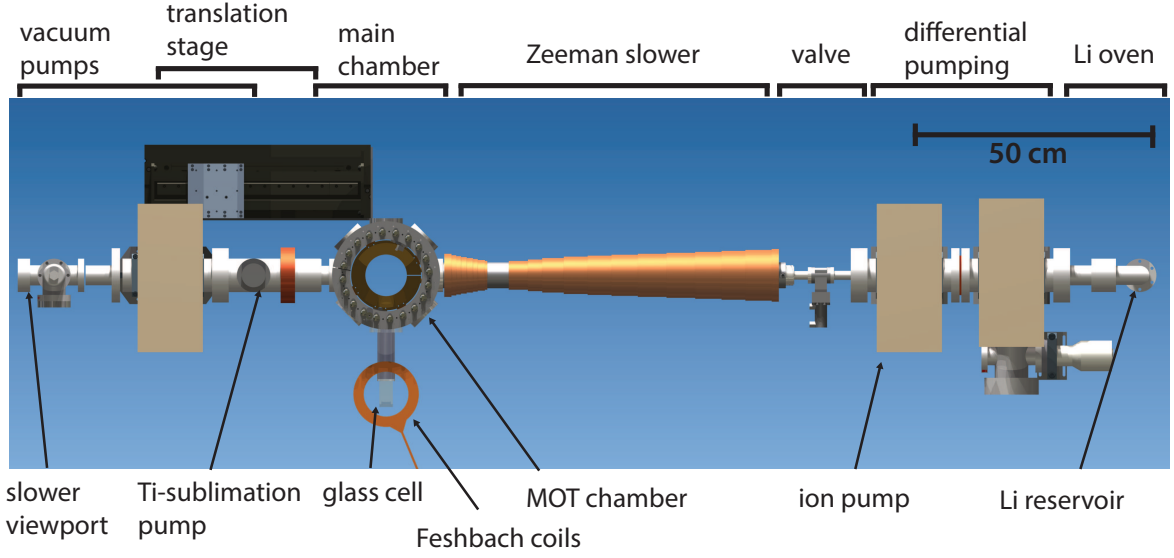


Figure 3.1.: Top view of the experimental setup. In addition to the vacuum setup, only the air bearing linear translation stage is shown, which is placed close to the MOT chamber. The different sections and key experimental components of the apparatus are indicated and described in the text.

species, which allows tuning of the interaction strength (Enomoto et al., 2008; Zhang et al., 2015).

Overview of all-optical experimental sequence

The general structure of our experimental setup is defined by our cooling and trapping scheme for ^6Li with the additional requirement of an unrestricted optical access to the quantum gas. An overview of the setup is shown in Fig. 3.1 and the different indicated sections are described in the course of this chapter. In order to realize a short measurement duty cycle and to keep the experimental complexity low, an all-optical cooling and tapping approach is chosen (Barrett et al., 2001). Therefore, the atoms are directly transferred into an optical dipole trap (ODT) after the laser cooling stage in the magneto-optical trap (MOT) without intermediate steps. This avoids the need for deep magnetic traps and, in the case of ^6Li , the need for a second atomic species for sympathetic cooling, as outlined by Ketterle and Zwierlein (2008).

Atom source In the oven section of the setup, a few grams of lithium are heated beyond the melting point in order to create a high partial pressure of atomic lithium. After a series of collimation tubes and differential pumping stages, an atomic beam enters the Zeeman slower, which is part of the main section of the vacuum assembly. The atoms are decelerated by a counter-propagating laser beam that enters the chamber via the slower viewport, as indicated

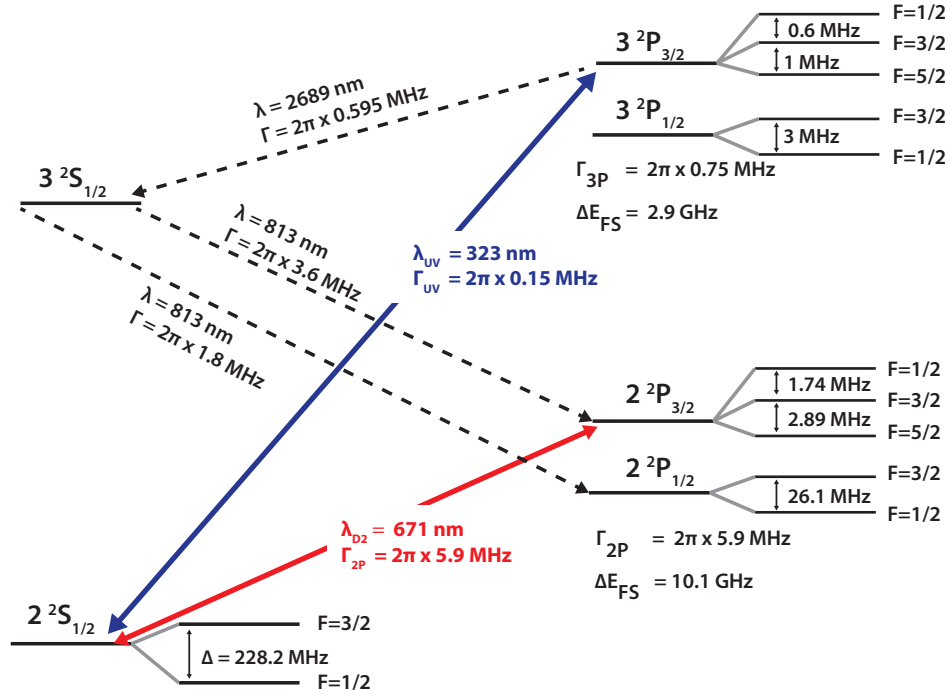


Figure 3.2.: Partial level structure of ${}^6\text{Li}$ highlighting the two laser cooling transitions at a wavelengths λ_{D2} and λ_{UV} . The natural linewidth Γ and the fine structure interval ΔE_{FS} of the respective excited state are provided and an alternative decay path for the $3P$ state is indicated (Kramida et al., 2016).

in Fig. 3.1. A spatially varying magnetic field compensates for the changing Doppler shift and keeps the atoms in resonance with the laser light during the propagation and slowdown along the Zeeman slower.

Standard magneto-optical trap The Zeeman-slowed atomic beam is then captured by a MOT consisting of three pairs of counter-propagating laser beams and a magnetic field gradient that is produced by two coils in anti-Helmholtz configuration, as illustrated in Fig. 3.3. In this initial phase the MOT is realized with light on the conventional D_2 transition at 671 nm, to which we refer to as the *red* MOT. Laser cooling is performed on the $2^2S_{1/2}, F = 3/2 \rightarrow 2^2P_{3/2}, F = 5/2$ line, as it offers a closed transition for circular polarized light. However, due to the largely unresolved hyperfine structure of the $2^2P_{3/2}$ state (see Fig. 3.2), the probability of exciting the $F = 3/2$ state is high and the atom can decay into the $F = 1/2$ ground state. Therefore, a repumping laser on the $2^2S_{1/2}, F = 1/2 \rightarrow 2^2P_{3/2}$ of similar intensity and equal polarization as the cooling beam has to be provided along all six directions. Both beams contribute significantly to the cooling process and the distinction between *cooling* and *repumping* light is mostly a convention for lithium. After a compressed

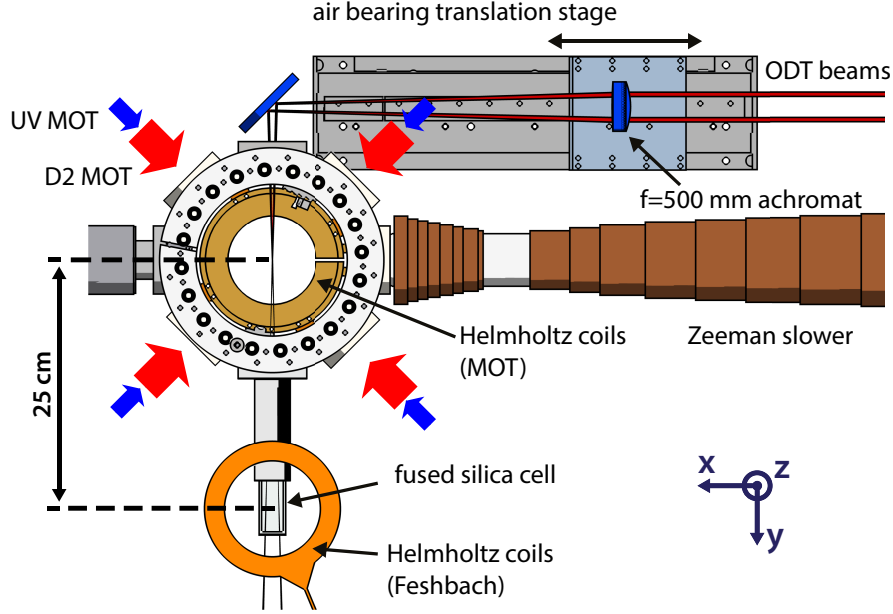


Figure 3.3.: Modular design of experimental apparatus. An atomic lithium cloud is laser cooled on the standard D_2 and on the narrow UV transition, and then transferred into a crossed ODT. Subsequently, the atomic cloud is transported from the MOT chamber into an attached fused silica cell by moving the focusing lens for the ODT with an air bearing stage. The true position of the stage in the experimental setup is shown in Fig. 3.1.

MOT (CMOT) phase, the temperature of the atomic cloud is typically on the order of $300 \mu\text{K}$, which is about twice the Doppler limit of $140 \mu\text{K}$ for ^6Li .

Unlike for other alkali-metal atoms such as rubidium or sodium, sub-Doppler cooling is absent for ^6Li due to the unresolved hyperfine structure of the excited state, as briefly discussed in Chapter 4. An efficient direct loading into an ODT requires therefore a comparatively deep potential to confine the atoms, because the depth should exceed the temperature of the atomic ensemble by a factor of about 5-10. A sufficiently deep trap for a lithium cloud at this temperature can be achieved by a small radius and a high optical power of the ODT beam (Gunton et al., 2013b; Huckans et al., 2009) or by a resonator enhanced optical dipole trap (Mosk et al., 2001; Zimmermann et al., 2011).

UV cooling of ^6Li In our all-optical approach we instead employ a second laser cooling stage after the red MOT in order to obtain lower temperatures of the atomic cloud and therefore to achieve better conditions for loading of the optical dipole trap. For this, we drive the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ MOT transition at 323 nm, which was first demonstrated by Duarte et al. (2011). This wavelength is in the ultraviolet (UV) regime and we refer to this stage as the *UV* MOT. The excited state of this transition has natural linewidth of $\Gamma_{3P}/(2\pi) = 754 \text{ kHz}$, which

is about 8 times smaller as compared to the one of the $2P$ state and has a correspondingly reduced Doppler temperature of $18\ \mu\text{K}$. Laser cooling on this transition also leads to higher densities and is described in detail in Chapter 4.

Loading of ODT and optical transport The enhanced phase-space density of the atomic sample after UV laser cooling facilitates loading of a large number of atoms into a small-angle crossed ODT with a moderate 22.5 W per beam. The wavelength of the trapping light is 1070 nm, which is close to a magic wavelength of the UV cooling transition (Safronova et al., 2012). Therefore, the differential ac Stark shift is small and allows continued laser cooling in the ODT (Duarte et al., 2011). In a next step, the atoms are transported into a glass cell that is attached to the MOT chamber, as indicated in Fig. 3.3. We can use the initial trapping configuration for this purpose, which is created by using a single lens, mounted on a linear translation stage, to cross and focus the two beams for the ODT. These beams are aligned through the center of both the MOT chamber and the glass cell. The ODT is initially crossed in the MOT chamber and the atomic cloud is transported by moving the lens, which displaces the focus and the intersection point of the two beams.

Glass cell The main motivation for such a modular design of the vacuum chamber is the excellent optical access provided by the glass cell. In addition to the possibility of high-resolution imaging, the optical access offers optimal conditions to create a wide range of optical potentials for the atoms via the introduction of laser beams. The good optical access in this approach is achieved because constraints imposed by magneto-optical trapping and pre-cooling are circumvented by a dedicated science chamber. Furthermore, the spatial separation from the region where the cold atomic cloud is produced increases the flexibility of the experiments that can be performed, which is an important factor in the rapidly evolving research field of quantum gases.

Evaporative cooling and Feshbach resonance The atomic sample is prepared in a $|1\rangle - |2\rangle$ spin mixture of the two energetically lowest hyperfine states of ^6Li and the s -wave scattering length a_{12} is tuned by applying a magnetic field, as shown in appendix A.2. A pair of coils in Helmholtz configuration around the glass cell allows the application of magnetic bias fields of up to 1300 G to access the broad Feshbach resonance at 832 G (Zürn et al., 2013) and the

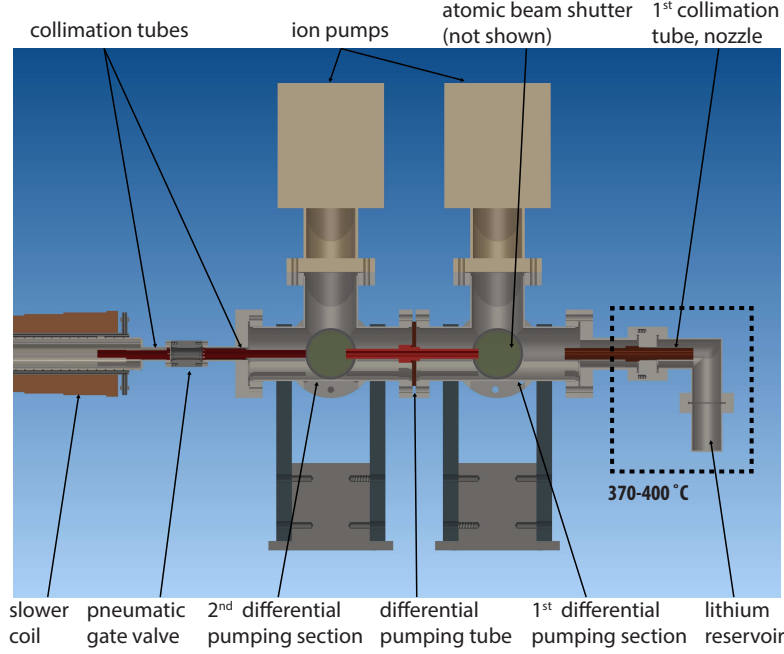


Figure 3.4.: Atom source of the experiment. The lithium reservoir is heated to 370 °C and produces an atomic beam. Two separate differential pumping sections with multiple collimation tubes ensure a large pressure drop to the main chamber with a background pressure on the order of 1×10^{-11} mbar.

region beyond. Forced evaporative cooling is initiated by lowering the optical power of the ODT and by applying a magnetic field to increase the elastic scattering rate. To create a weakly interacting Fermi gas, evaporation is performed at 330 G, where the scattering length a_{12} has a local minimum, as shown in appendix A.3. Evaporation is performed near the Feshbach resonance to produce a strongly interacting sample in the BEC-BCS regime.

3.2. Vacuum chamber and magnetic field coils

3.2.1. Atomic ^6Li source

The atom source for the experiment consists of a lithium reservoir, a differential pumping section and the Zeeman slower, as illustrated in Fig. 3.1. These components are based on the apparatus described in the PhD thesis of Taglieber (2008) and, with the exception of the extended differential pumping stage, are very similar to the current setup.

Lithium reservoir The lithium oven consists of a capped, vertically arranged stainless steel tube that is connected to the next chamber section via a 20 cm long nozzle with an inner diameter of 6 mm, as illustrated in Fig. 3.4. Around 5-10 g of enriched ^6Li with an isotopic purity of 95 % (Sigma-Aldrich Co.) are heated to 370 °C, which is well beyond the melting

point of 185 °C. This leads to a calculated partial pressure of around 4×10^{-5} mbar in the oven section (Alcock et al., 1984). In order to avoid deposition of lithium in the nozzle and a clogging of the tube, its temperature is regulated to be 40 °C above temperature of the lithium sample. This nozzle is machined from oxygen free copper to ensure an optimal temperature uniformity and a low outgassing rate.

Differential pumping The high temperature of the oven section, highlighted by the dashed rectangle in Fig. 3.4, leads to an increased outgassing rate from the vacuum components on either side of the nozzle. This severely compromises the quality of the vacuum and limits the attainable background pressure to roughly 1×10^{-8} mbar.

To reduce the diffusion of molecules of the background gas into the main section of the experiment without compromising the flux of the directional atomic beam, a narrow tube is used to connect the different chambers. The conduction through the tube of length l and diameter d is described by molecular flow and can be calculated by $C = \frac{\pi}{12} \bar{v} \frac{d^3}{l}$ (Moore et al., 2009). The mean velocity $\bar{v}$ depends on the composition of the background gas, which is dominated by molecular hydrogen. The pressure ratio in the different sections of the chamber is determined by the relation $P_1/P_2 = S/C$, where S is the pumping speed of the vacuum pump in the section with pressure P_2 .

The tube connecting the first with the second differential pumping section, illustrated in Fig. 3.4, has a length of 17 cm and a diameter of 7 mm. The two differential pumping tubes at the beginning of the Zeeman slower have a diameter of 7 mm and a length of 13 cm and 9 cm, respectively. All ion pumps (VacIon Plus 75 StarCell) have a nominal pumping speed for hydrogen of 65 l/s, resulting in an overall pressure ratio of about 1×10^4 . This value is consistent with the observation that the pressure reading from an ion gauge in the main chamber is independent on the state (open/closed) of a gate valve that is placed between the oven section and the Zeeman slower. This gate valve allows us to seal the main chamber from the oven section in order to refill the lithium reservoir, if this should be required in future.

Zeeman slower The number of windings for the Zeeman slower increases towards either end, as shown in Fig. 3.1. This configuration is called a spin-flip Zeeman slower, because the direction of the magnetic field is reversed along the axis. The differences and advantages of this design, as compared to a Zeeman slower with a monotonically decreasing magnetic

field strength (Barrett et al., 1991), are described in the PhD theses of Taglieber (2008) and Chikkatur (2002). On the technical side, this configuration reduces the required absolute field strength, however, an additional repumping laser beam on the $2^2S_{1/2}, F = 1/2 \rightarrow 2^2P_{3/2}$ transition has to be provided because of the zero crossing of the magnetic field.

The magnetic field strength $B(0)$ at the entrance of the Zeeman slower and the frequency detuning δ of the counter-propagating laser beam define the maximum velocity of an atom that can be decelerated. These values are experimentally optimized for the number of trapped atoms in the MOT and we obtained values of $B(0) = 580$ G for the magnetic field, corresponding to a current of 10 A, and $\delta = -520$ MHz for the detuning. This results in a calculated capture velocity of 900 m/s for the atoms.

3.2.2. MOT Chamber

Vacuum chamber The *MOT* or *main* chamber is a commercial stainless steel octagon (Kimball Physics Inc., MCF800). We use quartz viewports due to the higher transmission of UV light as compared to standard glass and due to the compatibility with high-power lasers in the infrared regime. The special design of the quartz viewports permits bake-out temperatures of more than 350 °C (Culham Centre for Fusion Energy). The anti-reflection (AR) coating covers a narrow spectral region around 323 nm and the full range from about 530 nm to 1100 nm with a reflectivity of less than 1% per surface (LENS-optics GmbH).

Magnetic field coils To generate a magnetic field gradient for the MOT and a bias field for evaporative cooling in the main chamber, a pair of coils in Helmholtz configuration is used. Each coil has 100 windings and is attached to a water-cooled mount. A switching circuit based on MOSFETs¹ allows us to reverse the polarity of one of the coils in order to change the magnetic field in the center of the chamber from a homogeneous field to a quadrupole configuration. The actively stabilized current generates an axial magnetic field gradient of $2 \text{ G cm}^{-1}/\text{A}$ or a bias field of 7.5 G/A .

An additional three pairs of coils are installed along the principal axes x , y , and z . These coils allow us to apply a magnetic bias field of up to 4 G in order to compensate for magnetic stray fields. Furthermore, a change of these fields during the experimental sequence shifts the position of the MOT, which is useful during the loading of the ODT.

¹Metal-oxide-semiconductor field-effect transistor

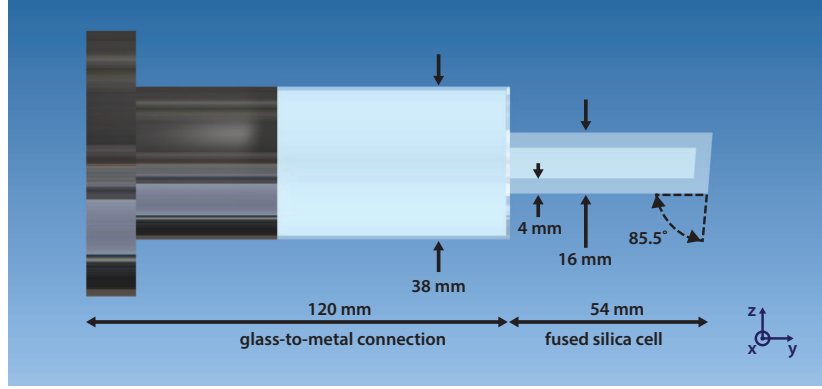


Figure 3.5.: 3D model of the fused silica science cell with relevant dimensions. The width of the cell (along the x axis) is 28 mm. A slight angle between the front face of the cell and the horizontal plane is introduced to prevent back-reflections of the trapping light onto the atomic cloud along the transport direction.

3.2.3. Science chamber

A small, custom-made fused silica cell (Starna Scientific Ltd.) is the final chamber for the atomic cloud. It is horizontally attached to the MOT chamber, as illustrated in Fig. 3.5, and in the following we refer to it as *science chamber* or *glass cell*. The atoms are transported from the MOT chamber into the glass cell in a crossed optical dipole trap, as illustrated in Fig. 3.3 and described in Section 3.6.

Design considerations High-resolution imaging of the atoms in the glass cell would be performed along the direction of gravity. For this reason, the height of the glass cell was chosen to be small. It is manufactured from 4 mm thick fused silica plates that are optically contacted and the distance from the center to the horizontal outer faces of the cell is 8 mm. This allows utilizing a microscope objective with a relatively short working distance, which is compatible with a system described by Zimmermann et al. (2011).

A requirement on the minimal width follows from the crossed optical dipole trap, which is used to transport the atoms, as shown in Fig. 3.3. A clipping of the beams at the edges of the front face of the cell should be avoided during the experimental cycle to minimize scattered light from the high-power ODT beam. However, a constraint on the maximum width follows from optical access considerations, in particular for the introduction of a vertical lattice to confine the atoms to two-dimensional layers. An ideal configuration to implement this, are two beams propagating in the xz -plane (see Fig. 3.5) that are crossed at the center of the cell. Based on the dimensions of our glass cell given in Fig. 3.5, an enclosed crossing angle of up

to 20° is possible, leading to lattice spacing of $3\text{ }\mu\text{m}$. Such a separation can be resolved with standard imaging techniques and allows for the characterization two-dimensional clouds, as demonstrated, for example, by [Martinyan et al. \(2010\)](#). Eventually, the length of 5 cm of the glass cell permits the introduction of a square optical lattice in the horizontal plane.

To attach the glass cell to the steel chamber, a glass-to-metal connection is required to match the thermal expansion coefficient of the different materials. To achieve this, a minimal length of about 12 cm from the flange to the fused silica cell is required ([Hulme, 2014](#)). Fused silica is preferred compared to the more standard borosilicate glass due to a higher transmission in the infrared regime and the lower thermal expansion coefficient. In this way, thermal lensing effects can be minimized when high optical powers are used ([Gunton et al., 2013b](#)). The outside surfaces of our glass cell are not AR coated due to prolonged defect of the manufacturer's coating facility. This is not a major experimental limitation, however, we observe fringes in the absorption images that are attributed to internal reflections within the glass plates.

Feshbach and levitation coils In order to access and investigate the strongly interacting regime near the Feshbach resonance of a $|1\rangle - |2\rangle$ spin mixture of ^6Li , magnetic fields of up to 1000 G should be accessible. These are provided by a pair of coils with 20 windings each that produce a field strength of 3.3 G/A. They are separated by 44 mm and centered around the glass cell. A hollow core copper wire with a cross-sectional area of $4 \times 4\text{ mm}^2$ is used and is water-cooled from the inside. The overall resistance of the coil assembly is $0.04\text{ }\Omega$ and the driving current is provided by a 10 kW power supply with a maximum of 500 A (TDK-Lambda Americas Inc., GENESYSTM 10KW). While the two coils are arranged in Helmholtz configuration, the magnetic field at the center is not perfectly homogeneous. We have determined the curvature of the field by measuring its effect on the trap frequencies of the atoms in the ODT and find a value for the curvature of $B'' = B \times 3.12 \times 10^{-3}\text{ cm}^{-2}$ in the radial direction, where B is the applied field strength. This measurement is described in Chapter 5.

A bias current of up to 10 A can be superimposed in the top coil, which is independent of the current used to produce the Feshbach field. This allows us to generate a vertical magnetic field gradient, which is positive along the z axis. At high magnetic fields, both states of the $|1\rangle - |2\rangle$ mixture are high magnetic field seeking states, such that the applied field gradient

can be used to compensate the gravitational force.

3.3. Laser system for the red MOT

Detection and initial laser cooling is performed on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition at 671 nm. The laser frequencies that are required for the various stages of the experimental sequence are indicated in a simplified level scheme in Fig. 3.6 and a short description of laser cooling and trapping is provided in Chapter 4.

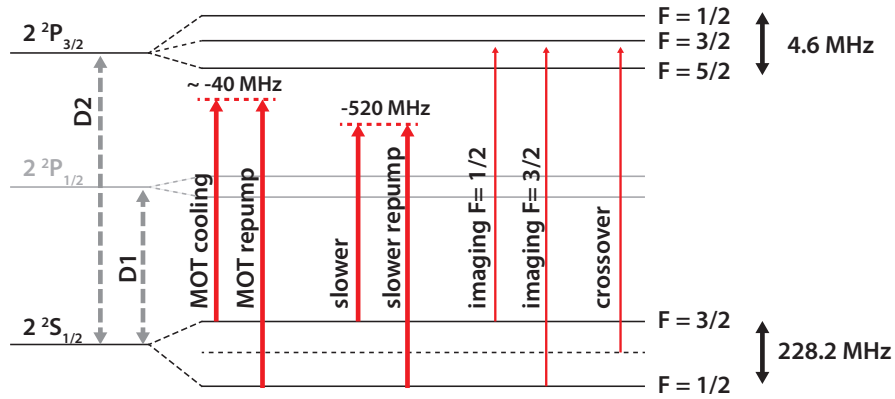


Figure 3.6.: Simplified level scheme of the D_2 transition. The arrows indicate transitions used in the experimental sequence and are described in the main text. The spacing between the levels are not to scale.

3.3.1. Laser setup

In order to efficiently drive an atomic transition, the linewidth of the laser should be smaller than the atomic natural linewidth. A very well established light source for this task is an external cavity stabilized diode laser (ECDL), which was described by Ricci et al. (1995). The light of such a laser can be amplified by seeding a diode laser (DL) or a tapered amplifier (TA). The laser setup for the 671-nm light is based on such semiconductor lasers and is arranged on a dedicated optical table (laser table), as schematically illustrated in Fig 3.7. Optical fibers are used to bring the light to the main table with the vacuum chamber (experiment table).

Reference laser and frequency stabilization The reference laser of the system is provided by a home-made ECDL, which is stabilized to an atomic transition. We use an anti-reflection coated laser diode (TOPTICA Photonics AG, LD-0670-0025-AR-2) with an output power of 15 mW. About 10 mW are used for Doppler-free frequency modulation (FM) spectroscopy

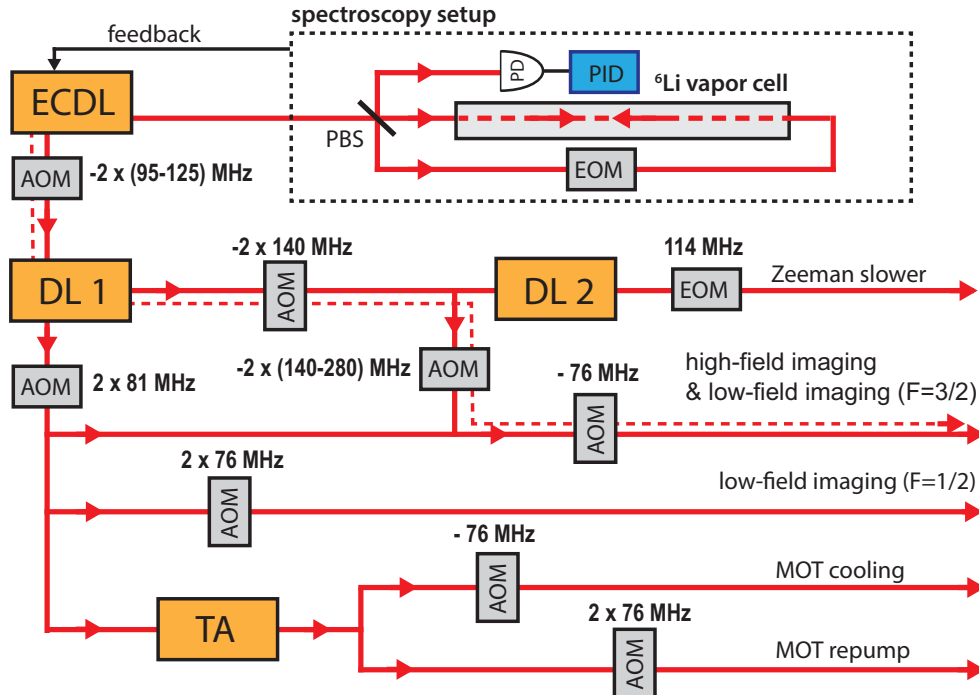


Figure 3.7.: Illustration of the laser system for D_2 transition. The reference light is provided by an ECDL that is locked to the atomic transition via Doppler-free FM spectroscopy. The light for all experimentally accessed transitions is derived from this laser. Injection seeded diode lasers (DL) and a tapered amplifier (TA) provide the required power and AOMs and EOMs are used to shift and modulate the laser frequency. The dashed line indicates the beam path for the high-field imaging light.

(Bjorklund et al., 1983) and the light is split into a probe and pump beam, as shown in Fig. 3.7. The probe beam is phase modulated with an electro-optic modulator (EOM) at a radio frequency (RF) of 30 MHz and overlapped with the pump beam in a lithium vapor cell. The photodiode signal of the transmitted probe beam is demodulated to generate an error signal, which is used to lock the frequency of the laser to the crossover feature between the two hyperfine ground states. The frequency of the stabilized laser is therefore 114 MHz blue-detuned with respect to the $2^2S_{1/2}, F = 3/2 \rightarrow 2^2P_{3/2}$ transition.

Part of the light from the reference laser is frequency shifted with an AOM in double-pass configuration and used for injection seeding of a 'slave' diode laser with an available output power of about 90 mW. This scheme allows us to tune its laser frequency within a range of 60 MHz, about ten times the natural linewidth, without a change in the output power. The light of this slave laser is used for injection seeding another diode laser and a tapered amplifier. In the following, the laser beams for the different experimental applications are briefly described in terms of the required frequency tuning range and optical power, and the technical implementation is discussed based on the schematic laser setup shown in Fig. 3.7.

Zeeman slower light In the Zeeman slower, a laser beam at a wavelength λ_L is counter-propagating to the atoms moving at a velocity $\mathbf{v}$. The frequency of the light in the rest frame of the atom is subject to a changing Doppler shift $\omega_D = -\mathbf{k} \cdot \mathbf{v}$, where the absolute value of the wave vector $\mathbf{k}$ is given by $\frac{2\pi}{\lambda_L}$. A fixed laser detuning δ and a spatially varying magnetic field keep the atoms in resonance with the laser light and lead to a deceleration of the atoms (Metcalf and van der Straten, 1999; Phillips and Metcalf, 1982). For the experimentally optimized laser detuning we find a value of $\delta = -520$ MHz.

A sufficiently high laser intensity is required for saturating the atomic transition in order to maximize the deceleration. To improve the overlap with the expanding atomic beam, the laser beam is focused, such that the light fully covers the final differential pumping tube that extends into the main chamber (see Fig. 3.4). For a calculated beam radius of 10 mm at the position of the MOT, a power of 4 mW is needed to obtain a saturation parameter s_0 of one. In addition to light on the cooling transition, also repumping light has to be provided, which was discussed in Section 3.2.1.

To meet these requirements, we use a dedicated diode laser. The light from the first slave laser is frequency shifted with a double-pass AOM configuration, resulting in a frequency that is 520 MHz red-detuned from the crossover transition. The beam is then passed through an EOM driven at an RF frequency of 114 MHz, half the value of the hyperfine interval of the ground state, such that the $+1^{\text{st}}$ and -1^{st} order sidebands have a detuning of 520 MHz from the repumping and the cooling transitions, respectively. The applied RF power is optimized for the loading rate of the MOT and we find that this coincides with an almost complete suppression of the carrier frequency after the EOM. The combined optical power for these two transitions is 35 mW after the optical fiber.

Cooling and repumping light for the MOT During the experimental cycle, the MOT evolves from a 'capture' into a 'cooling and compression' phase. In the first few seconds of the experiment, the MOT parameters are chosen to maximize the number of collected atoms from the diverging atomic beam. This is achieved by choosing a large $1/e^2$ radius for the six MOT beams of 0.9 cm and by optically saturating the atomic transition. Furthermore, a laser frequency detuning δ of about $-7 \times \Gamma_{2p}$ leads to a large effective trap volume, which optimizes the capture velocity of the MOT. After the loading phase, the trapping parameters are rapidly changed to values that are optimized for temperature and density of the atomic

cloud. This is realized by reducing the laser detuning and by lowering the optical power to a small fraction of the saturation intensity, as described in more detail in Section 4.

The MOT light is provided by a tapered amplifier with an output power of about 300-350 mW. The seed light for the TA is supplied by the diode laser DL1, as illustrated in Fig. 3.7. Due to the small hyperfine splitting of the ground state, both cooling and repumping light can be derived from the same laser source by dividing the power into two arms and by frequency shifting the light with AOMs. In addition to the applied frequency shift, the AOMs are used to regulate the optical power for the compressed MOT stage. We use a polarization maintaining optical fiber coupler (Evanescence Optics Inc.) with two input and six output ports to combine the two frequencies and to bring the light to the experiment table. The light from each input port is equally ($\pm 3\%$) split among the output fiber ports and is used to provide the MOT light along all 6 directions. The power ratio between cooling and repumping light is set to 2 : 1 and a combined power of 10-15 mW is available per beam.

Detection light For absorption imaging the atomic cloud is exposed to a resonant or near-resonant laser beam that is partially absorbed and analyzed with a CCD camera. In general, imaging is performed at a magnetic field strength of about 1-2 G, which is applied in order to define a quantization axis for the atoms. In the following we refer to this type of imaging as low-field imaging. However, for certain measurements it can be advantageous or even necessary to image the atomic cloud at a high magnetic field. This applies in particular to experiments in the region of the Feshbach resonance at 832 G and we refer to it as high-field imaging. For instance, this facilitates the observation of a molecular Bose-Einstein condensate of lithium dimers, as discussed in more detail in Section 5.4.2. The required optical power for the imaging beams is low as we require $I/I_{\text{sat}} \ll 1$, such that saturation effects can be neglected (see Section 4.1.1).

The generation of the light for low-field imaging is analogous to the one for the MOT light, as shown in Fig. 3.7. Two AOMs are used to provide light for the $2^2S_{1/2}, F = 1/2 \rightarrow 2^2P_{3/2}$ and the $2^2S_{1/2}, F = 3/2 \rightarrow 2^2P_{3/2}$ transition, such that both ground states can be imaged. At high magnetic fields the imaging transition from the state $|1\rangle$ ($|2\rangle$) of the ground state to the state $|3\rangle$ ($|2\rangle$) of the $2^2P_{3/2}$ excited state is a cycling transition due to selection rules. The notation and numbering of the respective states is provided in Appendix A.2. To detect the atoms at magnetic fields close to the Feshbach resonance, a large range of laser detunings

with respect to the cooling transition is needed, with values of up to -1100 MHz. In order to achieve this, we use a dedicated AOM with a bandwidth of 140 MHz (IntraAction Corp. Model ATD-2001A1) in double-pass configuration. In addition to that, we change the RF frequency of other AOMs in the laser setup that are not used otherwise during the absorption imaging sequence (see dashed line in Fig. 3.7). In this way, imaging can be performed within a range from 0 - 870 G.

3.4. Laser system for the UV MOT

In the experimental sequence to produce a quantum degenerate sample, the UV light is only used to drive the MOT cooling and repumping transitions. The laser system for the 323 -nm light is therefore comparatively simple, which allows us to place the setup on the experiment table without a need for an optical fiber. This is preferably because of the limited available optical power.

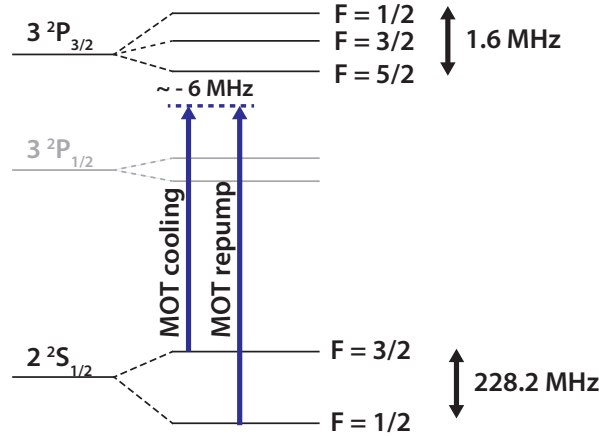


Figure 3.8.: Simplified level scheme of the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ UV transition. In the standard experimental sequence we drive the UV cooling and repumping transition.

Light source The UV light is generated by a commercial frequency doubling system (TOP-TICA Photonics AG, TA/DL-SHG pro). The fundamental light at 646 nm is produced by an ECDL and amplified with a tapered amplifier to an output power of 180 mW. The light is coupled into a bow-tie-ring resonator with two flat and two spherical mirrors. A frequency doubling crystal is placed at the focus between the concave mirrors for optimum conversion efficiency, resulting in a power of up to 35 mW at 323 nm.² The frequency lock to an

²Over time the output power continuously decreases. The most important factor leading to this deterioration of the power arises due to stains accumulating on the optics inside the doubling cavity. These optical

atomic transition consists of a fast and a slow proportional integral differential (PID) loop, as schematically illustrated in Fig. 3.9 and described in the following.

PDH lock to cavity The fast loop involves a Pound-Drever-Hall (PDH) lock (Black, 2001; Drever et al., 1983) of the fundamental 646-nm light to an external Fabry-Perot cavity with a finesse of about 400. Transmitted light from a mirror after the tapered amplifier is phase modulated with an EOM and coupled into the cavity, as shown in Fig. 3.9, and the photodiode signal of the reflected light is demodulated to generate an error signal. A fast PID regulator (TOPTICA Photonics AG, FALC 110) provides a feedback to the piezo element of the grating and the current of the ECDL. When locked to the cavity, the linewidth of the fundamental laser light is about 30 kHz, which was inferred from a beat-note measurement with a narrow frequency comb, and is small compared to the natural linewidth of the UV transition.

Modulation transfer spectroscopy The frequency stabilization to the atomic transition is implemented via modulation transfer spectroscopy (Shirley, 1982), while the initial locking scheme was based on standard FM spectroscopy, as described in Section 3.3 for the D_2 laser system. However, we observed drifts in the offset voltage of the error signal, which lead to corresponding fluctuations of the laser frequency. An advantage of the subsequently implemented modulation transfer method is the stability of this baseline, which was discussed by McCarron et al. (2008).

About 2 mW of the UV power is used for the spectroscopy setup, which is split into a pump and probe beam. Both beams are frequency shifted by -228 MHz with AOMs in double-pass configuration. The RF signal to drive the AOM of the pump beam is mixed with a local oscillator at 200 kHz to generate sidebands in the RF power spectrum, which are reduced by 6 dB relative to the carrier frequency. This introduces a modulation of the pump beam that is overlapped with the probe in a lithium vapor cell. Via a four-wave mixing process described by Snyder et al. (1980), the modulation is transferred to the probe beam. The resulting beat signal with the carrier frequency of the probe light is extracted with a lock-in amplifier and generates an error signal. This signal is used to regulate the length of the Fabry-Perot cavity to lock the UV laser to the $2S_{1/2}, F = 3/2 \rightarrow 3P_{3/2}$ transition. Furthermore, the RF signal for the AOMs in the spectroscopy setup determines the output frequency of the UV laser and

elements can be cleaned with standard optics cleaning methods.

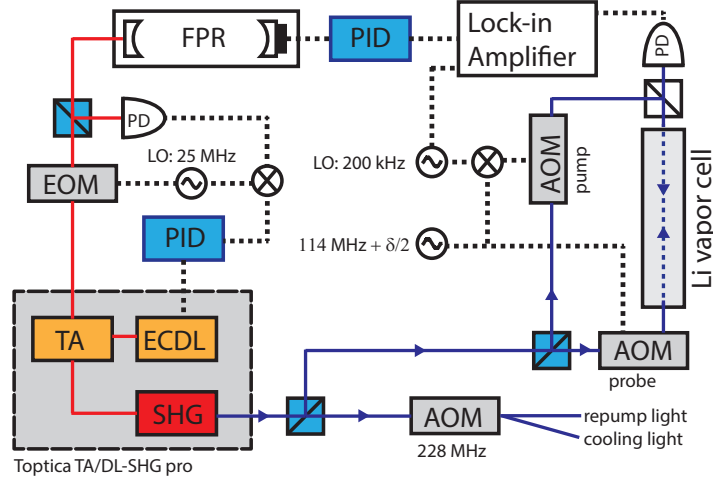


Figure 3.9.: Schematic laser setup for the laser cooling on the UV transition. The 323-nm light is supplied by a second harmonic generation (SHG) system. An external cavity diode laser (ECDL) provides the fundamental light at 646 nm that is amplified with a tapered amplifier (TA) and is locked to a Fabry-Perot resonator (FPR) to reduce the short-term linewidth to about 30 kHz. For long-term stability, the FPR is locked to the atomic UV transition frequency by modulation transfer spectroscopy performed in a lithium vapor cell.

results in a tuning range of about 10 MHz.

Overlap of UV and red MOT beams The main output of the laser passes through an AOM driven at an RF signal of 228 MHz to generate the cooling and the repumping light. The two UV beams are combined on a polarizing beamsplitter and expanded to a $1/e^2$ radius of 4.3 mm. This combined light is split into three beams, which are overlapped with the red MOT beams on dichroic mirrors. The UV beams are retro-reflected after passing the vacuum chamber, which increases the effectively available power. The dichroic mirrors (Bernhard Halle Nachfl. GmbH) that are used reflect 323-nm and transmit 671-nm light with a loss of less than 2%. We use $\lambda/4$ wave plates (ELAN Ltd.) that work at both wavelengths simultaneously to produce circular polarized light for the MOT.

3.5. Imaging

To investigate and extract thermodynamic properties of the atomic cloud, methods are required to probe the physical system. The most commonly applied technique is absorption imaging, where atoms are illuminated with a weak probe beam that is partially absorbed, as reviewed, for example, by [Ketterle et al. \(1999\)](#). The analysis of the transmitted beam with a charge-coupled device (CCD) camera provides information on the density distribution and

the total number of atoms. Also in our experiment this is the primary technique to probe the atoms. An alternative implemented method is the detection of ions, which can serve as a sensitive probe for spectroscopy measurements, as described in Section 3.7.

Principle of absorption imaging The principle of absorption imaging is based on the Beer-Lambert law and can be expressed according to

$$\frac{dI}{dz} = -\sigma I n(x, y, z), \quad (3.1)$$

which describes the intensity I of the probe beam as it propagates along the z axis through a medium of density $n(x, y, z)$ (Svanberg, 2004). The photon absorption cross section σ is given by (Metcalf and van der Straten, 1999)

$$\sigma = \underbrace{\frac{3\lambda^2}{2\pi}}_{\sigma_0} \frac{1}{1 + \left(\frac{2\delta}{\Gamma}\right)^2}, \quad (3.2)$$

which is valid for a two-level atom in the limit of $I/I_{\text{sat}} \ll 1$, and σ_0 is the atomic absorption cross section. For the imaging of multilevel atoms, the absorption cross section in Eq. (3.2) has to be corrected with a normalization factor in order to account for the different transitions that are accessed. The effective transition strength can be estimated by averaging the squared Clebsch Gordan coefficients of all possible transitions for a given polarization of the imaging light. This results in a prefactor of $2/3$ for the $2^2S_{1/2}$, $F = 1/2$ ground state of ^6Li and is used for imaging of the atomic cloud after release from the MOT.

The intensity profile $I_{\text{abs}} = I_{\text{abs}}(x, y, z)$ of the partially absorbed laser beam is recorded with a CCD camera and can be related to the optical density $\text{OD}(x, y)$ of the cloud according to

$$\text{OD}(x, y) = -\text{Log}\left(\frac{I_{\text{abs}}}{I_{\text{ref}}}\right) = \sigma \int n(x, y, z) dz = \sigma \eta(x, y), \quad (3.3)$$

where I_{ref} is the laser beam profile that is recorded without atoms. The column density $\eta(x, y)$ is the integrated density distribution of the atomic cloud along the line-of-sight. The total atom number N is an important experimental quantity and is determined by an integration of the optical density:

$$N = \frac{1}{\sigma} \int \text{OD}(x, y) dx dy. \quad (3.4)$$

In order to determine the full density profile $n(x, y, z)$ of an atomic cloud, one generally has to obtain a second image from a different direction. However, often the atomic cloud is a cylindrically symmetric ellipsoid, which allows reconstructing the three-dimensional density profile from a single absorption image.

Time of flight imaging The temperature of a harmonically confined ideal gas can be measured as follows. The trapping potential is rapidly switched off such that the cloud expands according to the velocity distribution of the atoms. The initial density profile is assumed to follow a Gaussian distribution (see Section 2.1), while a Maxwell-Boltzmann distribution is assumed for the velocity. Under these conditions it follows that the density distribution remains Gaussian and evolves according to (Weiss et al., 1989)

$$R^2(t) = R^2(0) + \frac{2k_B T t^2}{m}, \quad (3.5)$$

where the $R(t)$ is the radius of the Gaussian cloud according to Eq. (2.4) after a free expansion time t , and m is the atomic mass. The temperature T of the atomic cloud is obtained by fitting Eq. (3.5) to a series of radii obtained after different expansion times.

Experimental implementation For absorption imaging, a collimated laser beam is directed onto the atoms and the partial absorption leads to a shadow in the center of the beam. A relay telescope creates an image of the atomic cloud outside of the vacuum chamber, which is projected onto a CCD chip by means of a camera objective. This objective, which in our current setup is a single lens, allows us to vary the magnification depending on the measurement, without other changes in the imaging setup. An illustration of this imaging technique was given, for example, by Dieckmann (2001).

The imaging setup for the science chamber is arranged such that the atomic cloud can be imaged along any of the three principal axes with the same camera. A similar layout, upon which ours is based on, was described and illustrated by Costa (2011). We use relay telescopes consisting of 2-inch diameter achromatic lenses with focal lengths of $f = 100$ mm and $f = 150$ mm, respectively, and arrange the 3 imaging paths along a cube. The actual imaging direction is selected by a suitable combination of interchangeable mirrors, mounted on optical rails to ensure a reproducible alignment, which determines the imaging path that is

projected onto the CCD camera. For the science chamber we use a 1024×1024 CCD camera with a pixel area of $13 \times 13 \mu\text{m}$ (PIXIS 1024BR_eXcelon CCD, Princeton Instruments) and a magnification of $M = 3.1$ for the measurements presented in Chapter 5.

Vertical imaging in the MOT chamber is performed in a similar way. The relay telescope consists of two $f = 100$ mm lenses and the images are recoded with a low-cost 1294×964 pixel CCD camera (Stingray, Allied Vision Technologies) with a pixel area of $3.75 \times 3.75 \mu\text{m}$. For the investigation of the UV MOT, which is discussed in Chapter 4, also imaging along the horizontal direction was employed. The imaging direction was along the y axis, which is used for the optical transport into the glass cell after an extension of the vacuum chamber.

3.6. Optical dipole trap and transport to the science chamber

After laser cooling, the atoms are transferred into a conservative confinement potential to further lower the temperature by evaporative cooling. As outlined in the beginning of this chapter, we follow an all-optical approach without intermediate magnetic trapping and transfer the atoms from the MOT directly into an ODT. In our setup, this trap is also used to transport the atoms into the glass cell and for evaporative cooling.

3.6.1. Optical dipole trap

Neutral atoms in a strong light field experience a force that originates from the interaction of an induced dipole moment with its driving field. In a classical picture, the electric field $\mathbf{E}(t)$ induces an electric dipole moment $\mathbf{d}(t)$ in the atom that is parallel to the external field and oscillates at the same frequency. The amplitudes are related by $d = \alpha E$, where α is the complex polarizability of the atom. The resulting potential seen by the atoms is given by (Grimm et al., 2000)

$$U_{\text{dip}}(\mathbf{r}) = -\frac{1}{2\epsilon_0 c} \text{Re}(\alpha) I(\mathbf{r}) \quad (3.6)$$

where the $I(\mathbf{r}) = 2\epsilon_0 c |\mathbf{E}(\mathbf{r})|^2$ is the laser intensity at the position $\mathbf{r}$ and ϵ_0 is the vacuum permittivity. The conservative potential for the neutral atoms $U_{\text{dip}}(\mathbf{r})$ is related to the real part of the polarizability, while the imaginary part is related to the absorbed power and

correspondingly to the photon scattering rate in the light field ([Grimm et al., 2000](#)):

$$\Gamma_{\text{sc}}(\mathbf{r}) = \frac{1}{\hbar \epsilon_0 c} \text{Im}(\alpha) I(\mathbf{r}) . \quad (3.7)$$

The atomic polarizability can be derived within the approximation of a two-level system. This leads to expressions for the energy shift of the ground state and the photon scattering rate, which are related to the properties of the atomic transition according to ([Grimm et al., 2000](#)):

$$U_{\text{dip}}(\mathbf{r}) = -\frac{3\pi c^2}{2\omega_0^3} \left(\frac{\Gamma}{\omega_0 - \omega_L} + \frac{\Gamma}{\omega_0 + \omega_L} \right) I(\mathbf{r}) = -\tilde{U} I(\mathbf{r}) \quad (3.8)$$

$$\Gamma_{\text{sc}}(\mathbf{r}) = \frac{3\pi c^2}{2\hbar \omega_0^3} \left(\frac{\omega_L}{\omega_0} \right)^3 \left(\frac{\Gamma}{\omega_0 - \omega_L} + \frac{\Gamma}{\omega_0 + \omega_L} \right)^2 I(\mathbf{r}) . \quad (3.9)$$

These equations are derived for a two-level atom with an angular transition frequency ω_0 and a natural linewidth Γ of the excited state, which is exposed to a light field of angular frequency ω_L . For laser detunings $\delta = \omega_L - \omega_0$ that are much larger than the hyperfine splitting of the ground and excited state, these expressions become also valid for multilevel atoms. Our optical dipole trap is operated at a wavelength of 1070 nm, such that this condition is well satisfied and all Zeeman states of the ground state experience an identical trapping potential.

The potential energy near the center of an ODT that is generated with Gaussian beams can often be approximated by a harmonic potential

$$U_{\text{dip}}(x, y, z) \cong U_0 + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) , \quad (3.10)$$

where $\omega_{x,y,z}$ are the angular trap frequencies along the respective spatial direction and m is the atomic mass. This approximation is well fulfilled under normal experimental conditions because the equilibrium temperature of an atomic cloud is on the order of a tenth of the trap depth ([O'Hara et al., 2001a](#)) such that atoms are predominantly in the center of the trap.

For a single Gaussian beam with a $1/e^2$ radius ω and an optical power P , which is propagating along the y axis, one obtains the following relations for the trap frequencies:

$$\omega_{x,z} = \sqrt{\frac{P}{m \omega^4} \frac{8}{\pi} \tilde{U}} , \quad \omega_y = \sqrt{\frac{P \lambda^2}{m \omega^6} \frac{4}{\pi^2} \tilde{U}} \quad (3.11)$$

This shows that the axial trap frequency rapidly decreases with an increased beam waist.

Furthermore, the aspect ratio of the atomic cloud increases because radial and axial trap frequencies scale differently with the beam radius.

3.6.2. Crossed ODT for optical transport

The requirements for the ODT in our approach are as follows. First, the potential has to be sufficiently deep and voluminous to facilitate an efficient transfer of the atoms from the MOT into the ODT. Second, as our scheme involves a transport of the atoms, it must be possible to translate the trapping geometry by about 25 cm without significantly heating the atomic cloud. Third, the trap frequencies have to be adequate to ensure a fast thermalization rate during evaporative cooling.

Trap depth Provided laser cooling of the atoms is not hindered by the presence of the optical dipole trap, O'Hara et al. (2001b) derived a scaling law for the loading process of an ODT. It suggests an essentially exponential increase in the final atom number with the truncation parameter $\eta = U_0/k_B T$, which is the ratio of trap depth to the temperature of the atomic cloud. While the model is not applicable for large values of η , a strong dependence of the atom number on the trap depth was observed, for example, by Kuppens et al. (2000). For previous all-optical implementations, values of generally about 5-10 were chosen for η , as summarized by Gunton et al. (2013b). Another important factor for the loading efficiency is the spatial overlap of the ODT with the atomic cloud in the MOT (Burchianti et al., 2014). The choice of the ODT beam waist is therefore a compromise between the trap depth and volume, since $U_0 \propto I_{\max} = 2P/\pi\omega^2$.

The temperature of the atomic cloud in the UV MOT is about $50 \mu\text{K}$, as described in Chapter 4, and the available optical power is 45 W at a wavelength of 1070 nm. For a crossed ODT, where the power is evenly split between two arms, a waist of $\omega = 60 \mu\text{m}$ ($70 \mu\text{m}$) leads to a trap depth of $U_0 = 480 \mu\text{K}$ ($350 \mu\text{K}$), while the actual size of our focused ODT beams is $66 \mu\text{m}$ (see Chapter 5).

Crossed ODT for transport In our transport scheme we translate a crossed ODT from the MOT into an attached science chamber. This is implemented by moving a lens, which simultaneously focuses and crosses the beams for the ODT, as illustrated in Fig. 3.10 (c). In traditional optical transport schemes, atoms are confined in a single, tightly focused ODT

beam (Gustavson et al., 2001; Léonard et al., 2014; Zimmermann et al., 2011). These confinement potentials are optimized for the transport, but are generally too small for an efficient direct loading of the atoms from a MOT. The small waist of these trapping beams is chosen to achieve a short Rayleigh length and correspondingly a high axial trap frequency, which follows from Eq. (3.11). The consequence for these schemes is that different ODTs are used in sequence during the experimental cycle, requiring multiple beams and laser sources. Instead, here we use a crossed ODT for the transport. To the best of our knowledge, this is the first such implementation for a long-distance transport of ultracold atoms. The central idea is that even a small crossing angle leads to a significant enhancement of the axial trap frequency, which voids the requirement for a small beam waist for the transport trap. This allows us to use the same ODT for loading and transport.

Geometric constraints The translation of the crossed ODT requires the two beams to enter the experimental chamber through a single viewport, as illustrated in Fig. 3.10 (c). This imposes a limit on the crossing angle and correspondingly on the axial trap frequency. For a beam waist of $66\,\mu\text{m}$ and a power of $22.5\,\text{W}$ per beam, the trap frequency is shown in Fig. 3.10 (a) as a function of the crossing angle. In order to achieve a trap frequency of about $75\,\text{Hz}$, which is similar to another efficient transport scheme demonstrated by Zimmermann et al. (2011), the two beams have to enclose an angle greater than 2.4° . Conversely, the clear aperture of the entrance viewport limits the crossing angle to less than about 3.2° , indicated by the green shaded area in Fig. 3.10 (b).

Optical setup The power for the optical dipole trap is derived from a single mode 1070-nm fiber laser (IPG, YLR-50-1070-LP) operated at a fixed output power of $50\,\text{W}$. It is split equally into two beams for the crossed ODT, as illustrated in Fig. 3.11. Each beam passes an AOM and is expanded to a $1/e^2$ radius of $2.6\,\text{mm}$ using a diverging and a converging lens. The AOMs are placed at the virtual focus of this telescope, which helps to improve the pointing stability of the beams when the RF power for the AOMs is ramped for forced evaporative cooling. We find that in this configuration an active compensation for the changing RF power, as described by Fröhlich et al. (2007), is not required.

Fluctuations in the ODT power can lead to parametric heating of atomic cloud (Gehm et al., 1998). To stabilize and regulate the power of each beam, we measure the transmitted

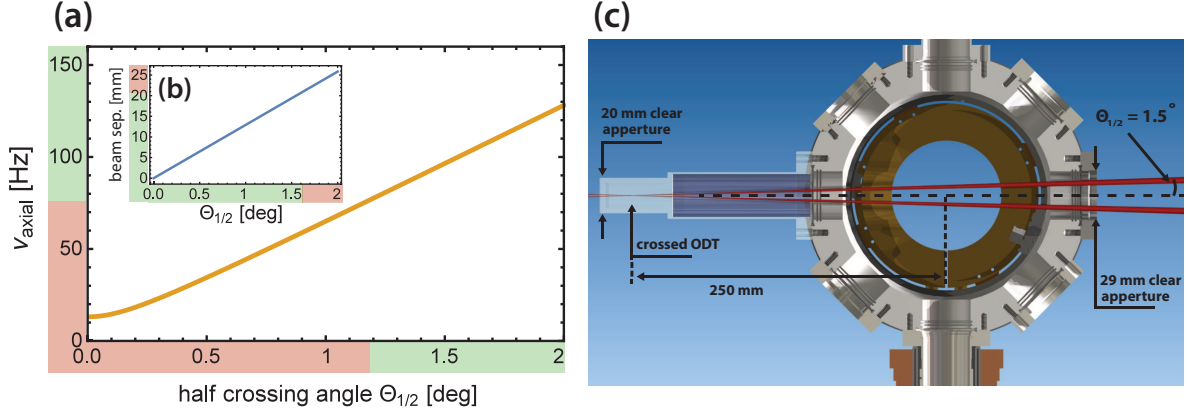


Figure 3.10.: (a) Axial ODT trap frequency versus crossing angle of ODT beams with a waist of $66 \mu\text{m}$ and 22.5 W per beam. The green shaded area indicates experimentally acceptable parameters. (b) Beam separation at the entrance viewport if the ODT is crossed in the center of the glass cell. The red shaded area indicates the excluded range due to the limited clear aperture of the viewport. (c) Illustration of experimental implementation.

light through one of the mirrors with a logarithmic photodiode. Based on this signal, a high-bandwidth PID regulator provides a feedback to the applied RF power for the AOMs. This allows us to regulate and stabilize the optical power for the experiment over four orders of magnitude, from a maximum of 23 W to a few milliwatts per beam.

Linear translation stage The lens that focuses the two beams of the ODT is placed on a linear translation stage, which allows us to shift the axial position of the trap, as shown in Fig. 3.3. The first implementation of the optical tweezers method for transporting ultracold atoms was demonstrated by [Gustavson et al. \(2001\)](#), where a BEC was moved by up to 44 cm . However, initially a severe heating of the atomic cloud was observed, which was attributed to parametric heating induced by vibrations of the mechanical stage. This could be solved by reducing the velocity and by increasing the payload of the moving part ([Chikkatur, 2002](#)). A suggested alternative was the use of an air bearing translation stage instead of a mechanical one. The absence of a firm contact between the moving platform and the support ensures a smooth and fast motion with high reliability. We use an air bearing stage from Nelson Air Corp. (Atlas-101-310-HD Stage) with a maximum travel distance of 310 mm and a specified repeatability of $0.04 \mu\text{m}$.

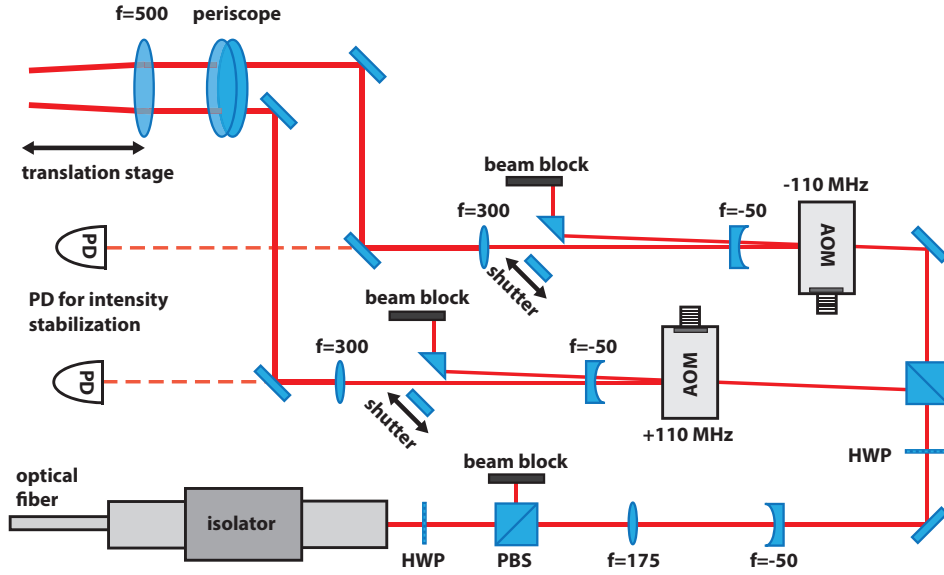


Figure 3.11.: Schematic laser setup for the crossed ODT. The optical power of the two beams is independently regulated with AOMs, and can be deflected into a water-cooled beam trap using mechanically controlled mirrors. The transmitted light through back-polished mirrors is used to provide a feedback to the applied RF power for the AOMs.

3.7. Ion detection

Motivated by the prospect of a photoassociation spectroscopy measurement to bound states below the $2S$ - $3P$ asymptote, we decided to integrate an ion detection system in the MOT chamber as part of a system upgrade. In typical PA measurements, described in more detail in Chapter 6, a spectroscopic transition manifests itself as reduction in the number of trapped atoms at a certain wavelength λ_{PA} of the probe laser. The experimentally most convenient detection method is to monitor the fluorescence from the trapped atoms in the MOT while the frequency of the probe beam is scanned (Jones et al., 2006). For such a measurement the PA transition strength must be sufficiently strong to result in an observable signal.

The PA transitions strength to the $2S$ - $3P$ asymptote is known to be weak and a detection via the MOT fluorescence is not feasible. For these transitions, however, we identified that a loss channel of atoms results in the production of ions. While the *loss* of a small fraction of atoms might not be traceable, the corresponding *production* of ions might be. This is because of the in-principle zero ion background in the chamber and the efficient detection of charged particles.

3.7.1. Ion detection with channel electron multiplier

Working principle We use a channel electron multiplier (CEM) (KBL5RS/90, Dr. Sjuts Optotechnik GmbH) for the detection of ions. The basic working principle is illustrated in Fig. 3.12 and a comprehensive description of a CEM in the context of a cold atom experiment was given by Henkel (2011). A CEM consists of a tube with an active inner surface that emits secondary electrons upon the impact of a primary particle. In this way, a single captured ion can generate a detectable current pulse. A CEM has a high surface resistivity and an applied voltage across the channel results in a continuously changing electric potential, which produces an electric field along the tube. This electric field directs and accelerates the secondary electrons further into the channel, as illustrated in Fig 3.12. Multiple secondary emission processes occur along the propagation of the tube and produce an electron cloud containing on the order of 100 million electrons per event at the end of the channel. This corresponds to a gain on the order of 1×10^8 for a single absorbed charged particle for the implemented CEM model (Sjuts, 2014a). A potential difference of about 100 V between the end of the CEM channel and the anode directs the electrons to the connected signal wire. This bias voltage is passively generated by the intrinsic resistance of the CEM channel of 200-300 M Ω and an additional load of 10 M Ω placed in series, as illustrated in Fig 3.12. The signal is amplified with a low-noise preamplifier (SRS, model SR570) with variable bandwidth and can be analyzed with an oscilloscope or a counter.

Interlock for CEM A CEM has a finite lifetime. After an ion count of about 1×10^{11} the gain starts to decrease (Sjuts, 2014a). To protect the CEM in case of an excessive exposure to ions or in the event of some electronic failure, the anode current is monitored by a specially designed interlock circuit. If triggered, the high-voltage power supply is switched off by means of the supplied analog control voltage. This process is slow and happens on a timescale of a second. In addition to that, the ionization process in the experiment is suspended and is described in Chapter 6. This is accomplished on a timescale of microseconds by extinguishing the relevant lasers with AOMs.

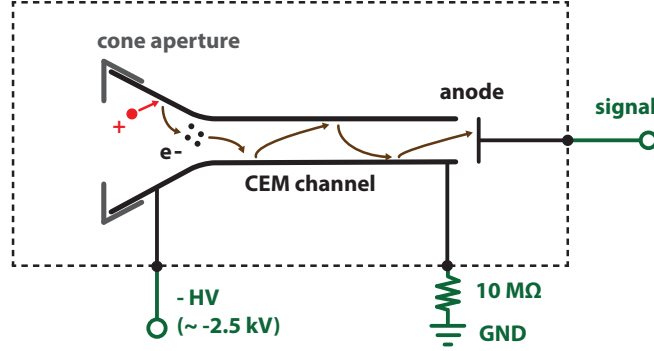


Figure 3.12.: Schematic illustration of the CEM setup. All components inside the dashed box are part of the vacuum chamber. A high negative voltage ($-HV$) is applied to the cone of the CEM, creating an electric field along the channel. Ions (red circle) impinging onto the surface of the cone, lead a cascade of secondary electron emission processes, generating a cloud of electrons collected by the anode. A custom made cone aperture ensures a well-defined electric field inside the cone and prevents a loss of secondary electrons.

3.7.2. Integration of ion detection in the MOT chamber

A challenge for the installation of the CEM into the existing chamber was to ensure not to compromise the performance of the MOT nor subsequent experiments with quantum degenerate gases. The CEM is placed in between two CF40 viewports of the octagon with the cone opening facing the MOT in a direct line, as shown in Fig. 3.13 (c),(d), to ensure that the full optical access in the horizontal direction is preserved.

Vacuum compatibility In addition to the optical access, the CEM assembly has to be ultra-high vacuum (UHV) compatible. The CEM is rated for this purpose and has a supposedly zero outgassing rate (Sjuts, 2014a,b). However, standard cleaning procedures for vacuum components cannot be applied because of the fragile inner surface of the CEM. For the bake-out procedure we heated the vacuum chamber to around 300°C for 2 weeks to attain a low background pressure that is required for quantum gas experiments. Despite exceeding the stated temperature limit of the CEM of 250°C for a rather long duration, the CEM performs fully according to the stated specifications.

Electric fields and ion trajectories The electric fields in the MOT chamber determine the trajectory of the atoms upon ionization. In our design we do not use specific guiding electrodes or ion-optical elements to direct the ions into the funnel of the CEM. The 'guiding' field is only defined by the voltage of up to -2.5 kV applied to the CEM cone and the surrounding metallic elements of the vacuum chamber. Omitting dedicated electron optics simplifies the

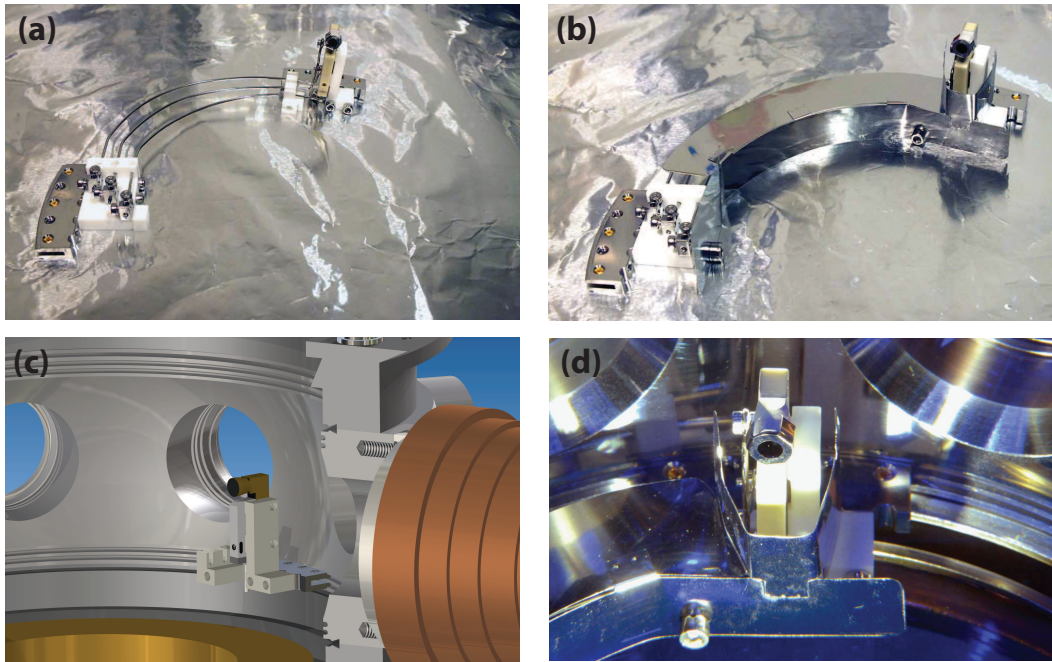


Figure 3.13.: (a),(b) CEM assembly before installation into the vacuum chamber with and without metal shield (see text). (c) Simplified 3D illustration of the CEM setup in the MOT chamber. It is placed between two viewports, without obstructing the optical access in the MOT chamber. (d) Photograph of CEM assembly in MOT chamber.

setup, however, electric stray fields cannot be compensated ([Henkel, 2011](#)). We use bare stainless steel wires for all electrical connections, including the one providing the high voltage. To avoid a deflection of the ions due to these electric potentials inside the chamber, the wire assembly is screened from the atoms with a shim metal that is connected to the ground potential, as shown in [Fig. 3.13 \(b\)](#).

The electric field inside the CEM channel is well-defined by the continuously changing electric potential of the inner surface. However, the entrance funnel is open, which can lead to a distortion of the electric fields. This can produce a saddle point potential for the secondary electrons and result in a reduced detection efficiency ([Sjuts, 2014a](#)). A metallic aperture on the CEM is used to provide a well-defined potential inside the funnel for the secondary electrons, which is illustrated in [Fig. 3.12](#) and was described by ([Henkel, 2011](#)).

A simplified 3D model of the assembly was used to simulate the electric fields in the steel chamber along the MOT-CEM axis. This was important for the design of the metal shield around the CEM assembly. This shield has to cover the wires and the CEM body, while the distance to the cone must be sufficient to prevent a strong vertical electric field component near the cone (see [Fig. 3.13 \(b\),\(d\)](#)), as this would deflect the atoms away from the center of the CEM funnel.

4. Two-stage laser cooling to high phase-space density

In this chapter we describe our laser cooling scheme of ${}^6\text{Li}$ on the atomic $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition at 323 nm. Among other alkali-metal atoms, laser cooling of lithium is special in the sense that sub-Doppler temperatures of the atomic clouds are not obtained with standard techniques. This is attributed to the unresolved hyperfine structure of the excited state. We begin the chapter with a brief summary of magneto-optical trapping, the associated temperature limit of Doppler cooling, and experimental considerations for laser cooling of lithium. Then, the first cooling stage of our experimental sequence is characterized, which is the red MOT on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition (see Fig. 3.2 for a level scheme). Because standard sub-Doppler cooling is not observed for lithium, temperatures on the order of $300\text{ }\mu\text{K}$ are experimentally obtained, which corresponds to about twice the Doppler limit. To reduce the temperature of the atomic cloud and to enhance the phase-space density for an efficient transfer into an ODT, we employ the second cooling transition, first demonstrated by Duarte et al. (2011). We present our measurements on the phase-space density optimization of the UV MOT on the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition, for which we obtain a value of up to 3×10^{-4} . Part of this chapter was published in *Physical Review A*, **90**, 033417 (2014) (Sebastian et al., 2014).

4.1. Laser cooling and trapping

Laser cooling of neutral atoms was first proposed by Hänsch and Schawlow (1975) and experimentally realized about 10 years later by Chu et al. (1985). This technique uses laser light to cool atomic clouds to temperatures in the micro-Kelvin regime, which are otherwise isolated from the environment. Today, laser cooling and trapping is a standard technique in the field

of atomic physics and is used for all experiments investigating quantum degenerate gases.

4.1.1. Doppler cooling

Laser cooling is based on the scattering force experienced by atoms that are exposed to a light field that is near-resonant with an atomic transition. The momentum of an absorbed photon is transferred to the atom, which experiences a change in momentum parallel to the propagation direction of the laser. If the excited atom returns to the ground state via spontaneous decay, then the direction of the emitted photon follows a random and isotropic distribution. The momentum transfer to the atom due to multiple spontaneous scattering events therefore averages to zero, while the absorption of photons from the laser beam leads to a directional force.

Two-level model The fundamental principle of laser cooling and associated quantities can be derived within the two-level approximation of an atom with an angular transition frequency ω_0 , which is interacting with laser light of angular frequency $\omega_L = 2\pi c/\lambda_L = 2\pi\nu_L$. In this description, the population of the excited state is given by

$$\rho_{ee} = \frac{1}{2} \frac{s_0}{1 + s_0 + \left(\frac{2\delta}{\Gamma}\right)^2}, \quad (4.1)$$

where $\delta = \omega_L - \omega_0$ is the detuning of the laser light with respect to the atomic transition (Metcalf and van der Straten, 1999). The lifetime τ of the excited state is linked to the natural linewidth Γ via $\Gamma = \frac{1}{\tau}$. The saturation parameter $s_0 = I/I_{\text{sat}}$ relates the laser intensity I to atomic properties of the transition via the saturation intensity according to

$$I_{\text{sat}} = \frac{2\pi^2 \hbar \Gamma \nu_L^3}{3 c^2}. \quad (4.2)$$

With this definition it follows from Eq. (4.1) that the occupation probability of the excited state is 0.25 for $I = I_{\text{sat}}$ and $\delta = 0$. In the limit of $s_0 \rightarrow \infty$, the excited-state fraction approaches a value of 0.5.

Light force Together with the natural linewidth, Eq. (4.1) for the excited-state fraction ρ_{ee} can be used to calculate the spontaneous photon scattering rate given by $\gamma_{\text{sc}} = \Gamma \rho_{ee}$. The average force exerted onto an atom due to spontaneous scattering events can be calculated in

a semi-classical approach (Metcalf and van der Straten, 1999) and coincides with the rate of change of momentum, therefore $F = \hbar \mathbf{k} \gamma_{\text{sc}}$, with $k = 2\pi/\lambda$. Further considering the effective detuning seen by a moving atom due to the Doppler shift, the total force induced by two counter-propagating beams in one dimension adds to

$$F = \hbar k \frac{\Gamma}{2} \left(\frac{s_0}{1 + s_0 + \left(\frac{2(\delta - \mathbf{k} \cdot \mathbf{v})}{\Gamma} \right)^2} - \frac{s_0}{1 + s_0 + \left(\frac{2(\delta + \mathbf{k} \cdot \mathbf{v})}{\Gamma} \right)^2} \right). \quad (4.3)$$

For a negative laser detuning δ , the frequency of the counter-propagating light is shifted closer to resonance, while the detuning for the co-propagating light is increased in the rest frame of the moving atom. This results in an imbalanced photon scattering rate from the two beams and leads to a net force acting on the atom. This force opposes the motion of the atom and is, because of the random character of the spontaneous emission process, dissipative.

Limit of Doppler cooling The attainable temperature of an atomic cloud via Doppler cooling can be determined by considering a balance of the cooling and heating mechanisms, as it was described, for example, by Lett et al. (1989). The damping of the momentum follows from the cooling process expressed in Eq. (4.3), while heating arises from the random character of the spontaneous emission. This leads to an increase in the momentum spread, similar to a random walk. Equating these contributions leads to an equilibrium temperature T_{eq} of

$$k_B T_{\text{eq}} = \frac{\hbar \Gamma}{4} \left(\frac{2|\delta|}{\Gamma} + \frac{\Gamma}{2|\delta|} \right), \quad (4.4)$$

where a negative detuning δ and a low light intensity with $s_0 \ll 1$ is assumed. The equilibrium temperature has a minimum at a laser detuning of $\delta = -\Gamma/2$, which is given by

$$k_B T_D = \frac{\hbar \Gamma}{2}. \quad (4.5)$$

T_D is called the Doppler temperature and depends only on the natural linewidth of the excited state. For lithium, the natural linewidth of the red MOT transition $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ is $\Gamma/(2\pi) = 5.9 \text{ MHz}$ leading to $T_D = 141 \mu\text{K}$. For the UV MOT transition $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ one finds $T_D = 18 \mu\text{K}$, as summarized in appendix A.1.

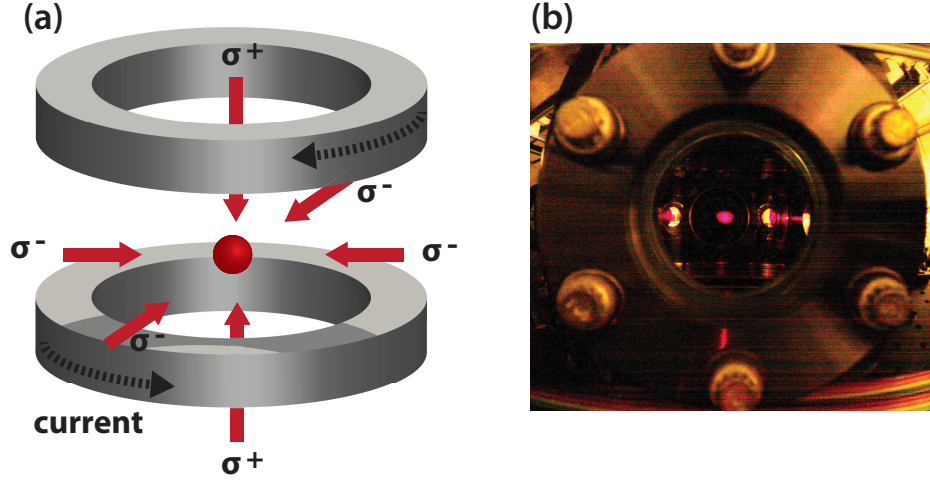


Figure 4.1.: Magneto-optical trap. (a) Illustration of the coils in anti-Helmholtz configuration and laser beams for the magneto-optical trap. (b) Photograph of the trapped ${}^6\text{Li}$ atoms in the red MOT.

4.1.2. Magneto-optical trap

The dissipative scattering force described in the previous section can be extended to three dimensions by providing counter-propagating laser beams along all 3 spatial directions. In such a configuration, an atomic cloud can be cooled but the atoms are not trapped because they can diffuse out of the intersection region of the six laser beams. In order to confine the atoms to that region, a spatially dependent force is required.

Spatial confinement In order to provide such a confinement for the atoms, a magnetic quadrupole field $B(\mathbf{r})$ is applied in addition to the six laser beams, as illustrated in Fig. 4.1 (a). This changes the effective detuning term in Eq. (4.3) for the scattering force to $\delta \mp \mathbf{k} \cdot \mathbf{v} \pm \mu' B(\mathbf{r}) / \hbar$, where μ' is the magnetic moment of the addressed atomic transition (Metcalf and van der Straten, 1999). The magnetic field dependent energies of the Zeeman levels, shown in appendix A.2, imply that for a small magnetic field strength the transition frequencies for σ^- (σ^+) light reduce (increase) with increased field strength.¹ With appropriate circularly polarized and red-detuned light, a restoring force to the center of the magnetic quadrupole field can be established. The first magneto-optical trap was realized with sodium atoms by Raab et al. (1987) and a photograph of our ${}^6\text{Li}$ MOT is shown in Fig. 4.1 (b).

¹The polarization of the light is defined with respect to the local orientation of the magnetic field. σ^- (σ^+) light drives transitions with $\Delta m_F = -1$ ($\Delta m_F = +1$).

4.1.3. Capture velocity

For the loading of the MOT from the Zeeman-slowed atomic beam, the atoms have to be decelerated close to zero velocity within the intersection region of the six laser beams. The maximum velocity of the incident atoms to remain trapped is called capture velocity v_c and depends on the experimental parameters. For instance, the natural linewidth sets a limit for the scattering rate and therefore for the maximum deceleration. Furthermore, Γ also restricts the velocity range for which an appreciable force acts on the atom (Chanelière et al., 2008; Metcalf and van der Straten, 1999).

Two-stage MOT Here, the capture velocity is estimated by numerically integrating the equation of motion in one dimension based on Eq. (4.3). The results for v_c are shown in Fig. 4.2 as a function of the detuning. For typical experimental parameters given in Table 4.1, we find a capture velocity of about 60 m/s for the red MOT, which is consistent with a value stated by Müller (2011) for a similar ^6Li MOT configuration. The capture velocity for the MOT on the narrow UV transition is much smaller and we estimate a value of about 5 m/s, which is not sufficient for a direct loading from the Zeeman-slowed atomic beam (Taglieber, 2008). This shows that a pre-cooling of the atoms on the standard D_2 transition is a necessary measure before Doppler cooling on UV transition can be employed.

	$2^2S_{1/2} \rightarrow 2^2P_{3/2}$	$2^2S_{1/2} \rightarrow 3^2P_{3/2}$
$1/e^2$ beam radius	0.9 cm	0.43 cm
Saturation parameter $s_0(x=0)$	4	0.4
Magnetic field gradient $\partial_x B$	6 G/cm	2 G/cm

Table 4.1.: Parameters used for calculating the capture velocity. These parameters are close to experimental values indicated in Fig. 4.5.

4.1.4. Laser cooling of ^6Li

The first magneto-optical trap for lithium was realized by Lin et al. (1991) and a temperature of $350 \pm 40 \mu\text{K}$ of the laser cooled atomic cloud was observed. This corresponds to about twice the Doppler temperature of $141 \mu\text{K}$, but the measurements were in good qualitative agreement with the detuning dependence of the temperature, as predicted by Doppler cooling (see Eq. (4.4)). Also in later experiments based on different laser sources and trap geometries,

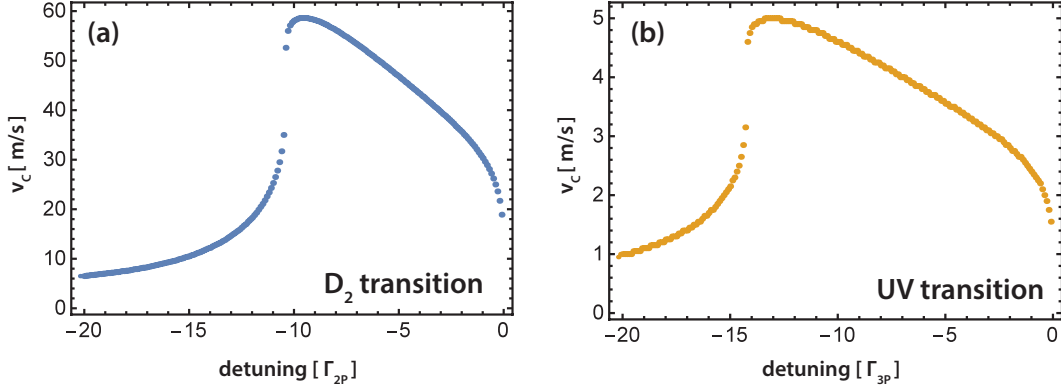


Figure 4.2.: Calculated capture velocity v_c for the (a) red and (b) UV MOT, with experimental parameters given in Table 4.1. The dependence of v_c is in qualitative agreement with results discussed in Metcalf and van der Straten (1999). The capture velocity for the UV transition would increase to about 9 m/s with a saturation parameter of $s_0 = 4$, which is considered for the D_2 transition.

similar temperatures were observed (Ritchie et al., 1994; Schünemann et al., 1998). This is in contrast to other alkali-metal atoms where early experiments resulted in temperatures far below the Doppler limit and was first reported for laser cooled sodium atoms (Lett et al., 1988).

Standard sub-Doppler cooling The mechanisms leading to temperatures below the Doppler limit involves the multiple hyperfine sublevels of the ground and excited states of the cooling transition. For atoms exposed to resonant or near-resonant light, the ground-state population distribution among the various hyperfine levels depends on the polarization of the light. Another effect is the light-induced energy shift of the atomic energy levels, which, for small detunings, also depends on the polarization of the light and is state dependent. Interference effects between different laser beams lead to a spatial variation of the light field and can induce optical pumping within the ground-state manifold. Different sub-Doppler cooling mechanisms can arise for an atom moving through such a light field and were first described by Dalibard and Cohen-Tannoudji (1989), Ungar et al. (1989) and Weiss et al. (1989).

Absence of sub-Doppler cooling for ^6Li Sub-Doppler cooling on the D_2 transition is absent for ^6Li . It was numerically shown for potassium that the efficiency of the sub-Doppler mechanism is reduced if the hyperfine splitting of the excited state is small or not well resolved when compared to the natural linewidth (Fort et al., 1998). However, for magneto-optical traps of ^{40}K with low atom numbers, temperatures below the Doppler limit were observed (Gokhroo et al., 2011; Modugno et al., 1999; Taglieber et al., 2006). For ^{40}K the splitting between the

two relevant levels of the excited state is only about 7Γ , while for ^6Li the hyperfine splitting is even smaller than the natural linewidth Γ .

Cooling below the D_2 Doppler limit In recent years different schemes have been developed or revisited to improve the laser cooling of lithium as well as potassium isotopes to sub-Doppler temperatures. The method of driving a MOT transition to a higher excited state with a smaller natural linewidth, which is realized in our setup, was first demonstrated for ^6Li by Duarte et al. (2011) and for ^{40}K and ^{41}K by McKay et al. (2011).

Another scheme uses gray optical molasses, where an atomic $J \rightarrow J' = J$ transition is driven with light that is blue-detuned from the atomic resonance, as it was proposed by Grynberg and Courtois (1994). This method was first experimentally realized by Boiron et al. (1996) for cesium on the D_1 transition and is called 'gray molasses' due to the reduced fluorescence as compared to the standard optical molasses method. Only much later, essentially in parallel to the work presented here, this method was applied to lithium and potassium (Fernandes et al., 2012; Grier et al., 2013; Salomon et al., 2013), where it was shown that sub-Doppler temperatures can be attained. Subsequently, all-optical schemes to produce quantum degenerate gases were demonstrated by Burchianti et al. (2014) and Salomon et al. (2014) for lithium and potassium, respectively.

4.2. Magneto-optical trap on the D_2 transition

4.2.1. Loading phase

Our experimental sequence begins with the loading of ^6Li atoms from a Zeeman slowed atomic beam into a MOT on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition at 671 nm. The experimental parameters for the initial phase of the MOT are optimized for the number of trapped atoms N , which reaches a steady-state value after a sufficiently long loading duration. The atom number is determined by a balance of the loading and loss rate of atoms from the MOT and is discussed below. In order to capture atoms from the atomic beam, we create a large volume MOT by applying a moderate magnetic field gradient of 12 G/cm (6 G/cm) in the axial (transverse) direction of the magnetic field coil. For a fixed gradient, the atom number is recorded as a function of the laser detuning δ of the MOT light with respect to the atomic transition, as exemplarily shown in Fig. 4.3. The shape of the obtained curve seems in qualitative agreement

with the numerical calculation of the capture velocity, which was discussed in Section 4.1.3. The optimal parameters for the loading phase of the MOT are found to be given by an axial magnetic field gradient of 12 G/cm and a laser detuning of $-7\Gamma_{2P}$ and are summarized in Fig. 4.5.

Dominant loss mechanisms in a magneto-optical trap are inelastic collisions, mainly involving a ground and an excited-state atom (Ritchie et al., 1995), and collisions with atoms and molecules from the hot background gas (Van Dongen et al., 2011). The loading dynamics is governed by a rate equation for the number according to (Weiner et al., 1999)

$$\frac{dN}{dt} = R - \gamma N - \beta \int n^2(\mathbf{r}, t) d\mathbf{r}, \quad (4.6)$$

where R is the loading rate, $n(\mathbf{r}, t)$ the atomic density, and γ and β are one- and two-body loss coefficients. During the initial phase of the loading process, the rate equation is dominated by R and the total number of atoms increases approximately linearly in time. For an increasing atom number, the contributions of the loss terms become more significant, eventually leading to a steady state value for the atom number. This characteristic time evolution is shown in Fig. 4.4 (a), from which we estimate a loading rate of $R \approx 2.4 \times 10^8$ atoms/s. The loading of the MOT can be interrupted by blocking the atomic beam, leading to a decay of the atom number according to Eq. (4.6). We infer a $1/e$ lifetime of the MOT of $\tau = 1/\gamma = 40$ s if the parameters for the detuning and the magnetic field gradient remain unchanged from the loading phase. This decay process is studied in more detail for the UV MOT and is discussed in Section 4.3.4.

4.2.2. Compressed MOT phase

The parameters during the loading phase of the MOT yield high atom numbers, however, densities are generally low and observed temperatures are on the order of 1-3 mK. To facilitate the transfer of the atoms into the small-volume UV MOT, a compression of the red MOT (CMOT) is carried out by simultaneously changing the detuning δ to $-2.7\Gamma_{2P}$, reducing the laser intensity to around $0.01 I_{\text{sat}}^{2P}$, and ramping the magnetic field gradient to 32 G/cm. The temperature of the atomic cloud after this CMOT stage is inferred from a time-of-flight measurement as discussed in Section 3.5 and is exemplarily shown in Fig. 4.6. We obtain a value of $274 \mu\text{K}$, which is about twice the Doppler temperature of $140 \mu\text{K}$. From absorption

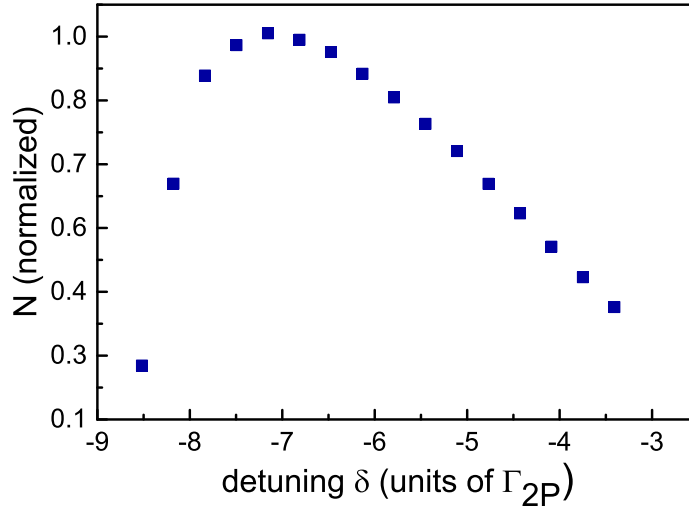


Figure 4.3.: Loading of the MOT on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition. The number of atoms N after a loading duration of 7.5 s is recorded as a function of the laser detuning δ . The magnetic field gradient is fixed at a value of 16 G/cm and N is normalized to unity.

imaging we infer an atom number of $N = 1.8 \times 10^9$ and a peak density of $n_0 = 6.4 \times 10^{10} \text{ cm}^{-3}$, where we generally estimate a systematic uncertainty of about 10% in the measured quantities. The corresponding phase-space density of the atomic cloud is calculated according to $\rho_0 = n_0 \Lambda^3$ (see Eq. (2.6)), where Λ is the thermal de Broglie wavelength, yielding a value of 5.1×10^{-6} for the atomic cloud after the red CMOT phase. This value is comparable with other lithium experiments (Zimmermann, 2010).

The temperature of the atomic cloud depends on the detuning of the laser cooling light, as implied by Eq. (4.4). Experimentally it is found that the temperature depends not only on the detuning from the atomic transition, but also on the magnetic field gradient and the laser intensity. A typical measurement of the temperature as a function of the laser detuning is shown in Fig. 4.4 (b). The trend of the temperature is characteristic for standard Doppler cooling with a clear minimum at a laser frequency close to the atomic transition. The actual position of the minimum does not coincide with the predicted optimal detuning of $-0.5 \Gamma_{2P}$, however, deviations from the simplified Doppler cooling theory are expected. For instance, spontaneously emitted photons of the cooling process can be absorbed by other atoms in the cloud, which can compromise the cooling efficiency, as described, for example, by DePue et al. (2000). Such effects are not included in the Doppler cooling theory and are difficult to be estimated. In our experiment, the parameters of the CMOT on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$

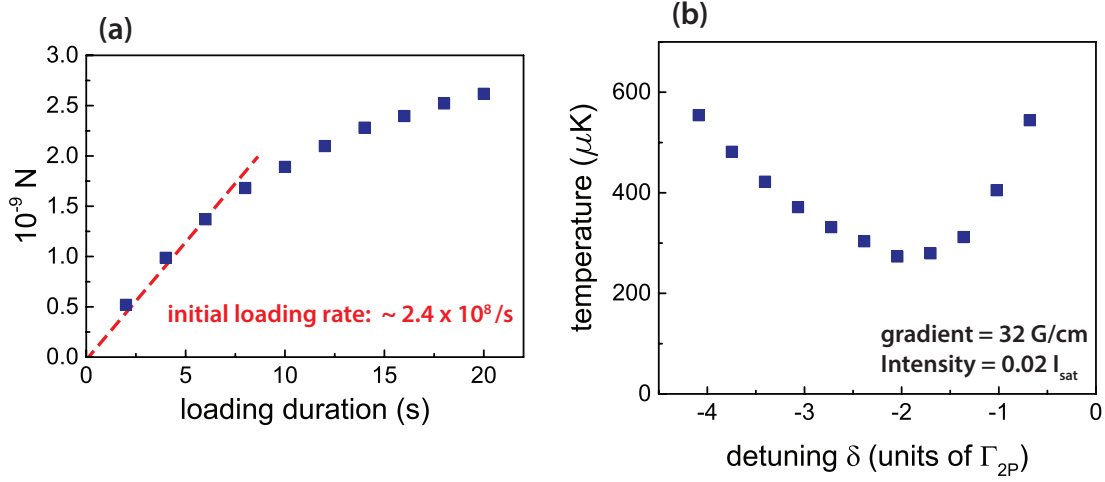


Figure 4.4.: (a) Loading of the MOT with experimental parameters given in the text. The initially linear increase in atom number is slowed due to loss mechanisms and the number of trapped atoms reaches a constant value after about 25 s. (b) Temperature of the atomic cloud after the CMOT phase on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition as a function of detuning δ .

transition are optimized for the transfer efficiency into the UV MOT and are summarized in Fig. 4.5.

4.3. UV cooling to high phase-space densities

UV MOT sequence After the compressed MOT phase on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition, the atoms are then transferred to the UV MOT by switching on the UV beams and rapidly reducing the magnetic field gradient while the red MOT light is extinguished. Each of the UV beams has a peak intensity of $0.4 I_{sat}^{3P}$ for the cooling and $0.01 I_{sat}^{3P}$ for the repumping transitions, where the saturation intensity of the UV transition is $I_{sat}^{3P} = 13.8 \text{ mW/cm}^2$. The experimental sequence with details on the relevant parameters is shown in a timing diagram in Fig. 4.5 and is described in the following sections.

We achieve the highest transfer efficiency with a reduced magnetic field gradient of 3.4 G/cm and a UV light detuning of $-8 \Gamma_{3P}$ during the UV MOT loading phase. At these parameters the lifetime of the atomic cloud is short, and we implement CMOT stage 1.5 ms after the transfer. For this, gradient and detuning are linearly ramped to the final values within 1.5 ms, while the light intensities are kept constant throughout the UV MOT phase. After a hold time τ of 16 ms, allowing for the spatial compression of the atomic cloud to be completed, the atoms are probed by standard absorption imaging on the D_2 line to infer atom number, density, and temperature.

stage parameters	Red MOT			UV MOT			TOF and Imaging
Axial gradient (G/cm)	12		32	3.4		15.8	Off
Red intensity (I_{sat}^{2P}) cooling/repump	3.7/1.6		0.01/0.01			0/0 (0/0.003)	Off
Red detuning (Γ_{2P})	-7		-2.7			-1	
UV intensity (I_{sat}^{3P}) cooling/repump						0.4/0.01 (0.4/0)	Off
UV detuning (Γ_{3P})				-8		-2.9	
Time interval (ms)	// 10^4	20	// 50	1.5	1.5	16	0.5 - 10

Figure 4.5.: Experimental sequence and corresponding parameters for red MOT, UV MOT, and imaging as explained in the text. In specifying the red and UV frequency detunings the values apply to both cooling and trapping transitions. The dotted lines for the red intensity and detuning indicate the realization of the UV MOT with the red repumping light, for which the parameters are given in parenthesis.

Repumping light Instead of using light on the UV transition to return atoms from the $2S_{1/2}, F = 1/2$ ground state back to the cooling transition, we also investigate the UV MOT by providing repumping light on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition for this purpose, to which we refer to as red repumper in the following. For standard laser cooling of lithium, the intensity requirements for cooling and repumping transitions are similar, as it was described in Section 3.1. This would suggest that using the red repumper would compromise the effect of the UV cooling because of the broad linewidth of the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ and the associated Doppler temperature. However, we find that efficient cooling with either repumping scheme can be achieved, as described below in Section 4.3.2.

4.3.1. Optimization of phase-space density

High atomic densities and phase-space densities in laser cooled clouds are of interest for different reasons and applications. For quantum gas experiments, the MOT is an intermediate step where high phase-space densities are beneficial for an efficient transfer of atoms to other traps (Lin et al., 2009; O’Hara et al., 2001b) and to provide good starting conditions for evaporative cooling. High densities are also of importance for studies of collisional processes, such as photoassociation spectroscopy measurements where the signal strength scales quadratically with the atomic density (Weiner et al., 1999).

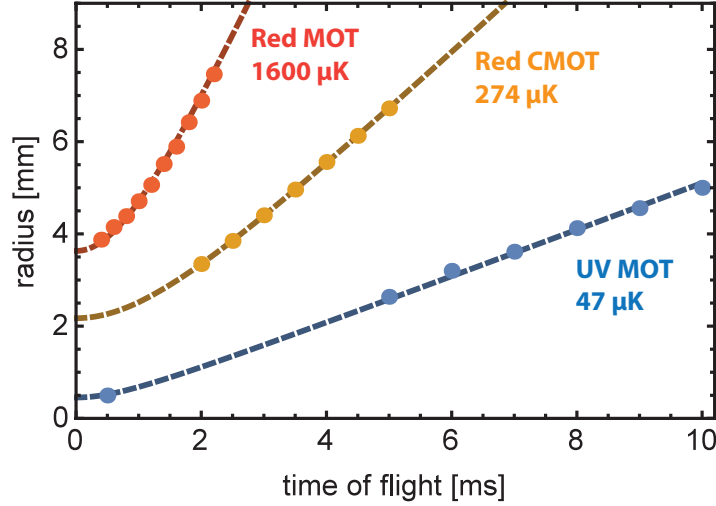


Figure 4.6.: Time-of-flight measurement after the red MOT, red CMOT, and the UV MOT. The temperature is inferred as described in Section 3.5. Here, the UV MOT is realized with repumping light on the UV transition.

The experimental parameters for the final stage of the UV CMOT are optimized by scanning the detuning of the UV light for various final magnetic field gradients. Peak density and temperature are measured by probing the atomic cloud at 0.5 ms and 8 ms time-of-flight, respectively. These values, together with atom number and phase-space density, are plotted in Fig. 4.7. A set of plots where the red repumping light replaces the UV repumper are also shown. In general we observe that different magnetic field gradients do not result in significantly different temperatures. Using the UV repumper, the highest peak density of $3 \times 10^{11} \text{ cm}^{-3}$ is achieved at a magnetic field gradient of 15.8 G/cm and a detuning of about $\delta = -2\Gamma_{3P}$. Lower gradients lead to a reduced confinement strength and to lower peak densities, as exemplarily shown for a gradient of 7 G/cm. However, increasing the magnetic field gradient beyond 15.8 G/cm does not further increase the peak density, as lower total atom numbers are attained.

Even higher peak densities are achieved by using the red repumper, as illustrated in Fig. 4.7. In this case the temperature is consistently higher as compared to the scheme where the UV repumper is used, and the combined effect leads to an overall reduced phase-space density when using the red repumper. The highest value for the phase-space density of the UV MOT is attained with the UV repumper at a temperature of $47 \mu\text{K}$ and an atom number of 1×10^8 , with a typical time-of-flight measurement shown in Fig. 4.6. The resulting value of $\rho = 3.3 \times 10^{-4}$ is approximately an order of magnitude higher as compared to previous reported values (Burchianti et al., 2014; Duarte et al., 2011) for ^6Li atoms involving the UV

transition or gray-molasses cooling.

4.3.2. UV and red repumping light

We find that for either the UV or red repumper, the peak density depends strongly on the power that is used to drive the repumping transition. This effect is studied at a magnetic field gradient of 15.8 G/cm and a UV detuning of $-2.9 \Gamma_{3P}$. While the cooling power is kept constant, the peak density is measured as a function of the repumping intensity, as shown in Fig. 4.8 (a). As the hyperfine structure of the optically excited states is not well resolved for lithium (see Fig. 3.2), the repumping light needs to be sufficiently strong and has to be provided along all 3 principal axes. At very low intensities of the repumping light, the trapping force is decreased due to the reduced scattering rate on the UV transition, and atoms are lost from the trap. This effect can be seen in Fig. 4.8 (b), where the atom number is shown as a function of the repumping intensity.

If we use the red repumper, we obtain the highest peak density of $3.8 \times 10^{11} \text{ cm}^{-3}$ at an intensity of $\simeq 0.003 I_{\text{sat}}^{2P}$, corresponding to only $10 \mu\text{W}$ per beam. At larger intensities of the repumping light, an increasing fraction of the atoms is optically pumped out of the $F = 1/2$ ground state. Therefore, the total scattering rate on the UV transition is increased and along with it density limiting factors like photon-reabsorption and light-assisted collisional two-body losses are enhanced. Obtaining high atomic densities at a comparatively low repumping intensity therefore resembles a situation that similar to a dark spontaneous-force optical trap (Ketterle et al., 1999). If the MOT is realized with the UV repumper, the peak density reaches a maximum value of $2.5 \times 10^{11} \text{ cm}^{-3}$ at $\simeq 0.009 I_{\text{sat}}^{3P}$. This corresponds to a ratio of only 44 : 1 between cooling and repumping intensity. At increased intensities the atom number decreases, while the density remains approximately constant. This is different to the situation with the red repumper, where a pronounced maximum of the density is observed in Fig. 4.8 (a). One reason for this different trend could be the overall lower observed peak density for the UV MOT with UV repumper, which leads to reduced two-body losses and correspondingly a slower decay in the total atom number.

Employing repumping light on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition alters the narrow-line character of the UV cooling scheme. The spontaneous scattering events on the red transition induce a heating that scales with the natural linewidth, as described in Section 4.1. However,

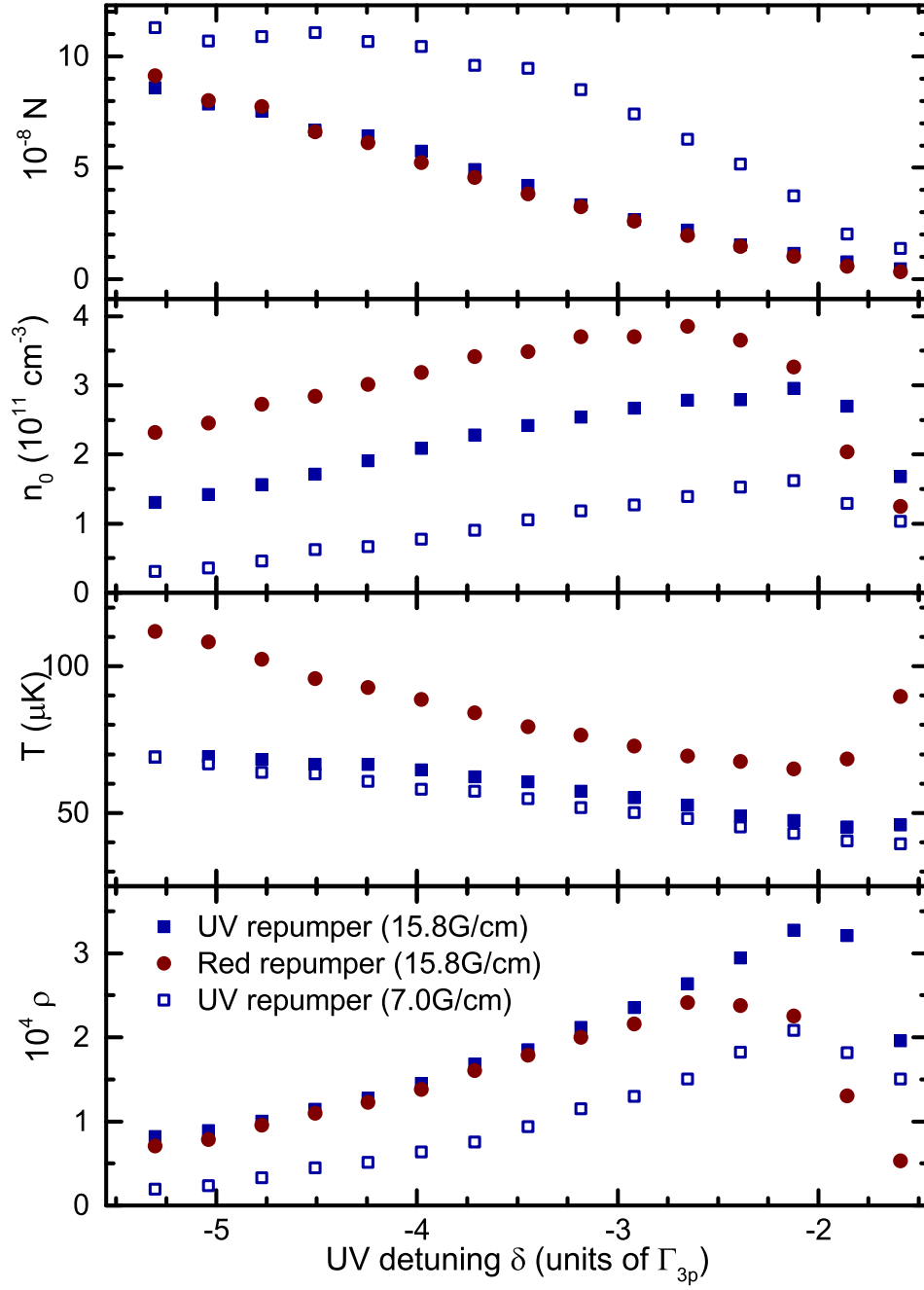


Figure 4.7.: Performance of the UV MOT. Atom number, peak density, temperature, and phase-space density are shown as functions of the detuning with respect to the UV cooling transition. The up/down triangles correspond to the UV MOT with UV repumper at magnetic field gradients of 15.8 G/cm and 7 G/cm, respectively. The open circles represent the UV MOT with red repumper at a gradient of 15.8 G/cm.

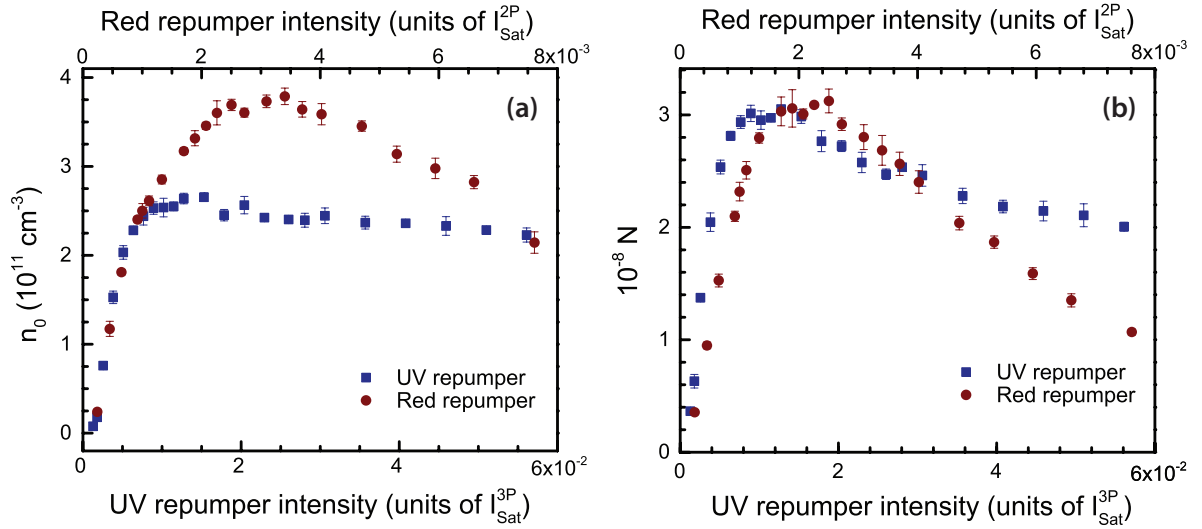


Figure 4.8.: (a) Peak density and (b) atom number as function of repumping intensity. The compressed UV MOT is realized with different intensities for the UV repumper (squares, x axis) and the red repumper (circles, upper x axis) at a magnetic field gradient of 15.8 G/cm and a detuning of $-2.9\Gamma_{3P}$.

the observed temperatures of the laser cooled atoms are well below the Doppler limit of the D_2 transition. For the experimental parameters that are used, this implies that the cooling strength of the UV light is large compared to the induced heating on the red transition.

4.3.3. Temporal evolution

It is important to note that the observed high peak density in the UV MOT is a transient effect. Shown in Fig. 4.9 (a) are measurements of peak density and atom number as functions of hold time τ after gradient and detuning reached the final values of the compressed MOT. In the initial phase we observe a fast contraction of the atomic cloud, resulting in a maximal peak density after approximately 16 ms, which then decays at a slower rate. This compression timescale seems consistent with a model in which an overdamped oscillatory motion is assumed for a single atom in the light field (Metcalf and van der Straten, 1999). With the parameters for the UV MOT as indicated in Fig. 4.5, a restoring time of 6 ms to the trap center is estimated. However, this simplified model neglects the effects of reabsorbed photons and the weak repumping light, which reduces the trapping force and leads to a longer relaxation time. In addition to this effect, we believe that the density buildup is limited by two-body losses. After changing the experimental parameters to initiate the compressed MOT phase, the atoms move to the center of trap, leading to an increased peak density. The increased two-body losses in the center are initially compensated by atoms propagating inwards. This

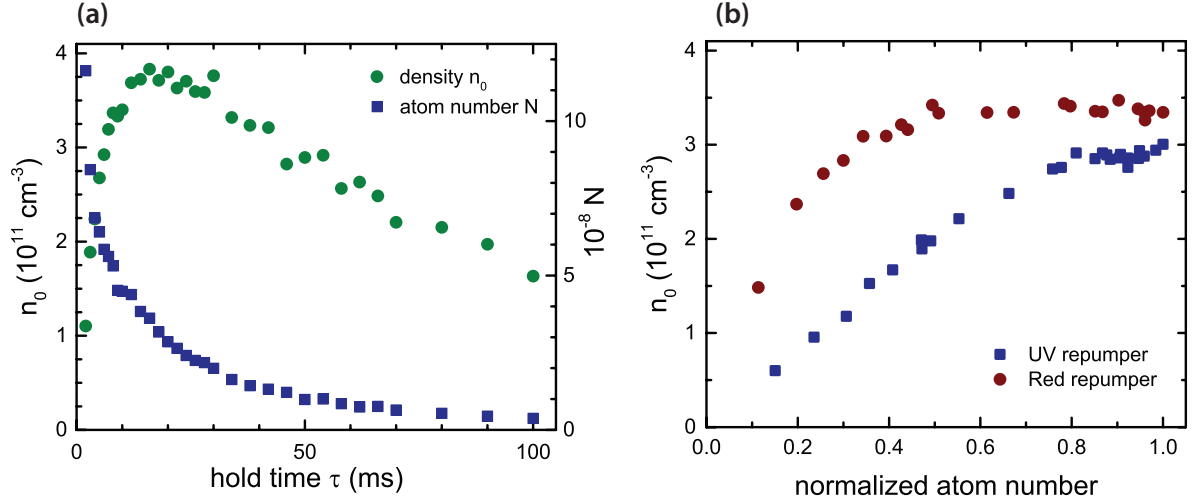


Figure 4.9.: (a) Transient dynamics of the UV MOT with red repumper after compression. Peak density and atom number are shown versus the hold time in the UV MOT with the final parameters as indicated in Fig. 4.5. (b) Peak density as a function of the atom number. The different atom numbers are attained by varying the loading duration of the red MOT between 0.2 s and 14 s.

process first leads to a reduction in the atom number and eventually also in the peak density, similar as described by DePue et al. (2000). The observed peak densities are therefore difficult to be increased by a higher atom number. We verified this by changing the loading time. For the case of the red repumper the atom number can be lowered by a factor of about 2, before the peak density is noticeably reduced, which is illustrated in Fig. 4.9 (b). The atom number was varied by changing the loading time of the red MOT.

4.3.4. Lifetime and 2-body loss rate of the UV MOT

In order to further study the limitations on density and atom number we perform lifetime measurements of the compressed UV MOT with either the UV or red repumper to determine the one- and two-body loss coefficients. This is done at repumping powers leading to high densities and at a gradient of 15.8 G/cm and detuning of $-2.9 \Gamma_{3P}$. The time evolution of the number of trapped atoms N is described by Eq. (4.6) and can be expressed for an atomic cloud with a Gaussian density distribution by

$$\frac{dN}{dt} = -\gamma N - \beta \frac{N^2}{(2\pi)^{3/2} \sigma_\rho^2 \sigma_z}, \quad (4.7)$$

where σ_ρ (σ_z) is the radial (axial) $1/e$ radius of the density distribution as defined in Section 2.1 and γ and β are the one- and two-body loss coefficients that were introduced in Eq. (4.6). The measurement is performed during the UV CMOT phase, where the atomic beam is blocked

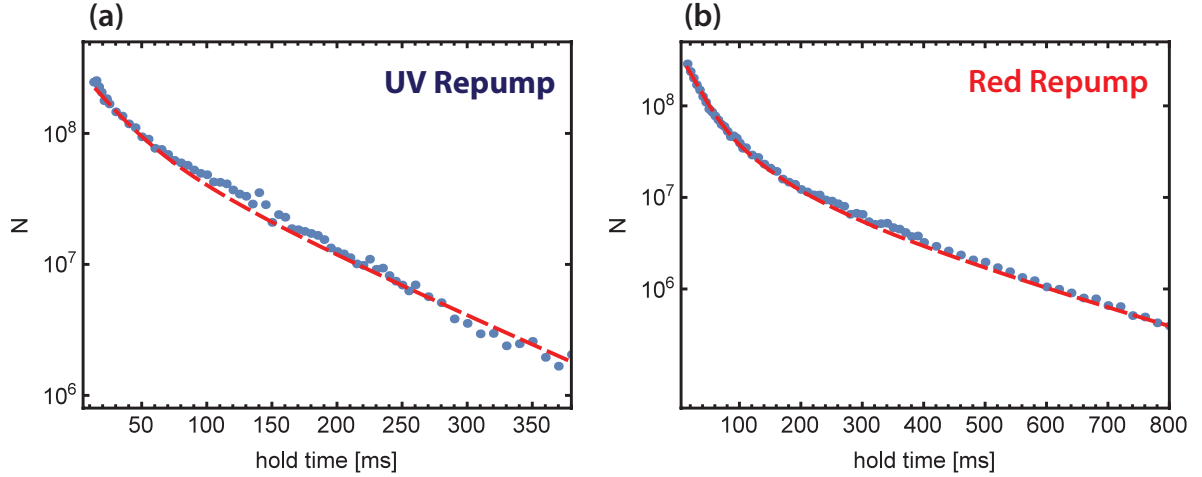


Figure 4.10.: Trap loss measurement for the UV MOT with (a) UV and (b) red repumper. The atom number (circles) is measured as a function of hold time in the compressed UV MOT and Eq. (4.7) is fitted to the data (dashed line). At long hold times the density is low and the atom number follows an exponential decay.

by a shutter and the loading rate R therefore vanishes. During the decay measurement we observe that the radius of the cloud is not constant, but changes with the atom number leading to a time dependence of the radius $\sigma_i = r_i(t)$, ($i = \rho, z$). This implies that Eq. (4.7) cannot be solved analytically. Instead, the differential equation is fitted directly to the experimental data, in order to extract the loss coefficients. We obtain $\beta = 1.3 \pm 0.4 \times 10^{-10} \text{ cm}^3/\text{s}$ if the UV repumper is used and $\beta = 2.1 \pm 0.6 \times 10^{-10} \text{ cm}^3/\text{s}$ for the red repumper, with the corresponding fits to the experimental data shown in Fig. 4.10. These values are high compared to previous measurements for the red MOT (Ridinger et al., 2011), but comparable to values reported for a potassium MOT driven on the narrow-line transition (McKay et al., 2011). We attribute the larger two-body loss rate in part to the reduced effective trap depth (Ritchie et al., 1995) and the small capture velocity, due to the low intensity of the MOT beams and narrow linewidth of the UV transition.

We obtain high one-body decay rates γ of $1/(84 \text{ ms})$ and $1/(224 \text{ ms})$ for using the UV and red repumper, respectively. We can exclude losses due to collisions with background atoms as a dominant contribution, as decay measurements of the red MOT yield lifetimes on the order of 40 s. We attribute the short lifetime to the finite capture velocity for the parameters after the compression ramp, which are optimized to achieve high phase-space densities. This is consistent with our observation of longer one-body decay times, if the gradient is reduced and the detuning increased. Driving the MOT on the UV transition introduces decay channels via photoionization, as described in more detail in Chapter 6. The loss rate due to ionization

is estimated based on a theoretical calculation of the ionization cross section of the excited states (Lahiri and Manson, 1993). We find approximately 1 s as a lower limit for the lifetime with respect to photoionization and conclude that this process is negligible on the timescale of the UV MOT and future loading into the ODT.

4.4. Summary

In summary, we have implemented and investigated a two-stage ^6Li MOT utilizing the narrow UV transition to achieve sub-Doppler temperatures with respect to the D2 transition. By compression in the UV MOT we achieve a transient phase of high density. This is possible as the rapid decay of the atom number is initially compensated by the contraction of the atomic cloud. We have measured high collisional two-body loss rates, which we identify as an important density limiting factor. Our optimization results in a high phase-space density for laser cooled lithium atoms. This is advantageous for efficient direct loading from the MOT into an optical dipole trap and facilitates further cooling for the production of a quantum degenerate sample.

5. Optical transport in a crossed ODT and cooling to quantum degeneracy

In this chapter the experimental sequence for the production of a large quantum degenerate sample of fermionic lithium is described. This approach is based on the efficient narrow-line laser cooling and trapping on the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition in the ultraviolet regime, which was discussed in Chapter 4. Due to the small linewidth, temperatures are achieved that are well below the Doppler limit for laser cooling on the D_2 transition, resulting in high phase-space densities. In addition, laser cooling remains effective when the atoms are loaded into an optical dipole trap.

We employ a small-angle crossed-beam trapping geometry with a large volume, leading to good loading efficiencies from the UV MOT, while simultaneously offering a suitable axial confinement for a fast transport of the atomic cloud. With this simple extension of the single-beam optical tweezers method no further optical trapping steps are needed, such as a resonator-enhanced ODT (Zimmermann et al., 2011) or a transfer between subsequent ODTs of decreasing volume (Omran et al., 2015). Our trapping configuration is used to transport the atoms into a science cell in order to facilitate good optical access. Furthermore, the optical confinement is sufficient for evaporative cooling of the atomic cloud into the quantum degenerate regime and the production of a Bose-Einstein condensate of Feshbach molecules. Part of this chapter was published in *Physical Review A*, **93**, 053424 (2016) (Gross et al., 2016).

5.1. Experimental approach

Different cooling and transport schemes Quantum gases have been widely studied with lithium and potassium because they both have fermionic and bosonic isotopes. For these

two species standard sub-Doppler laser cooling is not observed or inefficient, as described in Chapter 4. More recently, however, alternative schemes of laser cooling such as narrow-line cooling (Duarte et al., 2011; McKay et al., 2011) and gray optical molasses techniques (Burchianti et al., 2014; Fernandes et al., 2012; Grier et al., 2013; Salomon et al., 2013, 2014) were successfully demonstrated. This led to significantly improved phase-space densities after laser cooling and the improved all-optical production of quantum degenerate samples. Especially, the loading of the atoms into optical dipole traps can be improved, as this process typically suffers from insufficient matching of trapping volumes and depths.

An often important aspect for quantum gas experiments is the transport of atomic clouds over long distances to facilitate advanced techniques in manipulating and probing ultracold gases that require good optical or mechanical access. This mitigates constraints generally imposed by magneto-optical trapping and pre-cooling. Several transport methods were developed, which include the translation of magnetic traps (Greiner et al., 2001; Lewandowski et al., 2003) and optical tweezers (Couvert et al., 2008; Gustavson et al., 2001; Léonard et al., 2014; Zimmermann et al., 2011), as well as 1D moving optical lattices (Middelmann et al., 2012; Schmid et al., 2006). In most of these experimental schemes the confinement of the atoms is optimized for the transport itself, which requires different measures for the loading of the atoms into the optical dipole trap and subsequent optimized evaporative cooling.

Cold atom source Our experimental sequence for the production of a quantum degenerate ^6Li gas starts with a two-stage MOT. At first, we employ a standard MOT on the D2 transition to obtain a large number of atoms. This is followed by Doppler cooling on the narrow UV $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition at 323 nm with a natural linewidth of the excited state of $\Gamma_{3P} = (2\pi) \times 754 \text{ kHz}$. After this two-stage MOT, we typically obtain a ^6Li cloud containing around 1.5×10^8 atoms at a temperature of $\sim 50 \mu\text{K}$ with a central density on the order of $3 \times 10^{11} \text{ cm}^{-3}$.

In the next step the atoms are transferred into a crossed optical dipole trap that comprises of two beams intersecting at a small angle. The laser wavelength of 1070 nm for the optical dipole trap is near a magic wavelength, where the differential ac Stark shift of the UV MOT transition vanishes (Duarte et al., 2011; Safronova et al., 2012). This permits continued cooling on the UV transition during the initial stage of optical trapping and allows us to take full advantage of the high phase-space density of the UV MOT.

Optical transport After loading we transport the atoms into a small glass cell that is attached to the MOT vacuum chamber, as it was shown in Fig. 3.3. As the atoms are loaded from a Zeeman-slowed atomic beam, the vacuum background is low and no differential pumping stage between the MOT and science cell is required. This allows the use of a linear optical transport. Our particular scheme demonstrates the displacement of a crossed optical dipole trap across a long distance, realized with an air bearing translation stage. This is a key feature of our simplified experimental approach, as efficient direct loading from the MOT, loss-free near-adiabatic transport, and efficient evaporative cooling are achieved in the same trap.

Cooling to quantum degeneracy Evaporative cooling of the atomic cloud is performed in the science cell with a spin mixture of the two energetically lowest Zeeman levels, commonly referred to as states $|1\rangle$ and $|2\rangle$ (see appendix A.2). In order to tune the s -wave scattering length a_{12} , magnetic bias fields of up to ~ 1300 G can be applied. For this work evaporative cooling is either carried out near the broad Feshbach resonance at 832 G (Zürn et al., 2013) to create a strongly interacting Fermi quantum gas in the BEC-BCS crossover regime (Bartenstein et al., 2004), or at around 330 G to obtain a weakly interacting Fermi gas.

5.2. Optical dipole trap

The setup to generate and power-stabilize two beams for the crossed optical dipole trap was described in Section 3.6.2 and illustrated in Fig. 3.11. In order to avoid interference effects, the two trapping beams have orthogonal polarization and differ in frequency by 220 MHz. They are aligned parallel with respect to each other, separated by 2.6 cm and pass, symmetrically offset from the center, a $f = 500$ mm achromatic lens that is placed on a translation stage. This leads to a crossing angle of 3° for the ODT and was illustrated in Fig. 3.10 (c). This angle is determined under the geometric constraint of the aperture of the vacuum viewport. The two beams intersect near their foci, which have measured waists of $65\ \mu\text{m}$ and $67\ \mu\text{m}$, respectively. On a CCD camera we observed a slight power-dependent astigmatism. In contrast to a single-beam dipole trap, this has a negligible effect on the position of the ODT during forced evaporation, as the axial position of the trap is predominantly defined by the crossing of the two beams.

5.2.1. Characterization of the trapping potential

The trap depth U_0 of the crossed ODT, as defined in Eq. (3.10), is inferred from the measured beam parameters and the optical power. The full trap depth with 22.5 W per beam is estimated to be $k_B \times 330 \mu\text{K}$, which takes the observed astigmatism into account. In this section we characterize the ODT and note that the presented measurements were performed in the glass cell. This relies on the loading of the ODT and the optical transport, which is only described in the subsequent sections. For now, these experimental steps should be assumed to have been properly implemented.

Trap frequencies of ODT

To establish the atomic density in the ODT and for calculating the temperature of a degenerate Fermi gas from a time-of-flight measurement, the trap frequencies have to be known, as described in Chapter 2. Similar to the trap depth, they can be estimated from the measured ODT beam parameters. However, for more accurate values, the trap frequencies are determined experimentally.

With an auxiliary coil close to the atomic cloud we apply a short magnetic field gradient pulse in order to displace the atomic cloud along a symmetry axis of the trap to excite a center-of-mass oscillation. Duration and strength of the pulse are balanced to result in an observable motion of the cloud, while curtailing the displacement to limit effects of the anharmonicity of the trapping potential. These parameters have to be adjusted for each optical power where the trap frequency is measured. The oscillatory motion of the cloud in the trap is damped and the displacement Δz from the trap center is described by

$$\Delta z(t) = K e^{-\gamma t} \cos(\omega' t + \phi) + \text{offset}, \quad (5.1)$$

where $\omega = \sqrt{\omega'^2 + \gamma^2}$ is the angular trap frequency and γ the damping coefficient. This model is fitted to the observed position of the atomic cloud after various oscillation durations t . To fully characterize the trap, this measurement is performed for a series of optical powers along all 3 principle axes $i = x, y, z$. Following from Eq. (3.11), the scaling of the trap frequency with optical power P can be expressed by

$$\omega_i = 2\pi \times A_i \sqrt{P}. \quad (5.2)$$

	Crossed ODT	Single-beam ODT	Single-beam ODT
$1/e^2$ waist	$66\ \mu\text{m}$	$36\ \mu\text{m}$	$21\ \mu\text{m}$
Optical power	45 W	45 W	2 W
U_0/k_B	$330\ \mu\text{K}$	1.3 mK	$173\ \mu\text{K}$
Γ_{sc}	0.46 Hz	1.9 Hz	0.24 Hz
$\omega_y/2\pi$	81 Hz	81 Hz	85 Hz
$\bar{\omega}_r/2\pi$	3.04 kHz	12.10 kHz	7.43 kHz
Aspect ratio	37.5	149	87.2

Table 5.1.: Parameters of the implemented crossed ODT (first column) are compared to calculated values for a single-beam configuration with identical total optical power and axial confinement (second column). As reference, in the last column the respective values are listed for an optical trap geometry used for transport as reported in Ref. (Zimmermann et al., 2011). The values given for our crossed trap include effects of imperfect alignment.

This model is fitted to the observed trap frequencies, as shown in Fig. 5.1 (a),(b). The proportionality constant A is determined along all 3 axes and we obtain $A_x = 644 \pm 9\ \text{Hz}/\sqrt{W}$, $A_z = 638 \pm 3\ \text{Hz}/\sqrt{W}$ for the transverse and $A_y = 17.1 \pm 0.2\ \text{Hz}/\sqrt{W}$ for the axial direction of the optical dipole trap. The resulting trap frequencies at full optical power, and other relevant parameters of our trap, are listed in the first column of Table 5.1.

Curvature of magnetic bias field

The magnetic bias field to tune the s -wave scattering length and to access the Feshbach resonance has a small residual field gradient. In the horizontal plane, which is transverse to the symmetry axis of the coil assembly, the magnetic field has a negative curvature B'' and a local maximum approximately at the center of the science cell. The magnetic field strength can be expressed by

$$B(r, z=0) \approx B(0) + B'' \frac{r^2}{2}. \quad (5.3)$$

For the atoms, which are prepared in a mixture of the two lowest hyperfine Zeeman states, this results in a radial confinement for bias fields that are experimentally relevant. The magnetic field induced energy shift is approximately linear for fields that are higher than $\sim 150\ \text{G}$, as illustrated in Appendix A.2, resulting in horizontal trap frequencies given by

$$\omega_{\text{mag}; x, y} = \sqrt{\frac{\mu_B |B''|}{m}}, \quad (5.4)$$

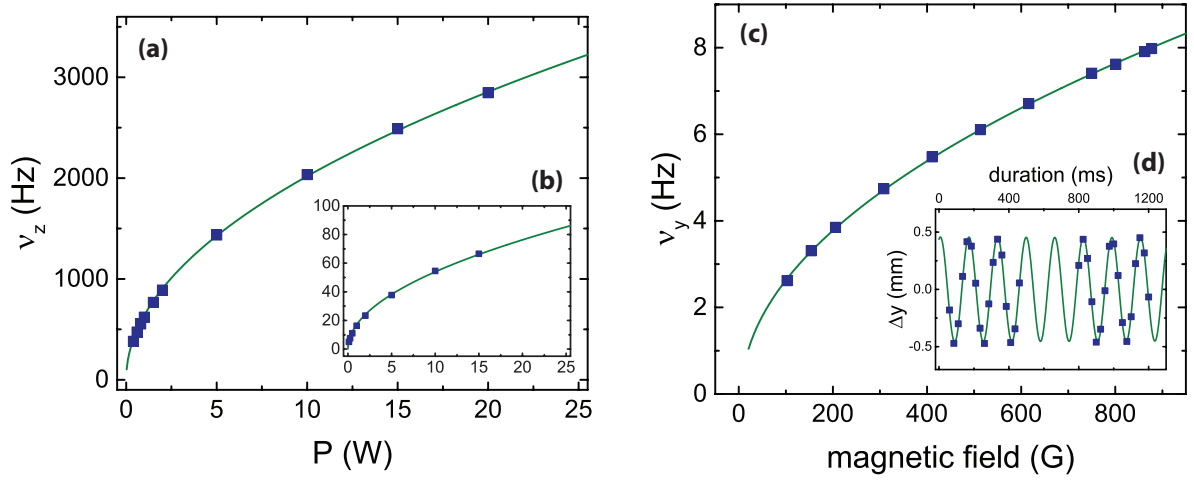


Figure 5.1.: (a) Transverse and (b) axial trap frequencies of the ODT for different optical powers. The squares are measured values and the lines are fits to the data using equation 5.2. (c) Residual magnetic trap frequency versus Feshbach field strength. The offset at $B = 0$ is due to a residual optical trap frequency of the single-beam ODT. (d) Center-of-mass oscillations of the atomic cloud in the single ODT beam at a magnetic bias field B of 500 G. After a variable duration of in-trap motion the position of the atomic cloud is determined (squares) and fitted to a damped harmonic oscillator model (line).

where μ_B is the Bohr magneton and m the atomic mass. Following from Maxwell's equations, the magnetic field curvature in the vertical direction has opposite sign and twice the magnitude of the value in the horizontal direction. This leads to an anti-confining potential that can formally be described by an imaginary trap frequency in the vertical direction, given by $\omega_{\text{mag},z} = i\sqrt{2}\omega_{\text{mag},x,y}$.

The contribution of the magnetic field curvature to the trap frequency can be measured experimentally as follows. Using the translation stage, the optical dipole trap is axially slightly displaced from the center of the glass cell and therefore from the center of the magnetic potential. Subsequently, the power of one of the ODT beams is ramped to zero, which transfers all the atoms into an optical potential defined by a single beam. This measurement is performed at an optical power of 0.25 W corresponding to an axial trap frequency of the single-beam potential of $\omega_y = 2\pi \times 1$ Hz, as compared to $\omega_y = 2\pi \times 8.6$ Hz for the crossed-beam configuration. The atomic cloud then oscillates in the combined potential and the trap frequencies are deduced using Eq. (5.1). The observed center-of-mass oscillations are exemplarily shown in Fig. 5.1 (d) for a magnetic bias field of 500 G. This measurement is performed at various magnetic fields, as illustrated in Fig. 5.1 (c), from which we deduce the horizontal trap frequency $\omega_{\text{mag},x,y} = 2\pi \times 0.271(1) \text{ Hz}/\sqrt{\text{G}}$ and the curvature of the field

$B'' = -3.12 \times 10^{-3} B \cdot \text{cm}^{-2}$ in the horizontal plane.

The addition of the magnetic potential alters the trap geometry for the atomic cloud significantly only along the axial direction of the crossed ODT and only for low optical powers. This follows from the quadratic addition of the different contributions to the trap frequency, expressed by $\omega_{\text{tot}} = \sqrt{\omega_{\text{mag}}^2 + \omega_{\text{opt}}^2}$.

5.2.2. Loading of the ODT

For the transfer of the atoms from the MOT into the crossed ODT, the optical power is linearly ramped up within 2 ms to the full trap depth during the compressed UV MOT phase. As described in Section 4.3.3, the peak density reaches a transient maximum value during this stage, at which point the ramp-up is initiated. After a combined loading and cooling duration of 10 ms, the UV MOT is switched off by extinguishing the repumping light 0.5 ms in advance of the cooling light. This optically pumps the atoms into the $F = 1/2$ hyperfine ground-state manifold, creating an incoherent balanced mixture of the $|1\rangle$ and $|2\rangle$ states. For the measurements presented in this chapter, the UV MOT is realized with repumping light on the D_2 transition. However, employing the UV repumping light instead leads to very similar loading efficiencies¹.

Transfer efficiency and plain evaporation

Immediately after the loading we measure an atom number N of 1.1×10^7 , which corresponds to a transfer efficiency on the order of 10 %. The temperature is observed to be anisotropic with a geometric mean of $T = 43 \mu\text{K}$. This results in an initial truncation parameter of $\eta = U_0/k_B T = 7.7$. Following the loading of the atoms into the ODT we allow for 1 s of plain evaporation. At small magnetic fields the s -wave scattering length between the states of the $|1\rangle$ - $|2\rangle$ mixture is vanishingly small, inhibiting efficient thermalization of the atomic cloud. To initiate evaporation, a magnetic bias field of approximately 200 G is applied, generated by inverting the polarity of one of the MOT coils. This tunes the s -wave scattering length to $a_{12} = -220 a_0$ between the two states (Zürn et al., 2013), which is below a local maximum

¹The preference of using the red repumper has a technical reason. As illustrated in Fig. 3.9, the light for the cooling and repumping transition passes the same AOM before it is used in the experiment and can therefore not be employed to individually regulate the power for both transitions simultaneously. Therefore, a mechanical shutter is used to initiate the optical pumping. While a small jitter in the shutter timing has no effect on the loading efficiency, it is experimentally preferable to use AOMs to ensure day-to-day stability.

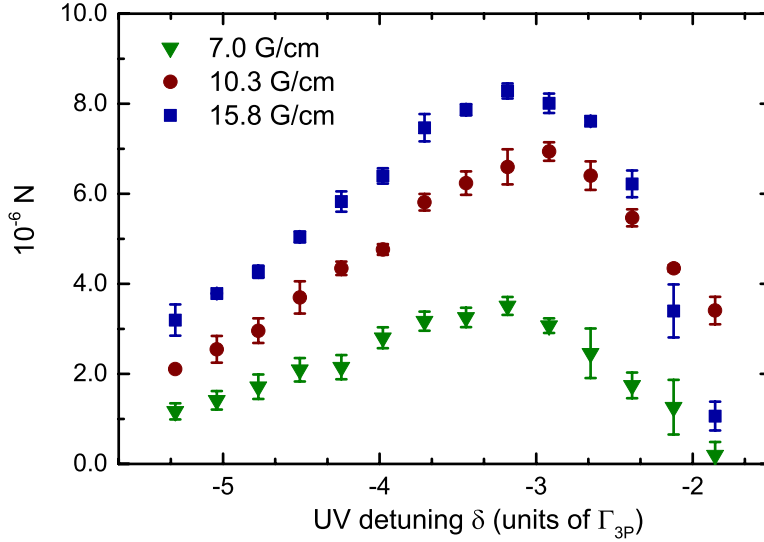


Figure 5.2.: Total number of atoms N in the ODT after plain evaporation as a function of the laser detuning with respect to the UV cooling transition for different axial magnetic field gradients of the MOT. The highest atom number is achieved with a detuning of $\delta \simeq -3.2 \Gamma_{3P}$ at a gradient of 15.8 G/cm. An increase of the magnetic field gradient beyond this value does not further improve the atom number.

of the absolute value of the scattering length that occurs at 320 G (see appendix A.3). This value is chosen to limit the heat load on the MOT coils.

After plain evaporation the balanced spin mixture in the ODT typically contains a total of $N = 8 \times 10^6$ atoms at a temperature of $T = 30 \mu\text{K}$ corresponding to $T/T_F = 2.4$. The Fermi temperature is defined as $k_B T_F = \hbar \bar{\omega} (3N)^{1/3}$, where $\bar{\omega} = (\bar{\omega}_r^2 \omega_z)^{1/3}$ is the mean trap frequency and $\hbar$ is the reduced Planck constant. This follows from the expression for the Fermi energy of a spin-polarized gas, given in Eq. (2.21). Using Eq. (2.5) for the harmonically trapped gas, we obtain an atomic peak density of $1.1 \times 10^{13} \text{ cm}^{-3}$. For the values stated here, we estimate a systematic uncertainty of about 10 % in the measured quantities.

Optimal UV detuning and simultaneous cooling and trapping

We investigated the effect of the UV detuning on the loading efficiency of the ODT, which is similar to the measurement discussed in Section 4.3.1 for the optimization of the phase-space density in the UV MOT. Shown in Fig. 5.2 is the atom number yield at the end of the plain evaporation stage for three different magnetic field gradients of the compressed UV MOT. Because the cloud thermalizes to the same temperature for all relevant detunings, the phase-space density follows the same curve and is not shown.

The UV frequency detuning of $\delta \simeq -3.2 \Gamma_{3P}$ for the maximum atom number differs from the

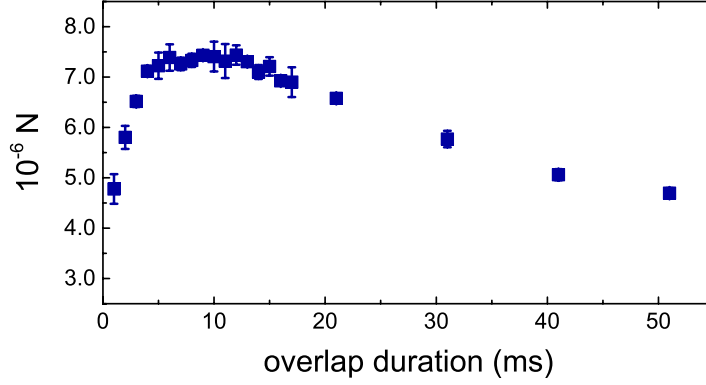


Figure 5.3.: Atom number vs. duration of continued UV cooling after the ODT is ramped up to full power. The initial increase in atom number demonstrates the effectiveness of UV cooling in presence of the 1070-nm trapping light, while the decrease at longer overlap durations is attributed to density dependent losses (see text). The error bars account for the statistical uncertainty of four repetitions.

detuning for the maximum phase-space density of the UV MOT, which was found to be $\delta \simeq -2.7\Gamma_{3P}$. The residual differential ac Stark shift of the cooling transition induced by the 1070-nm light cannot explain this difference, since it is small and increases the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition frequency (Duarte et al., 2011; Safronova et al., 2012). A possible reason for this observed difference could be due to enhanced light-assisted collisional loss on the UV transition, because the density is strongly increased in the presence of the optical dipole trap. In this case, the highest atom number is achieved for a larger laser detuning, which leads to a lower photon scattering rate and therefore a reduced atom loss from the trap.

The duration of the combined cooling and optical dipole trapping phase affects the loading efficiency, as shown in Fig. 5.3. Initially the atom number increases significantly with the overlap duration, demonstrating the efficiency of UV cooling in presence of the 1070-nm trap light. After a few milliseconds the atom number saturates and remains constant for about 10 ms. We assume that during this time the influx of atoms from the UV MOT into the ODT is approximately balanced with two-body losses occurring at high densities (DePue et al., 2000; Kuppens et al., 2000).

Furthermore, we measured the dependence of the transferred number of atoms on the optical power that is used to drive the UV MOT transition. A reduction of the optical power that is used for the 3 retro-reflected UV MOT beams leads to a reduced number of atoms transferred to the ODT, as shown in Fig. 5.4 (a). This shows that the experiment is not operated in a saturated regime. However, we find that even with just 1 mW of total UV power, an atom number of 2×10^6 is obtained in the optical trap before plain evaporation.

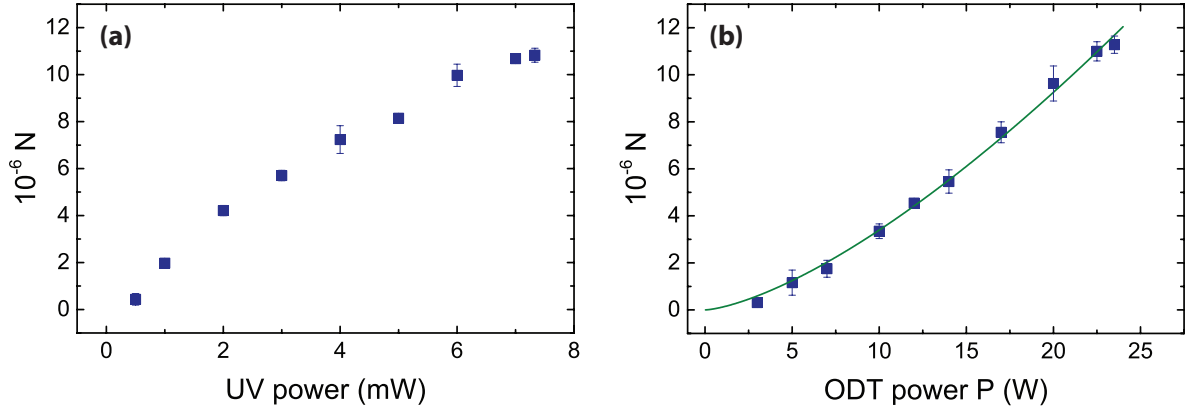


Figure 5.4.: (a) Number of atoms transferred into the ODT as function of the optical power for the UV MOT. The ODT is operated at full trap depth and the repumping intensity for the MOT is adjusted to maintain a constant ratio for the cooling and repumping power. (b) Dependence of the number of tapped atoms as function of the ODT power. The solid line is a fit of a power law function to the observed number of atoms before plain evaporation.

This demonstrates the effectiveness of laser cooling on the UV transition and shows that also low-power laser sources could be used to realize a UV MOT. For comparison, if we load the ODT directly from the red compressed MOT, less than 1×10^5 atoms are transferred. In Fig. 5.4 (b), the atom number is shown as a function of the available ODT power. No saturation of the atom number is observed at full trap depth, which suggests that a deeper trap could further improve the transfer efficiency. From a fit to a power law function we find an atom number dependence of $N(P) \propto P^{1.44^{(5)}}$, which is similar to another experimental observation (Zimmermann, 2010), but different to an exponential scaling as derived by O’Hara et al. (2001b) based on a simplified model.

Additional ODT beam at 1070 nm

In an effort to further improve the initial phase-space density in the ODT, we used an additional trapping beam to enhance the axial confinement of the trap during the UV cooling stage. This is motivated by the observation of continued UV cooling in the ODT and the relation between the phase-space density and the trap frequencies, as described by Eq. (2.6). For this purpose the frequency of one of the ODT beams is shifted by 115 MHz and directed back into the chamber to cross the existing trap under an angle of 51° . The additional beam has a maximum power of 15 W and a waist of $54 \mu\text{m}$ at the focus. This enhances the trap depth to around $k_B \times 500 \mu\text{K}$ and the axial trap frequency to $\omega_z = (2\pi) \times 1.8 \text{ kHz}$.

However, with this configuration we find that the temperature along the axial direction of

the atomic cloud before plain evaporation is increased by a factor of 3, despite the continued UV cooling. Furthermore, after plain evaporation and adiabatically extinguishing the auxiliary trapping beam, we find only a negligible enhancement of the phase-space density of the atomic cloud. A possible reason are interference effects between the ODT beams, as their polarizations are no longer mutually orthogonal and a spurious moving optical lattice is formed.

Additional ODT beam at 1064 nm

In an initial attempt we instead used a 1064-nm laser² to provide the third ODT beam, which was aligned along the same direction as the 1070-nm beam described in the previous paragraph. We used similar beam parameters and a maximum power of 35 W was available for the experiment. We observed that with the additional beam the number of trapped atoms is reduced, and decreases to 40% at full trap depth of the 1064-nm beam, as compared to the original configuration of two crossed beams. Furthermore, the mean temperature of the atomic cloud is increased by about a factor of two.

Overall, despite the increased density of the atomic cloud, the phase-space density is reduced by the introduction of the 1064-nm beam. A probable reason for these effects is the differential ac Stark shift on the cooling transition. Based a theoretical calculation by [Safronova et al. \(2012\)](#) we estimate a shift of the UV transition of -320 kHz/W for the 1064-nm trapping beam, as compared to 18.5 kHz/W for light at 1070 nm ([Duarte et al., 2011](#)). Relative to the natural linewidth of the $3^2P_{3/2}$ state, the induced shift of the transition frequency is large and negative, which can cause a heating of the trapped atoms. For the measurements discussed in the following, the ODT configuration consists only of two trapping beams, as described in Section 5.2.1.

5.3. Near-adiabatic and loss-free optical transport

In our experimental setup we realized a long-distance transport of the atomic cloud over 25 cm in 0.9 s in a crossed ODT from the MOT chamber into the glass cell. This is achieved by moving the lens that simultaneously focuses and crosses the beams for the optical dipole trap by means of a compact air bearing translation stage, as illustrated in Fig. 3.3.

²This laser will be used for the generation of an optical lattice in future.

5.3.1. Trajectory for optical transport

To transport the atomic cloud without inducing heating, spilling, or excitations of center-of-mass oscillations, it is favorable to operate the transport trap in the adiabatic regime. This requires the restoring force of the ODT in the axial direction, which is the direction of transport, to be large in comparison to the inertial force due to the translation of the trap (Zimmermann, 2010). Furthermore, the oscillation period in the trap should be short with respect to the transport duration (Couvert et al., 2008).

Suppression of center-of-mass oscillations A fast transport of atoms without heating can in principle also be achieved in the non-adiabatic regime (Torrontegui et al., 2011). Such a transport scheme was investigated by Couvert et al. (2008), where an atomic cloud is confined in an optical dipole trap with an axial trap frequency of only 8 – 9 Hz. The amplitude $\mathcal{A}$ of center-of-mass oscillations of the atomic cloud after the transport was studied as a function of the transport duration and compared to a one-dimensional model for a harmonic confinement, which predicts (Couvert et al., 2008)

$$\mathcal{A} = |\mathcal{F}[v_c(t)](\omega_0)| = \left| \int_{-\infty}^{\infty} v_c(t) e^{-i\omega_0 t} dt \right|. \quad (5.5)$$

Here $\mathcal{F}[v_c(t)]$ is the Fourier-transform of the velocity profile $v_c(t)$ of the moving confinement potential, which has an axial angular trap frequency of ω_0 . It is found that even for a weak axial confinement, residual oscillations can be avoided by an appropriately chosen duration of the transport. However, if experimentally possible, it seems more straightforward to transport the atoms in the adiabatic regime.

S-curve velocity profile To determine a suitable range of the axial trap frequency that ensures a fast and robust transport of the ultracold atoms, Eq. (5.5) is evaluated assuming a translation of the trap by 25 cm in 0.9 s, which corresponds to the current experimental implementation. The trajectory is defined by a symmetric S-curve velocity profile: The acceleration is linearly increased to 2.45 m/s² in 0.45 s leading to a maximum velocity of 0.55 m/s, directly followed by the deceleration. The corresponding acceleration and velocity profiles are illustrated in Fig. 5.5 (a). The maximum residual oscillation amplitude, estimated based on Eq. (5.5), decreases to below 1 μ m for trap frequencies above about 70 Hz, which

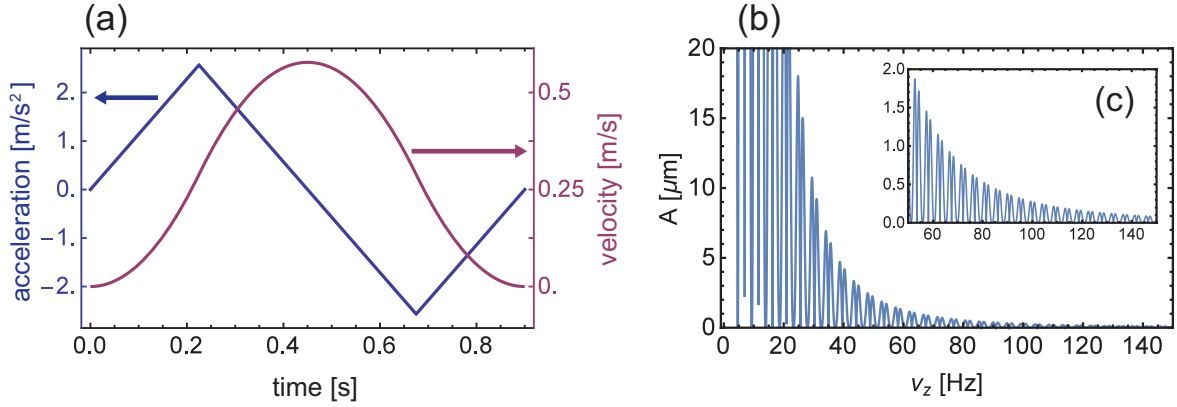


Figure 5.5.: (a) Acceleration and velocity profile for the optical transport of the atomic cloud. The trap is translated by 25 cm in 0.9 s. (b),(c) Calculated amplitude A of center-of-mass oscillations of the atomic cloud after the optical transport versus axial trap frequency, based on Eq. (5.5) and on the velocity profile shown in (a). The inset shows a magnified view of A for axial trap frequencies larger than 50 Hz.

are assumed to be negligible for our experiments. The equivalence of the strong modulation of the amplitude with changing trap frequency was experimentally observed by [Couvert et al. \(2008\)](#) by varying the transport duration.

The large maximum acceleration and the short transport duration in our scheme is taking advantage of the strong axial confinement of the crossed optical dipole trap, as compared to single-beam traps with comparable waist. The transport duration is only bound by technical limitations of the translation stage.

5.3.2. Characterization of the optical transport

During the transport, the optical power remains at the initial 22.5 W per beam. If the ODT is kept stationary in the MOT chamber, we measure a heating rate of $0.53(3) \mu\text{K/s}$ of the atomic cloud. This is in good agreement with a model estimating the heating rate as described by [Grimm et al. \(2000\)](#), for which we find a value $0.43 \mu\text{K/s}$ based on the parameters given in Table 5.1. As the observed heating rate is small compared to the initial temperature, a forced evaporation stage in the MOT chamber in order to reduce the optical power during the transport is therefore not required.

Heating rate In a typical experimental sequence the atomic cloud undergoes a single transport trip from the MOT chamber to the science cell. In order to test the performance of the optical transport, we use return trips and compare temperature and atom number to a sequence of identical duration, but without transport. For a single return trip with the

standard parameters discussed above, the differences between the transport and the reference measurement lie within normal fluctuations of the experiment.

To measure small heating rates we lower the initial temperature of the atomic cloud. For this, the optical power of the trap is first reduced for a forced evaporation stage and then ramped up to full power for the transport measurement. At this point the temperature of the atomic cloud is $6.1(2) \mu\text{K}$. Subsequently, the atoms are transported multiple times, up to twelve return trips, before the atoms are probed. From this measurement a small additional heating rate of approximately $0.04 \mu\text{K}$ per single trip induced by the transport at full optical power was determined.

Comparison to a single-beam configuration Table 5.1 shows the parameters of our crossed-beam transport configuration in comparison with a single-beam optical dipole trap. If equal laser power and axial confinement strength are assumed the crossed-beam trap offers the advantage of larger beam diameters and trapping volume, which can be beneficial for the loading efficiency (Burchianti et al., 2014). Furthermore, the crossed-beam configuration offers a four-fold smaller aspect ratio. The larger photon scattering rate of the single-beam trap can be avoided by using a lower power. However, to maintain the same axial confinement and to limit the aspect ratio, an even smaller beam waist would be required in this case. For example, the single-beam transport trap for ^6Li employed by Zimmermann et al. (2011) offers also optimal parameters for the transport, as summarized in the third column in Table 5.1. However, probably even with a UV MOT phase, additional measures would be required to obtain a good loading efficiency of the small-volume ODT.

5.4. Evaporative cooling to quantum degeneracy

In the following we describe how quantum degeneracy in the trapped lithium sample is achieved in the same crossed-beam configuration as previously used for capturing atoms from the UV MOT and for optical transport. For this trap, the evaporative cooling schemes are optimized for the cases of weak and strong interactions in the Fermi gas. To access the two regimes, forced evaporation is performed at different magnetic fields, which are generated by the Feshbach coils around the glass cell.

5.4.1. Weakly interacting Fermi gas

To produce a weakly interacting quantum degenerate Fermi gas, we apply a magnetic bias field of 330 G to increase the magnitude of the $|1\rangle$ - $|2\rangle$ s -wave scattering length to $a_{12} = -290 a_0$ (Zürn et al., 2013), where a_0 is Bohr's radius. To initiate the forced evaporation process, the trap depth U_0 is lowered by reducing the optical power of the ODT. Logarithmic photodetectors allow the stabilization and control of the optical power over four orders of magnitude, as described in Section 3.6.2.

Evaporative cooling in an optical potential

In contrast to evaporative cooling in a magnetic trap with constant trap frequencies, the optical potential becomes more shallow as the evaporation sequence progresses and the trap frequencies decrease. According to Eq. (2.15), this leads to a reduced elastic collision rate in the trap and correspondingly a slower thermalization rate. However, due to generally high initial trap frequencies in optical potentials and the large attainable scattering length for ^6Li , efficient evaporation can be achieved.

The trap depth during evaporation follows a power law that was derived by O'Hara et al. (2001a) for evaporative cooling in a time-dependent optical potential and is given by

$$U_0(t) = U_0(0) \left(1 + \frac{t}{\tau}\right)^{-2(\eta'-3)/\eta'}, \quad (5.6)$$

where τ is a time constant and η' is related to the truncation parameter $\eta = U_0/k_B T$ via $\eta' = \eta + (\eta - 5)/(\eta - 4)$. The model is derived under the constraint of a constant value of η during evaporation, which leads to a scaling law for the atom number N as function of the trap depth U_0 according to

$$\frac{N(t)}{N(0)} = \left(\frac{U_0(t)}{U_0(0)}\right)^{\frac{3}{2} \frac{1}{\eta'-3}}. \quad (5.7)$$

The time constant τ in Eq. (5.6) can be calculated using $\eta = 10$, which is commonly observed for evaporation in optical potentials (Jochim et al., 2003b; Luo et al., 2006), and the elastic scattering rate $\bar{\gamma}_0$ at $t = 0$ via $\frac{1}{\tau} = \frac{2}{3} \eta' (\eta - 4) \exp(-\eta) \bar{\gamma}_0$ (O'Hara et al., 2001a). Using the atom number and temperature of the atomic cloud after plain evaporation and the s -wave scattering length of $a_{12} = -290 a_0$, we obtain a trap-averaged scattering rate $\bar{\gamma}$ of 2.7 kHz from

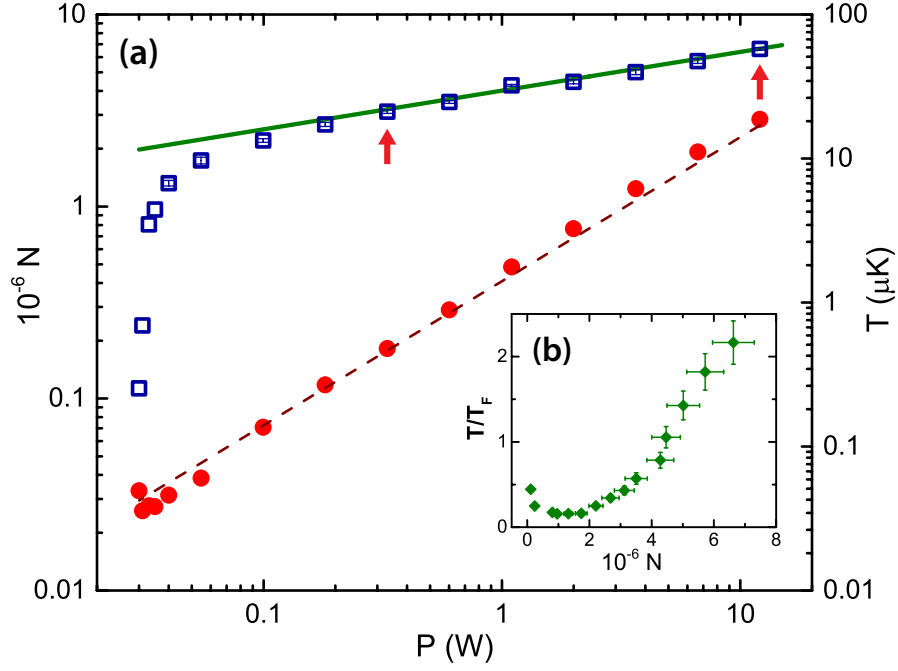


Figure 5.6.: (a) Total number of atoms N (blue squares) and temperature T (red circles) at various points during forced evaporative cooling performed at 330 G. P is the optical power per ODT beam at which the evaporation ramp was halted. The solid line is a fit of Eq. (5.7) to the data range that is indicated by the arrows. The dashed line corresponds to $0.1 U_0/k_B$, which is in close agreement with the measured temperature of the atomic cloud, indicating an approximately constant truncation η parameter throughout the evaporation. (b) T/T_F vs N for the same measurement. The error shown in (b) includes, in addition to the statistical error of 10 repetitions for each point, a systematic uncertainty of 10 % in the measured quantities.

Eq. (2.15). Based on this rate, one finds a value of 0.2 s for the time constant τ . Lowering the trap depth by a factor of 45 using this time constant, corresponding to an evaporation duration of 2.9 s, we obtain a sample with 2.1×10^6 atoms at $T/T_F = 0.8(1)$.

Characterization of the evaporation process

We employ a different time constant in order to cool the Fermi gas to lower temperatures, because with $\tau = 0.2$ s a rapid atom loss is observed for continued evaporation. We use a time constant of 4.2 s, which is experimentally optimized for maximum atom number at a final evaporation power of 0.1 W. This corresponds to a fraction of 1/225 of the initial trap depth. To characterize the evaporation, we probe the atomic cloud at various intermediate optical powers during the ramp.

For this purpose, the magnetic bias field and the optical potential are rapidly switched off and the density distribution is determined by standard time-of-flight absorption imaging. The

projected density profiles are fitted to a Fermi distribution function, from which we extract atom number, temperature, and T/T_F , with the results shown in Fig. 5.6. We observe efficient cooling of the cloud down to a laser power of $P = 50$ mW/beam, where 8.7×10^5 atoms in each spin state remain trapped at a temperature of 60 nK, corresponding to $T/T_F = 0.16$ (2).

We fit the power law of Eq. (5.7) to the measured atom number and determine a value of 9.6(3) for η , which agrees well with the expected value of 10. This shows that the evaporation trajectory is efficient in terms of atom number. However, the total evaporation duration with this time constant to the final power of 50 mW is 26.6 s. This duration is mainly limited by the comparatively weak axial confinement of the ODT and the aim for a high atom number. For future experimental sequences, the atomic cloud can be adiabatically compressed along the axial direction with an auxiliary beam in order to enhance the scattering rate, similarly to the third ODT beam described in Section 5.2.2. The atom loss due to background gas collisions during the evaporation seems negligible. From a decay measurement of the trapped atom cloud we estimate a $1/e$ lifetime on the order of 300 s.

5.4.2. Evaporation near the Feshbach resonance

To create a strongly interacting quantum gas in the BEC-BCS crossover, evaporation is performed near the broad Feshbach resonance at 832 G. As shown in Appendix A.3, it is possible to change sign and strength of the interaction between the atoms by applying a magnetic bias field. Above the resonance, the s -wave scattering length is negative and the effective interaction between the atoms is attractive, corresponding to the BCS side. The s -wave scattering length is positive below the resonance, which indicates the presence of a bound state below the two-body interaction continuum. For low enough temperatures bosonic dimers are created and a BEC can be formed, as discussed in Section 2.3.1.

Evaporative cooling of unitary Fermi gas

The strongly interacting atomic cloud is evaporatively cooled by reducing the trap depth according to

$$U_0(t) = U_0(0) \left(1 - \frac{t}{\tau_u}\right)^{2(\eta'-3)/(\eta'-6)}, \quad (5.8)$$

with a time constant $\tau_u = 3$ s. This evaporation trajectory was derived by Luo et al. (2006) for a Fermi gas mixture with a unitarity-limited s -wave scattering cross section. Analogous

to the model described in Section 5.4.1 for the weakly interacting Fermi gas, the assumption is a constant truncation parameter throughout the evaporation process. This results in the same power law for the atom number as function of the trap depth, as shown in Eq. (5.7). The difference is the energy dependent scattering cross section, which leads to a different time dependence for the elastic scattering rate and therefore also for the evaporation rate (Luiten et al., 1996). The unitarity-limited cross section increases during the cooling process because the Fermi wavelength increases, as it follows from Eq. (2.13). This sustains the elastic scattering and evaporation rates while the trap is relaxed and the atom number is decreasing. As a result, faster evaporation is possible as compared to the case of a constant scattering cross section.

In order to characterize the efficiency of the evaporation process, we perform identical evaporation ramps above and below the Feshbach resonance at magnetic bias fields of 940 G and 770 G, respectively. At these fields the s -wave scattering lengths are of similar absolute value, but of opposite sign. The atom number as function of the final laser power is shown in Fig. 5.7 (b). Down to a power of about 0.1 W, or a fraction of 1/225 of the initial trap depth, the two evaporation ramps result in an almost identical atom numbers. As shown in Fig. 5.7, we fit the power law function given in Eq. (5.7) to the measured atom number and determine a value of 9.8(1) for the truncation parameter η .

However, there is a distinct difference for lower optical powers. For evaporative cooling above the Feshbach resonance, the atom number rapidly decreases, which indicates the spilling from the trap due to the limited number of states that are available for the fermions at low optical powers. Evaporation below the resonance leads to higher atom numbers at identical optical powers. This can be attributed to the formation of bosonic dimers, while the spilling is a result of the repulsive interaction between the Feshbach molecules, as observed and described by Jochim et al. (2003b).

Observation of a molecular BEC

For the production of a molecular BEC we generally follow the procedure described by Jochim et al. (2003b). The magnetic field is ramped to 770 G, where the s -wave scattering length reaches approximately $a_{12} = 5100 a_0$, and $k_F a_{12} = 4.8$, where k_F is the Fermi wave vector. The binding energy of the Feshbach molecules at this magnetic field is on the order

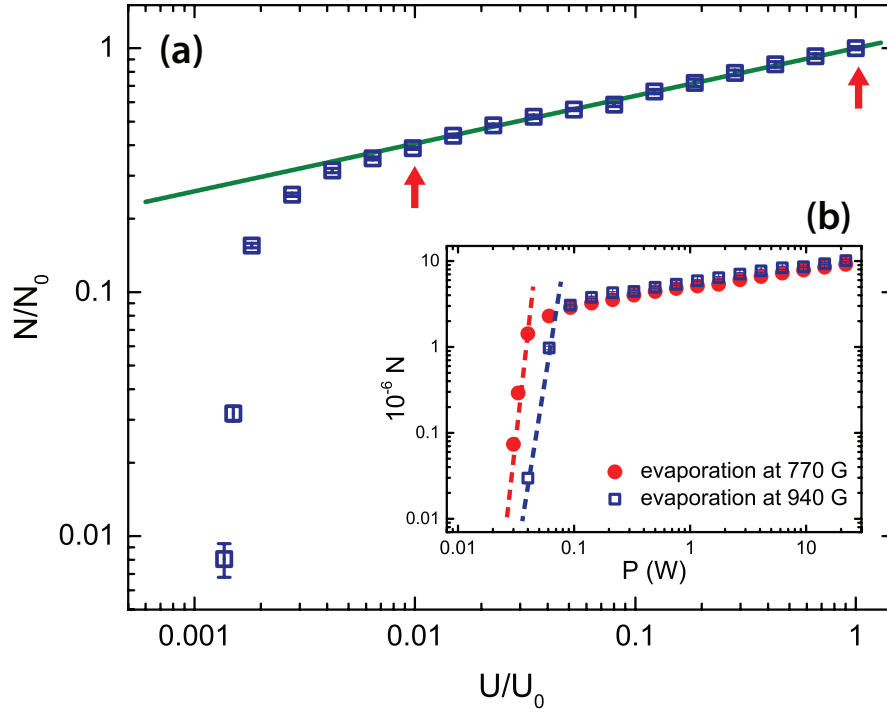


Figure 5.7.: (a) Scaling of atom number with trap depth for evaporative cooling at 940 G. Shown is the normalized atom number versus the normalized trap depth and a fit of a power law function to the data range that is indicated by the arrows (see text). (b) Atom number as function of the power P of the ODT for evaporative cooling at 940 G (squares) and 770 G (circles). The dashed lines are a guide to the eye.

of $k_B \times 1.1 \mu\text{K}$ (Zürn et al., 2013). The temperature of the atomic cloud decreases during the evaporation process and for temperatures on the order of and below the molecular binding energy, three-body recombination processes lead to the formation of Feshbach molecules (Chin and Grimm, 2004; Jochim et al., 2003a; Petrov, 2003). While the reverse process is also possible, at temperatures far below the binding energy an almost pure sample of Feshbach molecules is obtained. Upon the creation of a molecular state, the binding energy is released into the trapped gas. This excess energy is removed by the continued evaporation process, which is enabled by the molecule-molecule and atom-molecule elastic scattering length which is of similar magnitude as the atom-atom interaction near the Feshbach resonance (Petrov et al., 2004).

The continued evaporative cooling of the molecular cloud eventually leads to the formation of a Bose-Einstein condensate, as described in Section 2.3. To increase the visibility of the bimodal density distribution, which is characteristic for the onset of Bose-Einstein condensation, the interaction strength between the molecules is lowered by linearly reducing the magnetic field to 690 G in 100 ms before TOF absorption imaging (Burchianti et al., 2014;

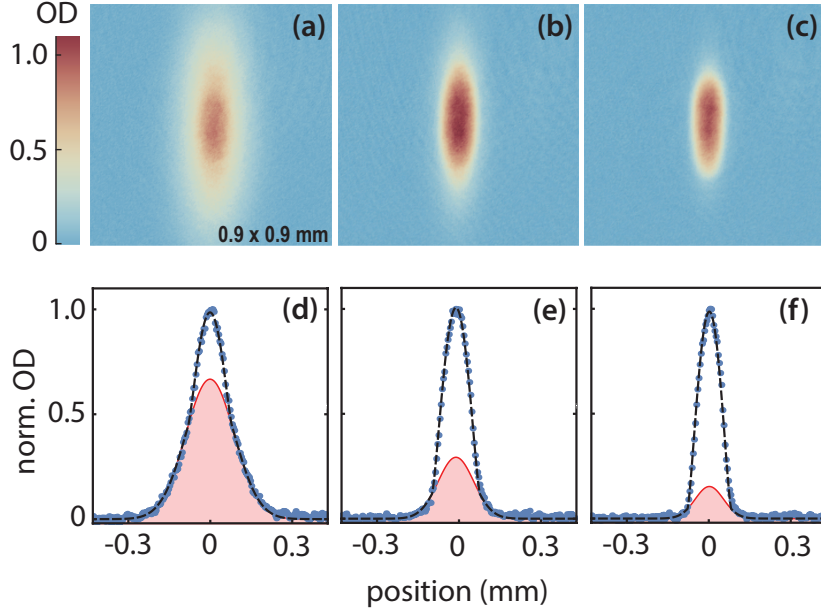


Figure 5.8.: Density distribution and individually normalized horizontal central profiles of the ${}^6\text{Li}_2$ cloud. Forced evaporative cooling is performed at 770 G to a final optical power of (a),(d) 100 mW, (b),(e) 45 mW, and (c),(f) 35 mW per beam of the ODT. The optical density (OD) of the cloud is recorded after a TOF of 6 ms at a magnetic field of 690 G. Each central profile (blue circles) is normalized to unity and the bimodal fitting function (dashed line) consists of a parabolic curve added to a Gaussian. The Gaussian component (solid line) illustrates the bimodal character of the density distribution.

Gunton et al., 2013b). This reduces the atomic scattering length a_{12} to around $1400 a_0$, which is related to the molecular s -wave scattering length via $a_{\text{mol}} = 0.6 a_{12}$ (Petrov et al., 2004). At this magnetic field absorption imaging of the molecules with light on the atomic imaging transition is still efficient (Bartenstein et al., 2004) and was discussed by Zwierlein et al. (2003). Trap depth U_0^{mol} of the ODT for the molecules is assumed to be twice as large as compared to the case for the atoms.

At $U_0^{\text{mol}}/k_B = 2.9 \mu\text{K}$ we observe 1.1×10^6 molecules and a deviation from a thermal density distribution, as shown in Fig. 5.8. This indicates the onset of condensation. At a final trap depth of $U_0^{\text{mol}}/k_B = 1.0 \mu\text{K}$ we observe a BEC containing around 3×10^5 Feshbach molecules, which is inferred from a fit to a bimodal density distribution. At this point the trap frequencies are $\omega_z = (2\pi) \times 7.8 \text{ Hz}$ and $\bar{\omega}_r = (2\pi) \times 120 \text{ Hz}$, leading to a critical temperature of $T_c = 170 \text{ nK}$ for an ideal Bose gas (see Eq. (2.24)). The axial confinement is enhanced by the residual curvature of the applied magnetic bias field, leading to a measured contribution to the axial trap frequency of $(2\pi) \times 4.6 \text{ Hz}$, while this effect can be neglected for the radial trap frequency.

5.5. Summary

In conclusion, we have demonstrated a refined scheme for an all-optical production of a quantum degenerate ${}^6\text{Li}$ gas that involves long-distance transport in a crossed ODT. Here we are taking full advantage of the high phase-space density obtained by the UV MOT for lithium and the possibility of continued laser cooling in the ODT. This allows an improved loading efficiency into optical dipole traps with lower trap depth and hence comparatively large volume. The benefit of UV cooling is demonstrated to be present even for a low optical power. In addition to loading with high atom number, our crossed-beam configuration also offers sufficient axial confinement for a rapid and near-adiabatic transport of the atomic cloud. By means of the same trap, evaporative cooling is performed to obtain a large quantum degenerate Fermi gas and a molecular BEC, which shows the efficiency of the approach. Our implementation facilitates experiments requiring unconstrained optical access, such as quantum gas microscopy.

6. Photoassociation spectroscopy (attempt) below the $2S$ - $3P$ asymptote

In this chapter, our approach for a photoassociation (PA) measurement to molecular states of potentials approaching the $2S$ - $3P$ asymptote of ${}^6\text{Li}_2$ is discussed. So far, no experimental data exist for the weakly bound states of these internuclear potentials. For this measurement we employ the laser that is normally used for the UV MOT and use an ionization detection scheme for the excited state. After an introduction to PA spectroscopy, the technical implementation and measurements on the atomic transition are presented, although no molecular transitions were observed within this work. However, the chapter is written with the intent to serve as a basis for a future, more refined and more successful approach to observe photoassociation transitions to the potentials approaching the $2S$ - $3P$ asymptote.

6.1. Photoassociation spectroscopy

Photoassociation refers to the formation of a molecule that emerges from two colliding atoms under the absorption of a photon. These molecules are electronically excited bound states that are supported by the interaction potential of the two atoms. In PA experiments, the main interest is the determination of the transition frequencies to these states, which serves as a spectroscopic method to investigate these potentials. Photoassociation experiments are generally performed with cold atoms such that the thermal energy is small compared to other energy scales, which makes it possible to probe the most weakly bound states. These levels are inaccessible to more traditional bound-bound spectroscopy methods and PA spectroscopy is therefore an important tool for the investigation of diatomic molecules and was reviewed in several articles ([Jones et al., 2006](#); [Masnou-Seeuws and Pillet, 2001](#); [Stwalley and Wang, 1999](#); [Weiner et al., 1999](#)).

6.1.1. Principle of photoassociation spectroscopy

In PA spectroscopy measurements, a cloud of trapped atoms is illuminated with a laser beam that is red-detuned relative to an atomic transition. For certain angular frequencies ω_{PA} of the light, two colliding atoms A and B can absorb a photon $\tilde{\gamma}_{\text{PA}}$ from this field and form a molecule in an electronically excited state $(AB)^*$, as formally expressed by



The binding energies E_B of these levels are defined with respect to the asymptotic value of the potential energy curve, as illustrated in Fig. 6.1. The locations of the resonances follow from energy and momentum conservation, as described by [Pillet et al. \(1997\)](#) and can be approximated according to

$$E_B = \hbar\omega_{\text{PA}} - \hbar\omega_A , \quad (6.2)$$

where ω_A is the atomic angular transition frequency ([Jones et al., 2006](#)). This approximation accounts for the low temperatures that are achieved in laser cooled atomic clouds, such that frequency shifts arising from the finite kinetic energy are small compared to typical binding energies. In addition, the recoil energy of the absorbed photon in the PA process is also neglected. Eq. (6.2) demonstrates that observed resonance frequencies are directly related to the absolute binding energies of the molecular states, which is an interesting feature of PA measurements because it complements experimental data obtained with different methods, such as Fourier transform spectroscopy. There, predominantly deeply bound states are accessed without direct relation to the binding energy ([LeRoy and Bernstein, 1970](#); [Linton et al., 1992](#)).

6.1.2. Decay and detection of photoassociated molecules

The lifetime of molecules created in a photoassociation process is short and is about half the lifetime of the corresponding excited atomic state. Specifically, for the weakly bound states of the potential correlated to the $2S$ - $2P$ asymptote of lithium, this corresponds to around 13.5 ns ([Côté and Dalgarno, 1998](#)). Possible radiative decay channels for the excited diatomic

molecules are described by



and involve the emission of a photon $\tilde{\gamma}_{d1(d2)}$ (Stwalley and Wang, 1999). The first process describes a bound-bound transition from the excited molecular state into a bound state $(AB)'$ of the ground-state internuclear potential. If the PA measurement is performed in a MOT, then the atoms bound in the molecular state are no longer susceptible to the trap light and will be lost from the atomic cloud. The second decay channel corresponds to a dissociation of the molecule into two free atoms and can be seen as the reverse process described by Eq. (6.1). However, the atoms can decay to ground-state continuum states with a different kinetic energy than the initial state.

Fluorescence trap-loss spectroscopy A straightforward method to observe PA transitions is to monitor the fluorescence of the atomic cloud confined in a MOT. The near-resonant trap light leads to scattered photons that can be detected with a photodiode and the signal strength is related to the number of atoms. If the PA laser resonantly excites molecular bound states, the two decay channels defined in Eq. (6.3) and (6.4) can induce a reduction of the atom number and correspondingly of the fluorescence level of the trapped cloud.

Because of the following considerations, the atomic loss rate induced by the PA process has to be sufficiently large, in order to be observable via this method. The atom number of a MOT under steady-state conditions is determined by a balance of the loading and the loss rate, as described in Section 4.2.1. The additional loss rate induced by PA processes has to amount to a significant fraction of the loading rate itself, in order to discernibly change the steady-state fluorescence signal beyond typical fluctuations. In practice it is rather difficult to constrain these fluctuations to below a few percent of the total fluorescence signal.

Detection via photoionization An important alternative method to detect PA transitions is photoionization. For this, a second photon ionizes the bound state and the charged particles are counted with an ion detector, such as a channel electron multiplier (CEM) described in Section 3.7. Two ionization channels, which were further described by Stwalley and Wang

(1999), are considered here. These processes are

$$(AB)^* + \tilde{\gamma}_{PI} \rightarrow (AB)^+ + e^- \quad (6.5)$$

$$(AB)^* + \tilde{\gamma}_{PI} \rightarrow A^+ + B + e^-, \quad (6.6)$$

where $(AB)^+$ is a molecular ion, A^+ an atomic ion, and e^- is the corresponding electron that is released. In our scheme, the energy of the photon $\tilde{\gamma}_{PI}$ has to be sufficient to drive the transition into the ionization continuum, as illustrated in Fig. 6.1.

The intrinsic advantage of this method was briefly indicated in Section 3.7. Instead of detecting a small loss of atoms from the trapped ensemble, the ion signal is directly related to the decay channels of interest. Ion detectors can provide single particle sensitivity, such that small numbers of ions can be measured. To illustrate this, a hypothetical ion production rate of 100 Hz can be assumed. Such a rate is observable with a standard ion detector, however, this number is negligible compared to the number of trapped atoms or even the loading rate of the MOT, which is on the order of 2×10^8 atoms per second (see Chapter 4).

6.1.3. Structure of diatomic molecules

The internuclear potential energy curve of a diatomic system may be derived from a combined Hamiltonian describing the isolated atoms and their mutual interaction. Within the Born-Oppenheimer approximation it is assumed that the electronic wave function adiabatically follows the nuclear motion, such that the resulting potential energy curve is a function of the internuclear separation R , as it was discussed, for example, by Brown and Carrington (2003). At large separations the system is asymptotically correlated to the configuration of two individual atoms in their respective electronic state, which is used to classify the various molecular potential energy curves, as exemplarily shown in Fig. 6.1.

Molecular term symbol The designation of the diatomic molecular states contains information on the symmetry of the electronic state as well as on the involved angular momenta. A diatomic molecule is cylindrically symmetric, such that the total electronic orbital momentum $\mathbf{L} = \mathbf{l}_a + \mathbf{l}_b$ is not conserved, but only its projection along the internuclear axis, represented by Λ . The absolute value of Λ is either zero or one for potentials correlated to the $2S$ - $2P$ or $2S$ - $3P$ asymptote and the molecular potentials that are relevant in the current discussion can

be labeled by

$$^{2S+1} |\Lambda|_{g,u}^{\pm}, \quad (6.7)$$

where S is the total electron spin. The absolute value of the projected orbital angular momentum Λ can assume values of $0, 1, 2, \dots, L$, which are represented by the capital Greek letters $\Sigma, \Pi, \dots$. The superscript $\pm$ denotes the parity of the orbital electronic eigenfunction under a reflection at any plane containing the internuclear axis. This symmetry is only indicated for the Σ states, as it was described by Herzberg (1950).

The label g/u , which stands for gerade and ungerade, indicates the parity of the electron wave function under a point reflection of only the electron wave function at the origin of the diatomic molecule. This symmetry arises because the electric field seen by the electrons remains unchanged under the exchange of the nuclei and exists only for homonuclear diatomic molecules. Equivalently, this symmetry can be defined as the parity of the electron wave function under the exchange of the two nuclei. A comprehensive discussion of these symmetries and notations was given by Herzberg (1950) and a concise summary was provided by Ulmanis et al. (2012).

Selection rules The knowledge of the relevant selection rules for electric dipole transitions allows one to establish the experimentally accessible potentials and helps to assign observed transitions. For the potentials and the range of binding energies that are considered here, the selection rules for Hund's case (a) and (b) are applicable and were given by (Herzberg, 1950):

$$\Delta \Lambda = 0, \pm 1 \quad (6.8)$$

$$\Delta S = 0. \quad (6.9)$$

In addition, only transitions between states of opposite gerade/ungerade symmetry are allowed. These rules can be applied to the experimental situation, where the ^6Li atoms are confined in a magneto-optical trap. As illustrated in Fig. 6.1, the atoms collide via the $X^1\Sigma_g^+$ and a $^3\Sigma_u^+$ interaction potentials, which limits the allowed transitions to symmetries of $^1\Sigma_g^+ \rightarrow \{^1\Sigma_u^+, ^1\Pi_u\}$ and $^3\Sigma_u^+ \rightarrow \{^3\Sigma_g^+, ^3\Pi_g\}$.

If the photoassociation measurement is performed in an optical dipole trap where the number of initial states may be reduced, or if the hyperfine structure can be resolved, a

more refined set of selection rules is required in order to assign observed transitions. The symmetry of the spin configurations and the bosonic or fermionic nature of the nuclei have to be considered, which was described for lithium, for example, by [Abraham et al. \(1995b\)](#) and [Semczuk et al. \(2013\)](#).

6.1.4. Significance of PA spectroscopy

Photoassociation transitions typically access the most weakly bound states of the electronically excited potentials, which extend to large internuclear distances. At short separations, the probability density of their wave functions diminishes such that these states are commonly referred to as long-range molecules.

Internuclear potential These long-range states are particularly sensitive to the properties of the potential energy curve at large internuclear separations R , because they spend most of the time near their outer classical turning point ([Jones et al., 2006](#)). An application of photoassociation spectroscopy is therefore the investigation of diatomic potentials. The long-range part of the potential energy can be expanded into a power series in $1/R$ according to

$$V(R) = D - \sum_n \frac{C_n}{R^n}, \quad (6.10)$$

where D is the dissociation limit of the potential and C_n are the corresponding dispersion coefficients, which represent different multipole interaction terms ([Marinescu et al., 1994](#)). This model potential asymptotically describes the configuration of two individual atoms and implies that the dispersion coefficients depend on the respective electronic state of the two atoms. PA spectra can be used to determine these coefficients ([McAlexander et al., 1995](#)), which can also be combined with other spectroscopic data to generate accurate analytic potential energy curves extending to short internuclear separations ([LeRoy et al., 2009](#)).

Radiative lifetime In most PA measurements, the potentials under investigation asymptotically correlate to a ground-state atom and an atom in the first excited state. For lithium this corresponds to the $2S$ - $2P$ asymptote and is shown in Fig. 6.1. For homonuclear atoms, the long-range part of this potential is dominated by the contribution of resonant dipole-dipole interactions, which is represented by the C_3 term in Eq. (6.10). This coefficient can be related to the atomic radiative lifetime τ via $C_3 = 3\hbar c^3 / (4\tau\omega_A^3)$ and can be inferred from

the analysis of PA spectroscopy measurements, as it was reviewed by [Bouloufa et al. \(2009\)](#). Interestingly, by probing the bound states of the internuclear potential, this property of the single atom can be determined with very high accuracy, as it was demonstrated, for example, by [McAlexander et al. \(1996\)](#).

Further applications Photoassociation spectroscopy can also be used to measure the ground-state s -wave scattering length that characterizes the collisional properties of the ultracold trapped atoms. This can be achieved by evaluating the variation of the PA transition strength to different molecular states of the same excited intermolecular potential and was demonstrated for lithium by [Abraham et al. \(1996\)](#). An alternative method is to use a two-photon spectroscopy method in order to determine the bound states of the ground-state interaction potential ([Abraham et al., 1995a, 1997](#)). PA spectroscopy is also an important element in the production of ultracold ground-state molecules. They can be formed by synthesizing a pair of cold atoms by employing an electronically excited state of the diatomic molecule, as described in a review article by [Ulmanis et al. \(2012\)](#). Furthermore, PA spectroscopy was used to probe the paired state of a fermionic lithium quantum gas in the BEC-BCS crossover ([Partridge et al., 2005](#)).

6.1.5. PA spectroscopy of lithium below the $2S$ - $2P$ asymptote

The investigation of lithium dimers and their internuclear potentials has received considerable attention from both theorists and experimentalist. An important reason is the relative simplicity of the system, because it is the smallest homonuclear molecule after the hydrogen dimer. Theoretical models for the investigation of heavier and more complex alkali-metal dimers can be applied to and tested on the lithium system, for which many *ab initio* calculations and spectroscopy measurements have been performed. A further discussion of this particular interest in lithium and references to a broad range of studies on the lithium dimer were provided by [Jasik and Sienkiewicz \(2006\)](#).

The $1^3\Sigma_g^+$ and $A^1\Sigma_u^+$ potentials of lithium, which are most relevant to photoassociation experiments ([Côté and Dalgarno, 1998](#)), are correlated to the $2S$ - $2P$ asymptote. The deeply bound molecular states of these potentials were spectroscopically investigated via bound-bound Fourier transform spectroscopy ([Linton et al., 1989, 1996](#)) and the binding energies of the states close to the dissociation limit were inferred from photoassociation measurement

(Abraham et al., 1995b). To further refine the knowledge of the internuclear potential curve, Gunton et al. (2013a) and Semczuk et al. (2013) performed a PA measurement to access the intermediate regime of the potential.

6.1.6. PA spectroscopy of lithium below the $2S$ - $3P$ asymptote

PA spectroscopy measurements with alkali-metal atoms, which employ a single photon to access bound states, are almost always performed below the first excited P state. This corresponds to potentials that asymptotically approach the nS - nP asymptote, where n is the principal quantum number of the ground state. A rather trivial reason is the readily available laser light for such measurements, because the required wavelength coincides with the one for laser cooling. As such, PA measurements have been performed for all laser cooled alkali-metal atoms. In order to directly drive transitions to higher P levels, laser light in the blue or UV range is required, for which the available laser power is generally low.

A further reason is the significantly reduced transition strength for alkali-metal atoms to the second excited P state, which is related to the dimensionless oscillator strength (Bethe and Salpeter, 2008). For lithium, the ratio between the oscillator strength of the $2S \rightarrow 2P$ and the $2S \rightarrow 3P$ transition is 137 (Martin and Wiese, 1976), which also reduces the excitation rate to bound states of the corresponding potential. The sole example of a PA measurement to potentials correlated to the nS - $(n+1)P$ asymptote was performed with cesium by Pichler et al. (2006). Only few spectroscopic features were observed below the dissociation limit and were not assigned to specific transitions. However, the main focus of that measurement was the investigation of spectroscopic features that are blue-detuned from the atomic resonance.

The reduced atomic transition strength profoundly influences the long-range part of the internuclear interaction potential of the $2S$ - $3P$ asymptote. Because of the weaker contribution of the resonant dipole-dipole interaction, the C_3 coefficient in Eq. (6.10) is reduced by a factor of more than 300 as compared to the one of the $2S$ - $2P$ asymptote, which leads to a more short-range character of the potential. As a consequence, the positions of the classical outer turning points R_c of the weakly bound states are shifted to smaller internuclear distances. Considering, for example, a bound state of the excited potential with $^3\Sigma_g^+$ symmetry and a binding energy of about -45 GHz, one finds a value of $111a_0$ ($42a_0$) for R_c for the $2S$ - $2P$ ($2S$ - $3P$) asymptote, where a_0 is Bohr's radius. This leads to a smaller spatial overlap with

the continuum wave function of the ground state and therefore to a further reduction of the transition strength to bound states of the $2S\text{-}3P$ potential, as discussed in more detail in Chapter 7.

So far, there are no experimental data on the long-range part for any of the lithium potentials correlated to the $2S\text{-}3P$ asymptote. Of particular interest for PA measurements are the excited states with $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ symmetry. For the former, deeply bound molecular states were observed with conventional bound-bound spectroscopy methods, while for the latter one, no experimental data exist even on the short range part of the potential (Dattani, 2015; Musial and Kucharski, 2014).

6.2. Experimental approach

Our scheme for the PA experiment to states below the $2S\text{-}3P$ asymptote is as follows. The atoms are loaded into the red MOT on the D_2 line and exposed to the UV PA laser. In order to ionize the weakly bound molecules, a high-power laser at 532 nm is superimposed to drive transitions to the ionization continuum, as illustrated in a simplified level scheme in Fig. 6.1. Atomic or molecular ions that are produced in this process are accelerated towards a channel electron multiplier (CEM), as described in Section 3.7. During an experimental sequence, the frequency of the PA laser is scanned and its wavelength is continuously measured with high absolute accuracy.

6.2.1. Photoionization of ^6Li

The ionization energy of the $3P$ state of lithium is 1.55 eV, which corresponds to a laser wavelength of 798 nm in order to reach the ionization threshold (Kramida et al., 2016). As illustrated in Fig. 6.1, different combinations of laser frequencies that are used in the experiment can drive a transition into the ionization continuum. The corresponding excitation rates γ_{PI} for a given atomic state can be calculated according to

$$\gamma_{\text{PI}} = \frac{I}{h\nu_{\text{PI}}} \sigma_{\text{PI}}(\nu_{\text{PI}}) , \quad (6.11)$$

where $\sigma_{\text{PI}}(\nu_{\text{PI}})$ is the photoionization (PI) cross section at a laser frequency of ν_{PI} and I is the intensity of the laser light. Here, the cross sections are estimated based on results of a

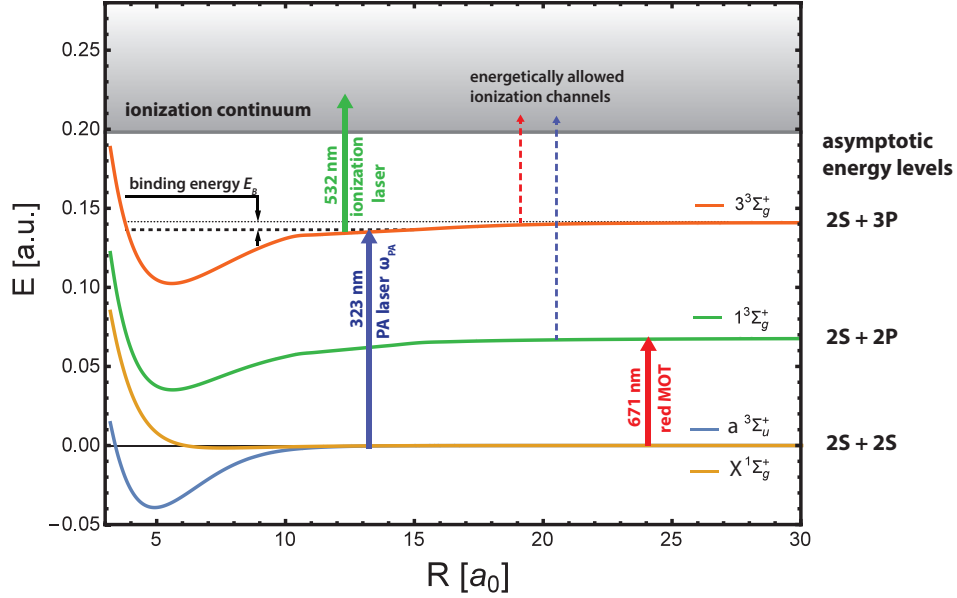


Figure 6.1.: Photoassociation level scheme. Shown are selected potential energy curves of the lithium dimer of the electronic ground state and of the first two excited P potentials as functions of the internuclear separation R (Jasik and Sienkiewicz, 2006). The solid vertical lines illustrate optical transitions that are driven and the dashed lines indicate additional possible ionization channels. The gray shaded area represents the ionization continuum. The energy difference between the asymptotic value of the potential (dotted line) and the eigenvalue of a molecular state (dashed line) defines the binding energy E_B .

theoretical calculation performed by Lahiri and Manson (1993) and the relevant values are summarized in Table 6.1.

Photoionization of $3P$ state with 532-nm laser The ion detection scheme for bound states of the $2S$ - $3P$ potentials, and of lithium atoms in the $3P$ state in general, requires a sufficiently high ionization rate. For the current experiment this simply means as high as possible and determines the selection of the laser (among the available options) that is used for this purpose.

The photoionization cross sections monotonically decrease with the photoelectron energy for excited P states, as discussed by Lahiri and Manson (1993), which suggests to use a laser close to the ionization threshold. This is near the wavelength that is used for laser cooling of rubidium and TA chips providing an optical power of 2 W are available.¹ However, one finds from the values given in Table 6.1 that the PI cross section is only reduced by a factor of four, if light at 532 nm is used instead. This is of interest because at this wavelength we have a continuous-wave (cw) laser with a nominal output power of 30 W.

The probability for ionizing an atom in the $3P$ state with the 532-nm light is calculated as follows. In the experiment we use an ionization beam with 30 W of optical power and

¹The TA chip TA-0780-2000-6 (TOPTICA Photonics AG) could be used, for example.

Ionization process	ϵ (a.u.)	σ (Mb)	Available power (W)
$2P + 323 \text{ nm}$	0.042	20	-
$3P + 671 \text{ nm}$	0.042	20	-
$3P + 323 \text{ nm}$	0.168	< 10	-
$3P + 532 \text{ nm}$	0.114	10	30
$3P + 780 \text{ nm}$	0.0027	40	2

Table 6.1.: Possible single-photon ionization processes into the continuum from the first two excited P states of lithium. The photoelectron energy ϵ is given in units of hartree E_h (atomic units) (Kramida et al., 2016) and the photoionization cross section in units of barn (Lahiri and Manson, 1993). In addition, the optical power of lasers are indicated that are available in our laboratory and which were considered as possible ionization lasers.

a $1/e^2$ radius of about 0.5 mm at the position of the atoms. After the transit through the atomic cloud, this beam is reintroduced into the chamber under an angle of 11° with respect to the first pass. This nearly doubles the available optical power and is illustrated as a simple retro-reflection in Fig. 6.2. The ionization probability of an atom from the excited state is calculated using $p_{\text{PI}} = \tau_{3P} \gamma_{\text{PI}}$, where τ_{3P} is the decay time of the $3P$ state. We find a value $4.1 \times 10^5 \text{ Hz}$ for γ_{PI} and a corresponding ionization probability of 9% with the PI cross section given in Table 6.1. With the applicable values for an ionization scheme using a 780-nm laser we find an ionization rate of 3%.

This probability was calculated for the *atomic* $3P$ state. It is assumed here that the ionization rate is of similar magnitude for the most weakly bound states of the corresponding internuclear $2S$ - $3P$ potential, but reduced by a factor of two due to the reduced lifetime of the diatomic molecule (Côté and Dalgarno, 1998). This assumption is further supported by a similar PA scheme with cesium reported by Pichler et al. (2006).

Photoionization of $2P$ state with 323-nm light Photoionization of the $2P$ state with 323-nm light is a possible ionization channel in the experiment, as indicated in Fig. 6.1 and discussed in the context of the UV MOT decay time in Section 4.3.4. While this effect is irrelevant for the normal operation of the UV MOT, it cannot be neglected for the PA measurement based on ion detection.

The photoionization rate for our experimental configuration can be estimated using Eq. (6.11). The radius of the 323-nm PA beam is 0.35 mm and the maximal optical power is 20 mW. If the PA beam passes the atomic cloud once, one finds an ionization rate of 420 Hz for an atom in the $2P$ state and an ionization probability of only 1.1×10^{-5} for a single excitation to the $2P$ state. However, the total number of ions produced by this process can be large because

in a MOT a significant fraction of the $\sim 10^9$ atoms is in the excited state (Fuso et al., 2000). This ionization channel leads to a background signal and has to be suppressed in order to observe weak atomic or molecular transitions.

Further photoionization channels The atomic $3P$ state can also be ionized by a 323-nm or a 671-nm photon, as illustrated in Fig. 6.1. If the $3P$ asymptote is spectroscopically investigated, these ionization channels contribute to the actual signal and not to the background. However, these effects are small, as shown in the following. Using the same parameters for the 323-nm beam as in the previous section, we find an upper limit of 210 Hz for the photoionization rate γ_{PI} from the $3P$ state.² Furthermore, the 671-nm MOT light can ionize atoms from this state and a value of 5.4 Hz is found for γ_{PI} if the beam parameters for the red MOT are used (see Section 3.3.1). These contributions to the ionization rate of the $3P$ seem negligible when compared to the corresponding values for the 532-nm high-power ionization laser.

The ground or excited state of the atom can also be ionized via an off-resonant multiphoton ionization. Considering only the high-power 532-nm laser, three (two) photons can ionize the ground state ($2P$ state) of lithium. The ionization rate for a K -photon transition scales with I^K and such experiments typically require large laser intensities I on the order of 10^{13} W/cm², commonly provided by pulsed-laser sources (Cohen-Tannoudji and Guéry-Odelin, 2011; Steinmann, 2007; Story and Gallagher, 1993). In our experimental implementation with a cw laser, we obtain intensities on the order of 1.5×10^4 W/cm² and we therefore assume the effects of multiphoton ionization to be insignificant. This is also supported by experimental observations.

6.2.2. Reduction of ionization background

For the spectroscopy measurement it is essential to suppress ionization processes that lead to a background signal and which are not related to the detection of states belonging to the $2S$ - $3P$ asymptote. This includes in particular the ionization of $2P$ atoms with 323-nm light because the photoassociation measurement is performed in a red MOT on the $2^2S_{1/2} \rightarrow 2^2P_{3/2}$ transition.

²In this ionization process the photoelectron energy ϵ is $0.168 E_h$, which is beyond the range considered in Lahiri and Manson (1993). However, as the photoionization cross section σ_{PI} is found to decrease monotonically with ϵ , a maximum value can be assumed for σ_{PI} .

Alternating trap and probe light This ionization channel can be eliminated by performing the PA measurement when all the atoms are in the ground state. To achieve this, we alternate the 671-nm MOT and the 323-nm PA probe light at a rate of 4.5 kHz. The duty cycle of the trapping light is 63%, which leads to a reduction of the atom number on the order of 25 %. In addition, we allow for a margin between the two phases to avoid any overlap and use a duty cycle of 30 % for the 323-nm beam, which is illustrated in Fig. 6.3 (a).

The cooling and repumping light for the MOT is switched with AOMs, however, we employ an optical chopper wheel for the PA beam. If only an AOM is used for the 323-nm laser beam, then about 10 nW of UV stray light remains overlapped with the beam path, originating from scattering in the AOM crystal.

Alternating spectroscopy and MOT loading phase An additional complication of the experimental sequence arises because the trapped atoms can be excited to the $2P$ state by the Zeeman slower light, which can then be ionized by the 323-nm probe beam. This requires the slower light to be blocked during a spectroscopy measurement. Consequently, the loading of the MOT is halted and prevents us from continuously scanning the laser frequency of the probe beam with a steady-state atom number. Instead, we employ a semi-continuous scheme which is implemented as follows. After initially fully loading the MOT, the atoms are exposed to the probe beam for 7 s during a spectroscopy phase, which is followed by a loading phase of 3 s. While the atom number decreases by about 10 % during the spectroscopy phase, this 10 s cycle can, in principle, be repeated arbitrarily often.

6.2.3. Experimental sequence for spectroscopy measurement

The experimental control for the spectroscopy measurement is illustrated in Fig. 6.2. It is based on the real-time experimental control that is also used for the production of the quantum gas and was described by Taglieber (2008).

Frequency scan The spectroscopy probe beam is provided by a frequency-doubling laser system that was described in Section 3.4. During a single measurement, we scan the frequency of the probe laser across a variable range of up to 4 GHz. The control signal for the frequency ramp is provided by an arbitrary waveform generator (AWG), which is programmed to account for the alternating MOT loading and spectroscopy phase of the experimental cy-

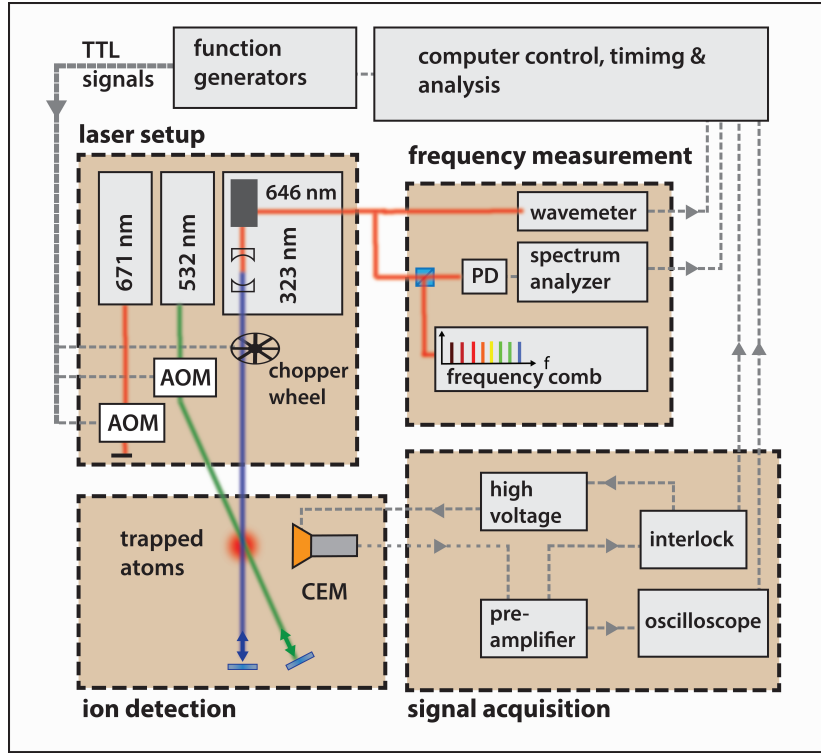


Figure 6.2.: Overview of spectroscopy setup. The 671-nm MOT light alternates with the 323-nm probe and 532-nm ionization light. In the depicted phase, the MOT light is blocked. The different highlighted sections are described in the text.

cle. Specifically, this implies that the frequency ramp during the intermediate loading phases of the MOT is halted. The ramp signal is directly supplied to the control unit of the piezo element of the ECDL, which then automatically provides a feed-forward signal to the laser diode current to ensure a mode-hop free frequency scan. Alternatively it is also possible to lock the laser to the Fabry-Perot resonator described in Section 3.4 and to scan the length of that resonator.

Laser frequency measurement of probe beam We determine the wavelength of the probe beam with a measurement setup based on an optical frequency comb, as illustrated in Fig. 6.2. While here only our measurement scheme is discussed, the frequency comb system that is used is described in the PhD thesis of Pal (2016). At the beginning of each spectroscopy scan, the absolute frequency of the laser is measured as follows. A wavemeter³ with an absolute accuracy of 60 MHz determines the number of the spectral line of the frequency comb that is closest to the frequency of the probe light with an uncertainty of ± 1 . The relative frequency is inferred by interfering the comb and probe light on a polarizing beam splitter and observing

³WS7, HighFinesse Laser and Electronics Systems GmbH

the beat-note with a fast photodiode and a spectrum analyzer. In addition, the frequency of the probe laser is shifted by about 5 MHz to the negative and to the positive side of the center frequency while the beat-note frequency is recorded. This allows us to unambiguously assign the number of the spectral line and to determine the frequency difference to the probe light, which then completes the measurement of the absolute laser frequency.

To accurately determine the wavelength of the probe beam during a spectroscopy scan, we measure the frequency of the beat-note at a repetition rate of 4 Hz. These measurements are synchronized with the experimental control and therefore occur in real-time.⁴ The knowledge of the initial absolute frequency, the direction of the frequency ramp and the timed beat-note measurements allow us determine the absolute laser frequency at any time during the scan with an estimated uncertainty on the order of 1 MHz, if a ramp rate of 20 MHz/s is assumed.

Data acquisition An ion that is absorbed by the CEM generates a current pulse, as described in Section 3.7, and the amplified ion signal is recorded with an oscilloscope at a sampling rate of 5000 points/s. A typical frequency scan contains nine repetitions of the scan and loading cycles of 10 s and covers a range of about 2 GHz. In a first processing step after the frequency scan, the sections of the intermediate loading phases of 3 s are removed from the acquired data set and the time axis is converted to the absolute frequency. Examples of such measurements are shown in Fig. 6.3 (b) and Fig. 6.4 (a).

The ion signal is also continuously monitored by the interlock, which was described in Section 3.7. The threshold is usually set to 100 nA, corresponding to a count rate of about 10^4 Hz. If triggered, the output of the high-voltage power supply is reduced. In addition, the MOT and the 532-nm ionization light are switched off with AOMs, which immediately interrupts the main ionization channels.

6.3. Ionization detection on atomic transition

The experimental scheme for the ionization-based spectroscopic investigation of the $2S-3P$ asymptote is first applied to the atomic transition. This allows us to test the integrated ion detection system and to verify the frequency measurement of the probe beam.

⁴While the spectrum analyzer is triggered in real-time, the acquisition duration is finite and introduces a maximum uncertainty of 12.5 ms (resolution bandwidth: 1 MHz, video bandwidth: 10 kHz, frequency span: 125 MHz). Assuming a scan rate of 20 MHz/s, this adds 0.25 MHz to the measurement uncertainty.

6.3.1. Atomic transition frequency and fine structure splitting of the $3P$ state of ${}^6\text{Li}$

For the observation of the atomic transition, we reduce the UV power from a maximum of 20 mW to 10 nW. Further, we only use a single-pass of the UV beam through the atomic cloud to limit the ionization rate. The power of the 532-ionization light is set to 10 W and the scan speed of the frequency ramp is 23 MHz/s. The atomic transitions $2^2S_{1/2} \rightarrow 3^2P_{1/2}$ and $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transitions are scanned separately and the obtained spectra are shown in Fig. 6.3 (b).

From this measurement we infer a value of 927 110 388.3 MHz for the $2^2S_{1/2}, F = 3/2 \rightarrow 3^2P_{1/2}$ transition, corresponding to a wavelength of 323.3622 nm. The absolute uncertainty of this value arises due to the presence of the magnetic field of the MOT and the unresolved hyperfine structure of the excited state, and is estimated to be on the order of about 5 MHz. The measured wavelength is consistent with the literature value (Radziemski et al., 1995), which, however, is stated with an uncertainty of 600 MHz. For the fine structure splitting we deduce a value of 2 883.2 MHz, which is calculated from the difference of the absolute frequency measurements. The literature value for the fine structure interval with the highest indicated accuracy for ${}^6\text{Li}$ is 2 882.7(15) MHz and was reported by Isler et al. (1969). Considering the systematic uncertainty of our measurement, the good agreement between the two values might be coincidental, but was not further investigated.

6.3.2. Detection and suppression of ASE

The observation of the atomic transition with an optical power of only 10 nW for the UV light demonstrates the applicability of the spectroscopy scheme based on the cw 532-nm ionization laser. For the photoassociation measurement, the UV power is increased to the maximum of 20 mW and retro-reflected, and the optical power of the ionization laser is set to 30 W. Furthermore, a higher negative bias voltage is applied to the CEM, which increases the gain by a factor of about 50, as compared to the gain of the previous measurement.

Observation of 'fake' lines

The sensitivity of our detection scheme to resonant light has led to the observation of a rather surprising multitude of well separated signals at detunings of dozens of GHz from the atomic

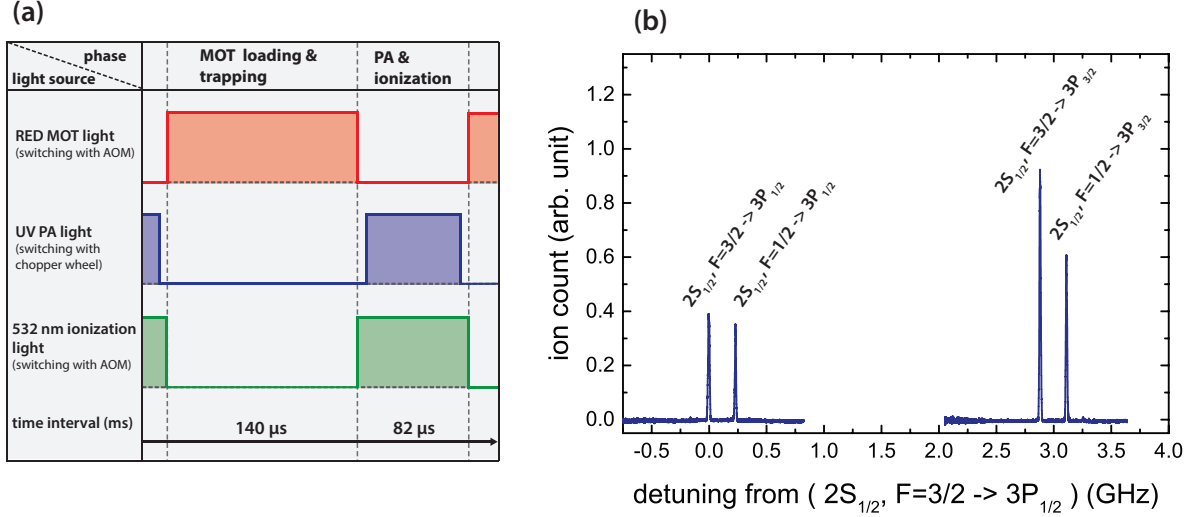


Figure 6.3.: (a) Alternating probe and trapping spectroscopy measurement. The atoms are exposed either to the trap (red) or the UV probe light (blue) in order to prevent ionization of atoms in the $2^2P_{3/2}$ state. In addition, the 532-nm light (green) is in general only applied in combination with the probe beam. (b) Observation of atomic transition with ion detection. The frequency is shown relative to the $2^2S_{1/2}, F = 3/2 \rightarrow 3P_{1/2}$ transition.

transition. These lines are not related to transitions to bound molecular states, as one might expect at these detunings, but originate from light that is resonant with the atomic transition.

The cause of these signals lies in the nature of the frequency doubling system that produces the 323-nm light. The fundamental light at 646 nm is provided by a diode laser setup and can, for most applications, be considered to operate at a single-frequency. However, while the linewidth of the laser is measured to be around 30 kHz, typical power spectra of diode lasers show finite light levels across a spectral range of a few nanometers, which is referred to as amplified spontaneous emission (ASE). For the implemented 646-nm system, the suppression of the ASE as compared to the carrier frequency is stated to be 40 dB.⁵

The frequency doubling stage consists of a crystal placed in a bow-tie-ring resonator, which has a free spectral range (FSR) of 1 092 MHz. Therefore, in addition to the carrier frequency, a discrete set of frequencies of the ASE light are coupled into the cavity. These various frequency components can be combined with the carrier frequency in the nonlinear medium to produce a photon in the UV range. As a result, the light after the doubling cavity consists of a carrier and a large number of sidebands that are separated by the FSR of the cavity, as illustrated in Fig. 6.4 (c).

For large detunings of the carrier frequency with respect to the atomic transitions, off-reso-

⁵Tapered amplifier chip TA-0650-0250-5 from Toptica Photonics AG.

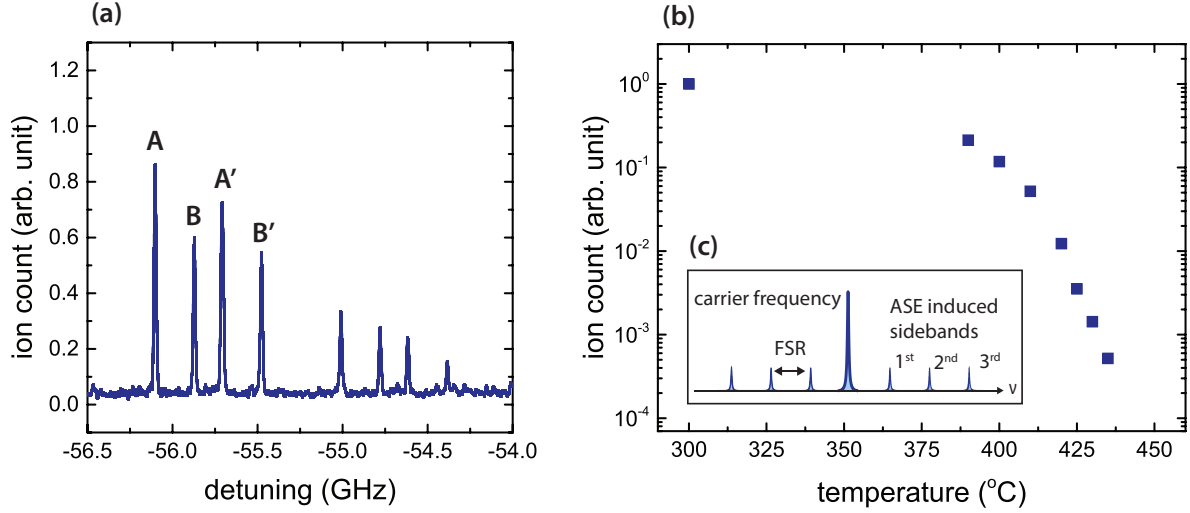


Figure 6.4.: (a) Ion signal due to ASE light. Peak A (A') arises due to light from the 54th (51st) sideband of the carrier that is resonant with the $2^2S_{1/2}, F = 3/2 \rightarrow 3^2P_{3/2}$ ($3^2P_{1/2}$) transition. B and B' are transitions from the corresponding second hyperfine ground state. (b) Amplitude of these spurious signals as function of the lithium-vapor-cell temperature. (c) Power spectrum of the probe beam after the frequency doubling stage. The optical power of the sidebands is shown largely exaggerated for illustrative purposes and are not to scale.

nant excitations are suppressed according to Eq. (4.1). However, as the carrier is scanned, the frequency of a certain sideband may become resonant with an atomic transition. This results in clearly observable ionization signals at well-defined frequencies, as exemplarily shown in Fig. 6.4 (a) for a detuning of more than 50 GHz.

Suppression of ASE with vapor cell

These spurious ionization signals have to be removed or greatly suppressed for a PA spectroscopy measurement. A possibility is to use a grating in order to spatially separate the frequency components or a second cavity with an FSR that is incommensurate with the one of the doubling cavity. Both solutions come at some technical cost. The cavity length would have to be actively regulated to follow the carrier frequency, while the grating would lead to a reduced available power and an incomplete suppression.

We use a method that is presumably simpler and more efficient for our particular application. After the frequency doubling stage, the UV light passes a lithium heat pipe, which is usually used for modulation transfer spectroscopy. Light that is resonant with the atomic transition is attenuated by the lithium vapor, while far-off-resonant light is transmitted. The small photon absorption cross section on the UV transition requires an elevated temperature

of the lithium vapor and a second passage of the beam to achieve a substantial reduction of the resonant light. The applicability of this scheme is demonstrated by measuring the signal strength of the spurious ASE signals as a function of the temperature of the heat pipe and is shown in Fig 6.4 (b). The amplitude is reduced by a factor of more than 10^3 and the ionization signal due to ASE light is no longer discernible at a cell temperature of 440 °C. The double-pass transmission through the heat pipe increases to about 85 % at laser detunings greater than 5 GHz from the atomic resonance.

6.4. PA scan below $2S$ - $3P$ asymptote

As indicated in the introduction to this chapter, we have not observed any signature of photoassociation transitions to bound states below the $2S$ - $3P$ asymptote within the scope of this work. Regardless of this, an example of a frequency scan is shown and discussed here.

6.4.1. Frequency range between -140 GHz to -35 GHz

The most weakly bound states of the internuclear potentials have the largest spatial extent and generally correspond to the strongest transitions in PA spectroscopy measurements. Furthermore, the energy spacing between adjacent molecular states increases rapidly with the binding energy (LeRoy and Bernstein, 1970). Therefore, the frequency range that is first experimentally investigated starts in the proximity of the asymptote of the $2S$ - $3P$ internuclear potential, which corresponds to the $2^2S_{1/2} \rightarrow 3^2P_{1/2}$ atomic transition. Compared to typical binding energies of molecular states, the fine structure interval of ^6Li is small such that the observation of states in between the two atomic asymptotes would be difficult. Accordingly, the indicated detunings and binding energies are with respect to the $3^2P_{1/2}$ level.

PA scan in vicinity of atomic resonance A frequency scan across the atomic resonances is shown in Fig. 6.3 (b). However, for the photoassociation frequency scan, the experimental conditions are different as indicated above. The total available UV power of the PA probe beam is increased to about 15 mW for the experiment and is retro-reflected, which raises the optical intensity by a factor of $\sim 3 \times 10^6$. With these parameters for the PA measurement, we scan a frequency range of detunings starting from -3 GHz up to about -30 GHz with respect to the atomic transition.

In this frequency range, the ionization rate due to off-resonant atomic excitations is sufficiently high such that the ion current produces a continuous signal. For this, we use a low-pass filter of 30 Hz, which effectively integrates the individual current pulses from the CEM. The frequency scan rate is 23 MHz/s, which should ensure a sufficient spectral resolution, if we consider the thermal broadening on the order of 10 MHz in the red MOT. A photoassociation transition would appear as a temporarily increased ionization rate and therefore as a deviation from the background of atomic excitations alone. However, with this method we could not identify any PA transition within this frequency interval. The ionization rate monotonically decreases in agreement with an off-resonantly driven atomic transition. In addition to the CEM signal, we also monitor the fluorescence of the MOT in order to ensure steady experimental conditions. At these detunings of the UV light, the introduction of the PA probe beam has no observable effect on the fluorescence signal.

PA scan for frequency detunings beyond -35 GHz Off-resonant atomic transitions can mask a weak PA signal and can make it difficult to distinguish it from other fluctuations in the ion signal. For frequency detunings on the order of -30 GHz, corresponding to $4 \times 10^4 \Gamma_{3P}$, the ionization rate decreases to a level which requires a different method to monitor the CEM current, if the same frequency scan rate is maintained. The reason is the following. Beyond this frequency detuning, we observe less than about twenty counts per second. Because of the random nature of the amplification process of the CEM, the amplitude of the current pulses fluctuates and follows some statistical distribution (Sjuts, 2014a). If the current is simply integrated, this effect will lead to additional fluctuations in the signal, which becomes relevant at a small count rate. To accommodate for this, the measurement scheme is changed from integrating the CEM current to counting of the ionization events, as illustrated in Fig. 6.5 (b).⁶ With this method we cover a frequency range from -35 GHz to -140 GHz with respect to the $2^2S_{1/2} \rightarrow 3^2P_{1/2}$ transition. We believe, as discussed in more detail in Chapter 7, that both the $3^1\Sigma_u^+$ and the $3^3\Sigma_g^+$ potentials support at least one bound state within this frequency interval.

The collected experimental data are shown in Fig. 6.5 (a). It comprises a total of 118 individual frequency scans, of which each covers a range of about 2 GHz. The observed

⁶In this scheme, the setting of the low-pass filter is adjusted such that individual ionization events are well resolved. For this measurement it would seem more appropriate to use a frequency counter, however, we use the oscilloscope and employ subsequently an algorithm to determine the event rate.

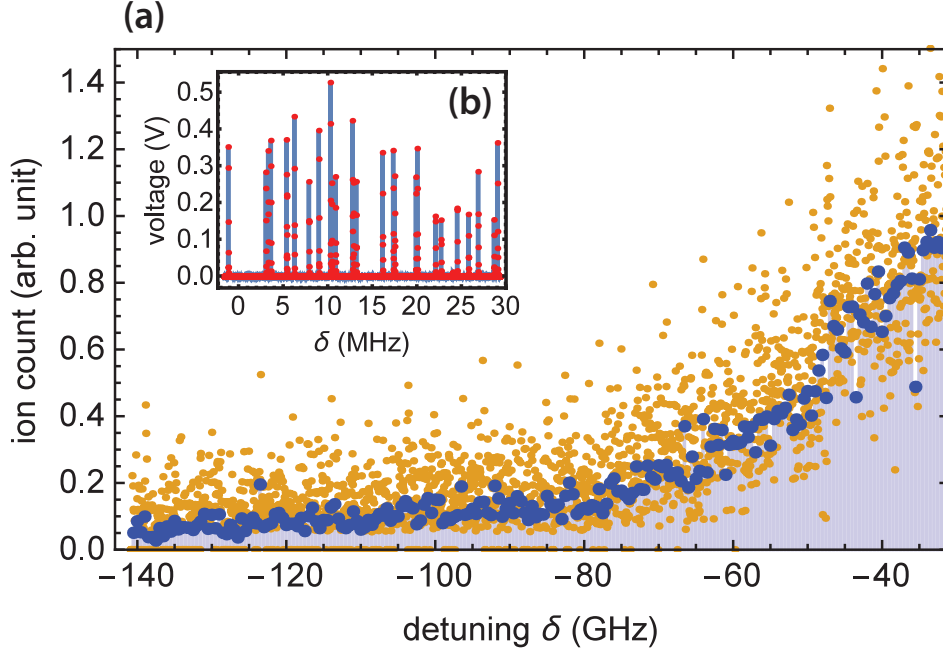


Figure 6.5.: (a) Photoassociation frequency scan. Ionization rate as function of the laser detuning with respect to the $2^2S_{1/2} \rightarrow 3^2P_{1/2}$ transition. The observed ionization events are displayed as a histogram, with a bin width of 500 MHz (blue circles) and 20 MHz (yellow circles). (b) Observed ionization signal (red circles) at a detuning of -45 GHz. The blue line connects subsequent measurement points and accents individual ionization events.

counts are grouped into bins of a width of 500 MHz and 20 MHz, respectively. Also in this frequency interval, we did not observe an evident signature of a PA transition that would clearly exceed the ionization rate due to off-resonant excitations of the $3P$ state. However, the fluctuations and the statistical error of the count rate in the individual bins is too high in order to observe transitions that would lead to ionization rates comparable to the background of off-resonant atomic excitations. The photoassociation transition strength to molecular states with higher binding energies, corresponding to larger frequency detunings from the atomic transition, is expected to diminish further. For this reason it was decided not to continue the frequency scan with the present method.

6.5. Summary

In summary, we have presented our failed attempt to observe transitions to bound states of potentials that are correlated to the $2S$ - $3P$ asymptote of ^6Li . In this approach, the atoms are trapped in a MOT on the D_2 transition and exposed to the 323-nm photoassociation beam, which is red-detuned from the atomic $2^2S_{1/2} \rightarrow 3^2P_{1/2}$ transition. Atomic or molecular excitations involving a $3P$ state are ionized with a high-power laser at 532 nm, and the

resulting ions are detected with a channel electron multiplier. The detection scheme, which involves a continuous and automated absolute frequency measurement, was successfully tested on the atomic transition. A PA scan covering a frequency interval of 140 GHz was performed, but the ionization rate showed no clear deviation from the atomic background due to off-resonant atomic excitations. In hindsight, the assumption that a PA resonance would be much stronger than the off-resonant excitation seems not justified, or rather naive. To gain a better understanding of the PA process to states of the $2S$ - $3P$ asymptote, we analyze the transition strength of this free-bound transition in the next chapter.

7. Photoassociation rate

In this chapter, photoassociation transition rates to bound states of the $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ potentials of Li_2 are calculated. The aim is to better understand the results presented in Chapter 6 and to evaluate the prospect of future PA measurements below the $2S$ - $3P$ asymptote. The evaluation of the free-bound transition strength requires the knowledge of the electronic transition moment and the wave functions of the initial and final states of the PA process. The different steps of the calculation are described and obtained results are compared to the literature values, where possible. For this purpose, the calculation is also performed for the $A^1\Sigma_u^+$ and $1^3\Sigma_g^+$ potentials of the $2S$ - $2P$ asymptote, which are well investigated. Following standard conventions, equations are generally expressed in atomic units, with conversion factors given in appendix B.1.

7.1. Photoassociation transition strength

The photoassociation process can be considered as a scattering phenomenon, in which laser light provides a coupling to electronically excited molecular states of the internuclear potential. If the energy difference between such a bound state and the ground-state continuum state equals the photon energy $\hbar\omega_{\text{Pa}}$ of the light field, then the scattering is resonantly enhanced (Napolitano et al., 1994). The photoassociation rate coefficient is proportional to the transition matrix element between the initial and final state according to

$$K_{\text{Pa}} \propto |\langle b | V_{\text{rad}} | u(E, J) \rangle|^2, \quad (7.1)$$

where $|u(E, J)\rangle$ is the continuum wave function of the ground-state potential with collisional energy E and angular momentum J , and $|b\rangle$ is the bound state. The radiative coupling term V_{rad} describes the electronic dipole interaction between the light field and the atomic and molecular states. The calculation of photoassociation transition rates requires the knowledge

of these three components, which are discussed in the following sections.

7.1.1. Transition dipole moment

The transition dipole moment between different molecular states depends on the electronic wave functions of the initial and final state. For diatomic molecules, these wave functions can be calculated in the Born-Oppenheimer approximation, where it is assumed that the electron configuration depends only on the separation of the two nuclei but not on their momenta. In a recent series of works, such *ab initio* calculations were performed for the ground state and several electronically excited state molecular potentials of Li_2 (Jasik and Sienkiewicz, 2006; Jasik, P. et al., 2007), and based on these results also transition dipole moments were calculated for various transitions of the lithium dimer (Jasik and Sienkiewicz, 2013).

The transition dipole moment operator can be written as a sum of the electronic and nuclear part according to

$$\mathbf{d}^{mol}(\mathbf{r}, \mathbf{R}) = \mathbf{d}^{el}(\mathbf{r}) + \mathbf{d}^{nuc}(\mathbf{R}) , \quad (7.2)$$

where $\mathbf{d}^{el/nuc}(\mathbf{r}) = \sum_i q_i \mathbf{r}_i$ with q_i the electronic or the nuclear charge and $\mathbf{r}$ and $\mathbf{R}$ are the respective position vectors. Here, the discussion by Jasik and Sienkiewicz (2013) is followed. The transition strength between different electronic states is proportional to the matrix element

$$\mathbf{d}_{f,i}^{mol} = \left\langle \Psi_f^{mol}(\mathbf{r}, \mathbf{R}) \left| \mathbf{d}^{mol}(\mathbf{r}, \mathbf{R}) \right| \Psi_i^{mol}(\mathbf{r}, \mathbf{R}) \right\rangle , \quad (7.3)$$

where $\left| \Psi_{i/f}^{mol}(\mathbf{r}, \mathbf{R}) \right\rangle$ is the initial and final molecular state, respectively. Following the Born-Oppenheimer approximation, the nuclear and the electronic part of the wave function can be separated, such that

$$\left| \Psi_{i/f}^{mol}(\mathbf{r}, \mathbf{R}) \right\rangle = \left| \Psi_{i/f}^{el}(\mathbf{r}; \mathbf{R}) \right\rangle \left| \Psi_{i/f}^{nuc}(\mathbf{R}) \right\rangle . \quad (7.4)$$

This relation can now be used in Eq. (7.3) and one finds that the contribution of $\mathbf{d}^{nuc}(\mathbf{R})$ vanishes. Formally, this follows from the orthogonality of the different electronic wave functions

and results in

$$\mathbf{d}_{f,i}^{mol} = \left\langle \Psi_f^{nuc}(\mathbf{R}) \left| \left\langle \Psi_f^{el}(\mathbf{r}; \mathbf{R},) \left| \mathbf{d}^{el}(\mathbf{r}, \mathbf{R}) \right| \Psi_i^{el}(\mathbf{r}; \mathbf{R},) \right\rangle \right| \Psi_i^{nuc}(\mathbf{R}) \right\rangle \quad (7.5)$$

$$= \left\langle \Psi_f^{nuc}(\mathbf{R}) \left| \mathbf{D}_{f,i}(\mathbf{R}) \right| \Psi_i^{nuc}(\mathbf{R}) \right\rangle, \quad (7.6)$$

where the second equation defines the electronic transition moment between states of different internuclear potentials. For diatomic molecules $\mathbf{R}$ is assumed to be parallel to the internuclear axis, commonly referred to as z axis, and R corresponds to the internuclear separation. Considering $\Sigma \rightarrow \Sigma$ transitions (see Section 6.1.3), it can be shown that only the matrix element along the internuclear axis is different from zero such that the expression in Eq. (7.6) reduces to $\left\langle \Psi_f^{nuc}(\mathbf{R}) \left| d_z \right| \Psi_i^{nuc}(\mathbf{R}) \right\rangle$. The integrand for the other components vanishes, which follows from symmetry arguments and was discussed by Herzberg (1950).

At asymptotically large internuclear distances, the mutual interaction between the atoms becomes negligible and the transition dipole matrix elements therefore have to approach the atomic values. Specifically, the square of these elements, which are related to the transition strength, converge to twice the value of an individual atom. This is because the considered system consists of two atoms (Ratcliff et al., 1987). As a first evaluation, this relationship can be used to approximate the relative strength of transitions to bound states of the $2S$ - $2P$ potentials and the $2S$ - $3P$ potentials, respectively, and is calculated according to:

$$\frac{\left| \left\langle 3^1\Sigma_u^+ \left| d_z \right| X^1\Sigma_g^+ \right\rangle \right|^2}{\left| \left\langle A^1\Sigma_u^+ \left| d_z \right| X^1\Sigma_g^+ \right\rangle \right|^2} \Big|_{R \rightarrow \infty} = \frac{\left| \left\langle 3^3\Sigma_g^+ \left| d_z \right| a^3\Sigma_u^+ \right\rangle \right|^2}{\left| \left\langle 1^3\Sigma_g^+ \left| d_z \right| a^3\Sigma_u^+ \right\rangle \right|^2} \Big|_{R \rightarrow \infty} \quad (7.7)$$

$$= \frac{\lambda_{323}^3 \Gamma_{UV}}{\lambda_{671}^3 \Gamma_{2P}} \quad (7.8)$$

$$= 3.0 \times 10^{-3} \quad (7.9)$$

The numerical values used in the second equation are given in Appendix A.1 and the result indicates that the transition strength to bound states correlated to the $2S$ - $3P$ asymptote is substantially smaller as compared to the one to the well investigated potentials correlated to the $2S$ - $2P$ asymptote. The transition dipole moments for the considered transitions $X^1\Sigma_g^+ \rightarrow \{A^1\Sigma_u^+, 3^1\Sigma_u^+\}$ ('singlet transition') and $a^3\Sigma_u^+ \rightarrow \{1^3\Sigma_g^+, 3^3\Sigma_g^+\}$ ('triplet transition') are shown in Fig. 7.1 (Jasik and Sienkiewicz, 2013).

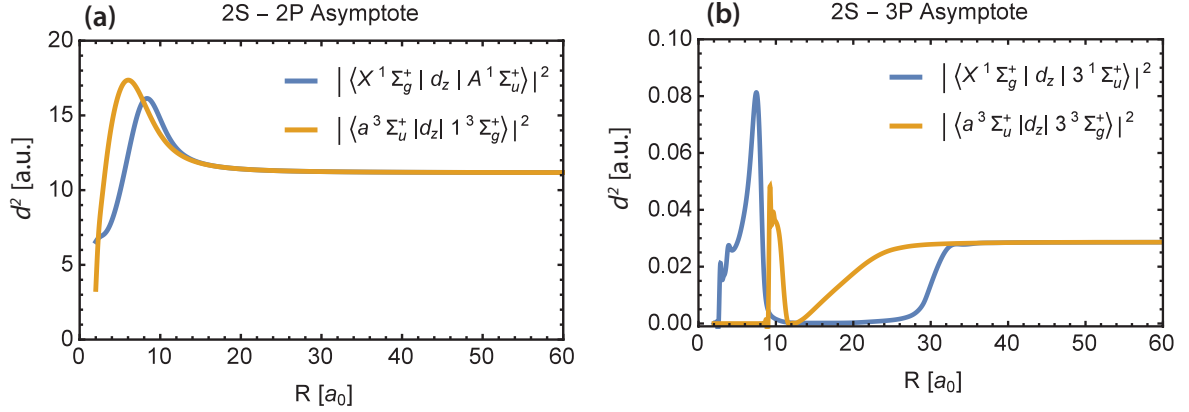


Figure 7.1.: Molecular transition dipole moment. (a) Shown are squared transition dipole matrix elements d^2 between states of the ground-state potential and states of the first excited P asymptote as a function of the internuclear separation R . (b) Values for transitions of the same symmetry but to potentials approaching the $2S$ - $3P$ asymptote. Only transitions relevant for the current calculation are shown with the data taken from [Jasik and Sienkiewicz \(2013\)](#).

7.1.2. Calculation of transition rates

While the prime interest for PA measurements is to determine the transition frequencies, experimentally relevant is also the rate at which these transitions occur and a measure for this quantity is the PA rate coefficient K_{PA} . Assuming a Maxwell-Boltzmann distribution at a temperature T for the colliding atoms, this coefficient can be expressed by ([Côté and Dalgarno, 1998](#); [Napolitano et al., 1994](#))

$$K_{\text{PA}} = \frac{k_B T}{h Q_T} \sum_{\nu} \sum_{J=0}^{\infty} (2J+1) \int_0^{\infty} |S_{\nu}(E, J, \omega_{\text{PA}})|^2 e^{-E/k_B T} \frac{dE}{k_B T}. \quad (7.10)$$

where $Q_T = (2\pi\mu k_B T/h^2)^{3/2}$ is the translational partition function and μ is the reduced mass. The S -matrix element $S_{\nu}(E, J, \omega_{\text{PA}})$ is related to the probability that a photon of angular frequency ω_{PA} drives a transition from a continuum state $|u(E, J)\rangle$, with a collisional energy E , to a bound state $|u_{\nu, J'}\rangle$ of the excited-state potential. To formally account for all possible transitions, a sum over the vibrational numbers ν of the excited state and all angular momentum numbers J of the ground state is performed. For laser intensities I where saturation effects can be neglected, it was shown by [Côté and Dalgarno \(1998\)](#) that the S -matrix element is approximately given by

$$|S_{\nu}(E, J, \omega_{\text{PA}})|^2 \approx 8\pi^2 \frac{\pi I}{c} |\langle u_{\nu, J'} | D(R) | u(E, J) \rangle|^2 \delta(E - \Delta_{\nu}). \quad (7.11)$$

The detuning $\Delta_{\nu} = E_{\nu} - \hbar\omega_{\text{PA}}$ is the difference between the photon energy $\hbar\omega_{\text{PA}}$ and the

bound state energy E_ν , which is measured relative to the atomic ground state, and δ is the Dirac delta function. The electronic transition moment $D(R)$ is a scalar function and was described in Section 7.1.1. Using this relation in the expression for the PA rate coefficient in Eq. (7.10), one finds

$$K_{\text{PA}} \approx \frac{8\pi^2}{3h} \frac{1}{Q_T} \frac{\pi I}{c} \omega_0 e^{-1/2} |\langle u_{\nu,1} | D(R) | u(k_B T/2, 0) \rangle|^2. \quad (7.12)$$

Several assumptions are made to arrive at this expression. First, photoassociation experiments are performed at low temperatures such that in most cases only s -wave collisions ($J = 0$) have to be included in the calculation. Second, only a single vibrational level is considered because the different levels are well separated at cold and ultracold temperatures of the atomic sample. Further, the factor of $1/3$ accounts for the polarization of the light and the maximum PA rate is generally obtained at a detuning of $\Delta_\nu = k_B T/2$, which determines the collisional energy of the continuum state in the expression for the matrix element (Gacesa and Côté, 2014). The factor ω_0 is the statistical weight for the considered transition, under the assumption of a mixture of hyperfine states in a magneto-optical trap. These values depend on the symmetry of the molecular states and on the nuclear spin of the atoms. The statistical weights were derived by Côté (1995) and are given for $^6\text{Li}_2$ continuum states with $J = 0$ by $\omega_0 = \frac{1}{6}$ for the singlet and $\omega_0 = \frac{1}{4}$ for triplet transition, respectively.

Spectroscopic signatures of a PA transition can be a reduction in the atom number or it can also be an enhanced ionization rate, as described in Chapter 6. These effects are based on additional physical processes that happen *after* the PA transition has occurred but are of course related to the PA rate itself. In order to use Eq. (7.12) for the calculation of the PA rate, the continuum wave functions of the ground state and the wave functions of the molecular states of the excited-state potential have to be calculated.

7.2. Numerical calculation of continuum states

The collisional properties of the elastic scattering of the two ground-state atoms can have a large effect on the PA transition rate and, in general, a detailed knowledge of the wave function is required for the calculation of the transition strength. However, it can be sufficient to approximate the ground state with the asymptotic form of the scattering wave function,

with the expression given in Section 2.2.1. The applicability of this approximation depends on the spatial extent of the addressed bound state and can be valid, in particular, for long-range states close to the dissociation limit (Côté and Dalgarno, 1998).

7.2.1. Radial Schrödinger equation and Numerov algorithm

However, the rather short-range character of the molecular potentials dissociating to the $2S$ - $3P$ asymptote, as discussed in Section 6.1.6, requires an accurate knowledge of the ground-state scattering wave function and the approximation indicated above cannot be applied. Therefore, the radial Schrödinger equation

$$\left(\frac{d^2}{dR^2} + \frac{2\mu}{\hbar^2} E - \frac{2\mu}{\hbar^2} V(R) - \frac{J(J+1)}{R^2} \right) u_{E,J}(R) = 0 \quad (7.13)$$

has to be solved numerically. Here, μ is the reduced mass of the lithium dimer, J the angular momentum number, $E = \frac{\hbar^2 k^2}{2\mu}$ the kinetic energy, $V(R)$ the internuclear potential energy curve, and $u_{E,J}(R)$ is the corresponding solution for these parameters.

This is a second-order differential equation and can be integrated using *Numerov's method* with appropriate boundary conditions, as discussed, for example, by Marchildon (2002). For this, the Schrödinger equation is written in the form

$$\frac{d^2 u(R)}{dR^2} = -g(R) u(R) \quad (7.14)$$

with $g(R) = -\frac{2\mu}{\hbar^2} \left(V(R) - E + \frac{\hbar^2}{2\mu} \frac{J(J+1)}{R^2} \right)$ and solved on a uniform grid. The recursion relation of Numerov's method for $u_{n+1} = u(R_{n+1})$, where R_n is the n -th grid point, is derived by expanding u_n up to fifth order on the finite grid and is given by

$$u_{n+1} = \frac{u_n(12 - 10f_n) - u_{n-1}f_{n-1}}{f_{n+1}} \quad (7.15)$$

with

$$f_n = \left(1 + \frac{g_n}{12} \Delta x^2 \right), \quad (7.16)$$

where Δx is the grid spacing. The recursive solution of $u(R)$ requires the knowledge of u_0 and u_1 , which are the boundary conditions of the problem. At small internuclear spacings R ,

the potential energy $V(R)$ diverges and exceeds the collisional kinetic energy by a few orders of magnitude and the probability density of the wave function is therefore exponentially small in this region. Together with the subsequent normalization of the wave function, this results in an uncritical choice for the values of the first two points u_0 and u_1 .

7.2.2. Ground-state potentials of ${}^6\text{Li}$

The numerical calculation of the scattering wave function is based on the knowledge of the potential energy curve of the system. The investigation of the interaction potentials of lithium has received considerable attention, both experimentally and theoretically. Fourier transform spectroscopy measurements (Barakat et al., 1986; Linton et al., 1989) and *ab initio* calculations (Jasik and Sienkiewicz, 2006; Konowalow and Olson, 1979; Konowalow et al., 1984; Musial and Kucharski, 2014) allow constructing potential curves in the short to intermediate regime from $\sim 3a_0$ to $\sim 20a_0$. At large internuclear spacings, the potential energy curve can be approximated by a power series of $1/R$ terms, as introduced in Section 6.1.4. The corresponding dispersion coefficients were calculated for the lithium dimer dissociating to atoms in the ground state but also to electronically excited states (Marinescu and Dalgarno, 1995; Marinescu et al., 1994; Yan et al., 1996). The relevant values are summarized in Table 7.1.

Potentials	C_3	C_6	C_8	C_{10}
$X\ ^1\Sigma_g^+ / a\ ^3\Sigma_u^+$	-	1.393 [3]	8.343 [4]	7.372 [6]
$A\ ^1\Sigma_u^+ / 1\ ^3\Sigma_g^+$	11.01 [0]	2.066 [3]	2.702 [5]	-
$3\ ^1\Sigma_u^+ / 3\ ^3\Sigma_g^+$	3.364 [-2]	3.814 [4]	2.702 [7]	-

Table 7.1.: Long-range dispersion coefficients of Li_2 for the potentials dissociating to the ground-state asymptote $2S-2S$ (Yan et al., 1996), and the excited-state asymptotes $2S-2P$ and $2S-3P$ (Marinescu and Dalgarno, 1995). The numbers in the squared brackets denote the powers of ten and the values are given in atomic units.

The ground-state potentials used in the present calculation are based on an analytic expression recently derived by LeRoy et al. (2009) for the singlet potential $X\ ^1\Sigma_g^+$ and by Dattani and LeRoy (2011) for the triplet potential $a\ ^3\Sigma_u^+$, respectively. The potential energy curves were generated by applying a fitting function to experimental data, with the model being constrained to asymptotically approach the long-range tail of the potential given in Eq. (6.10) with values for the dispersion coefficients from Yan et al. (1996). The complete analytic ex-

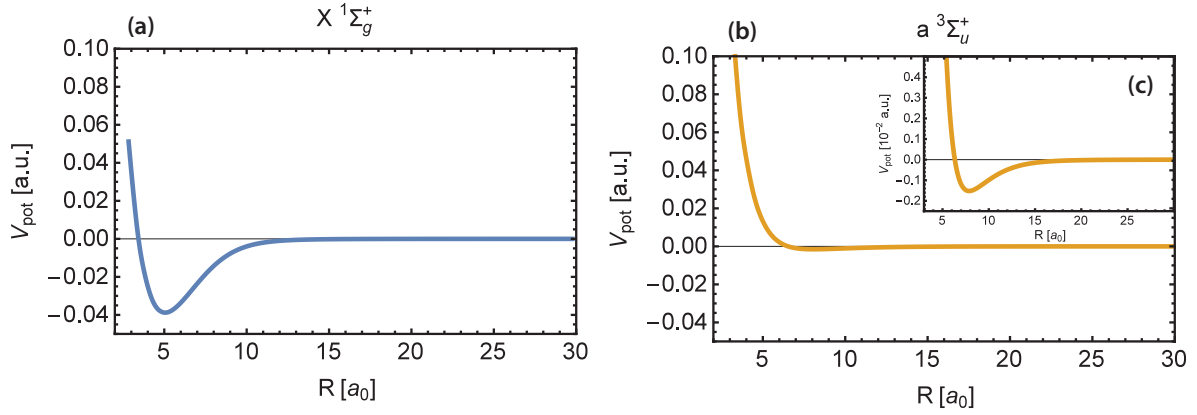


Figure 7.2.: Ground-state potential energy curves of lithium dimer. (a) Singlet potential $X^1\Sigma_g^+$ and (b) triplet potential $a^3\Sigma_u^+$ of Li_2 are shown as function of the internuclear separation and are given in atomic units (Dattani and LeRoy, 2011; LeRoy et al., 2009). (c) To better illustrate the shape of the $a^3\Sigma_u^+$ potential, the displayed energy range is reduced by a factor of 20. The difference between $^6\text{Li}_2$ and $^7\text{Li}_2$ would not be discernible on this energy scale, but is taken into account for the calculation of the ground-state scattering wave functions.

pressions are rather involved and are not given here, however, the corresponding potential energy curves are shown in Fig. 7.2.

7.2.3. Scattering cross section

With the knowledge of the potential energy curves of the lithium dimer and Numerov's algorithm, the wave functions of the continuum states can now be calculated. Energy normalized solutions (see Eq. (2.9)) of the radial wave function $u_{E,J}(R)$ for different collisional energies E and for zero angular momentum J are shown in Fig. 7.3 (e),(f). The calculation was performed for ^6Li atoms colliding under the influence of the singlet and triplet ground-state potentials and the solutions at low collisional energies reveal the positive (negative) s -wave scattering length of the singlet (triplet) potential. Apart from the wave function itself, derived quantities such as scattering phase shifts and scattering cross sections can be calculated for the different potentials. In the context of this work, comparison with literature values primarily serves as a verification for the implemented numerical method.

The scattering phase shift, which was introduced in Section 2.2.1, can be obtained by comparing the numerical solution $u_J(R)$ of Eq. (7.13) with the regular solution $v_J(R)$ of the free radial Schrödinger equation, obtained with $V(R) = 0$. The solution to that equation is given by $v_J(R) = kR j_J(kR)$, where $j_J(R)$ correspond to the spherical Bessel functions. The

phase shift δ_J can then be calculated according to

$$\sin\delta_J(k) = - \int_0^\infty j_J(kR) V(R) u_J(R) R dR, \quad (7.17)$$

which was discussed, for example, by [Burke \(2011\)](#). For this equation to be valid, the form of the asymptotic radial scattering wave function has to be $u(R) \approx \sin(kR + \delta_J - \frac{1}{2}J\pi)$, implying that the amplitude of the wave function must be normalized to unity. The associated total elastic scattering cross section follows from $\sigma_{tot} = \sum_{J=0}^\infty \sigma_J = \frac{4\pi}{k^2} \sum_{J=0}^\infty (2J+1) \sin^2\delta_J$ ([Landau and Lifshitz, 1977](#)), where σ_J is the partial wave scattering cross section for an angular momentum number J . With the implemented numerical method, these quantities are calculated for the singlet and triplet ground-state potentials for ^6Li and ^7Li , respectively. Collisional energies over a wide energy range and partial waves up to $J = 20$ were considered, and the results are shown in Fig. 7.3 (a)-(d). The obtained values for ^7Li can be compared with a numerical simulation reported by [Côté et al. \(1994\)](#) and are in good agreement with the current calculation.

Typical MOT temperatures for lithium are on the order of 1 mK, which corresponds to an average collisional energy of 4×10^{-9} a.u. . In this regime, scattering occurs predominantly via elastic s -wave collisions because the repulsive rotational contribution to the effective potential prevents the atoms from reaching short internuclear separations. Contributions from higher partial waves are nearly frozen out, as it follows from Fig. 7.3. Therefore, for the following calculations on the PA rate, only the $J = 0$ is considered for the scattering wave function.

At increased collisional energies, higher partial waves contribute to the total scattering cross section, leading to pronounced features, as shown in Fig. 7.3. These are scattering resonances and occur due to quasi-bound states that are supported by the J -dependent rotational barrier. From the preceding discussion it is clear that this energy range is not relevant for ultracold atoms, however, these characteristic features provide an ideal indication for the good agreement with previous calculations ([Côté et al., 1994](#)).

7.3. Numerical calculation of bound states

The PA transition strength depends profoundly on the shape of the excited-state wave function. Its overlap with the continuum wave function of the ground state is generally highest for

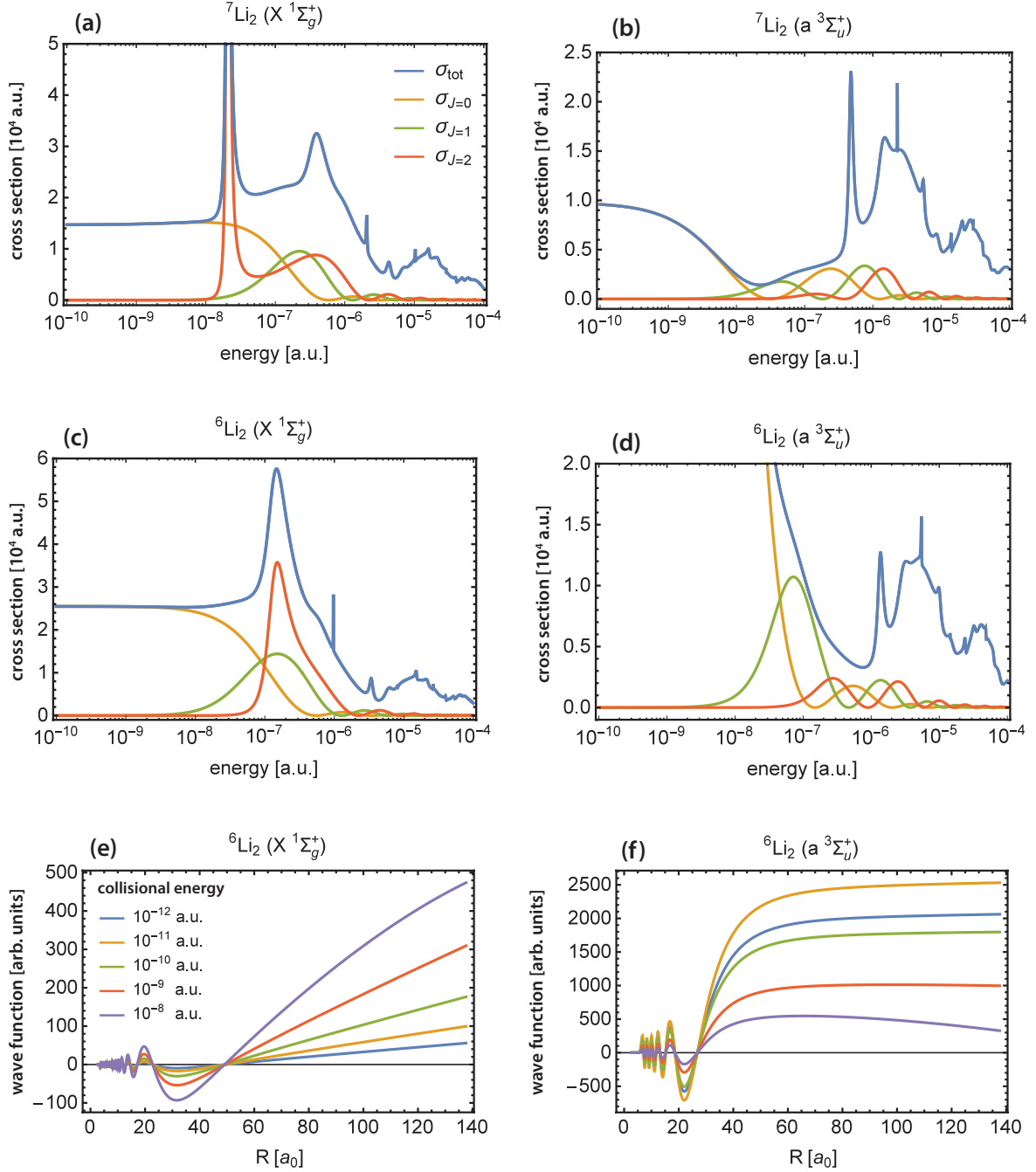


Figure 7.3.: Elastic scattering of lithium atoms. Calculated scattering cross sections for ${}^7\text{Li}_2$ (a),(b) and ${}^6\text{Li}_2$ (c),(d) via their respective $X {}^1\Sigma_g^+$ and $a {}^3\Sigma_u^+$ potentials. The partial wave cross sections are shown individually up to values of $J = 2$, while for the calculation of the total scattering cross section values of up to $J = 20$ were considered. For ${}^6\text{Li}$ atoms interacting via the $a {}^3\Sigma_u^+$ potential, the s -wave scattering cross section assumes very large values and converges to $\approx 1.5 \times 10^8$ a.u. at low collisional energies. (e),(f) Energy normalized wave functions of continuum states of the singlet and triplet potential for different collisional energies and zero angular momentum.

states with an outer classical turning point occurring at large internuclear spacings. Therefore, the PA process favors the creation of weakly bound long-range molecules. However, for potentials approaching the $2S\text{-}3P$ asymptote, the comparatively small C_3 dispersion coefficient leads to a more short-range character of the potential (see Eq. (6.10)). Correspondingly, the spatial extent of the molecular bound states of these potentials is smaller than the ones correlated to the $2S\text{-}2P$ asymptote.

7.3.1. Excited-state potentials

In the current calculation, only transitions with symmetries of the form $X\ ^1\Sigma_g^+ \rightarrow ^1\Sigma_u^+$ and $a\ ^3\Sigma_u^+ \rightarrow ^3\Sigma_g^+$ are considered. This implicitly excludes the most weakly bound states, for which spin-orbit coupling becomes relevant. This range would correspond to Hund's case (c) (Herzberg, 1950) and follows a different notation as compared to the one introduced in Section 6.7. Because of the small fine structure splitting of lithium, the excluded range of detunings corresponds to only around 20 GHz (10 GHz) for states dissociating to the $2S\text{-}2P$ ($2S\text{-}3P$) asymptote (Côté and Dalgarno, 1998). Symmetry considerations would also allow for transitions to the $^1\Pi_u$ and $^3\Pi_g$ states, as described in Section 7.3.1, but are not considered here. These potentials are expected to be repulsive at large internuclear distances (Marinescu and Dalgarno, 1995) and to lie below the asymptote only for short and intermediate distances (Musial and Kucharski, 2014).

The potential energy curves for the $2S\text{-}2P$ states are well investigated. Analytic expressions are available for the $A\ ^1\Sigma_u^+$ and the $1\ ^3\Sigma_g^+$ potentials (Dattani and LeRoy, 2011; LeRoy et al., 2009) and the resulting potential energy curves are shown in Fig. 7.4 (a),(b). These expressions are based on fits to experimental data, which also include data from PA spectroscopy measurements.

However, for states dissociating to the $2S\text{-}3P$ asymptote, the potential energy curves are based on *ab initio* calculations. At short to intermediate interatomic distances, values calculated by Jasik and Sienkiewicz (2006) were used and extended with the asymptotic form given in Eq. (6.10) for distances of $R \geq 70\ a_0$ (Marinescu and Dalgarno, 1995). The resulting potential energy curves are shown in Fig. 7.4 (a),(b). The uncertainty of such *ab initio* calculations is large compared to the accuracy of standard photoassociation measurements such that predictions on the precise transition frequencies are inherently difficult. However, it is

assumed that the relative spacings between the transitions can be estimated and therefore also the number of transitions within a given frequency interval.

7.3.2. Bound states of $2S$ - $3P$ potential

The total depth of the potentials dissociating to the two different P asymptotes are comparable, as illustrated in Fig. 7.4 (a),(b). However, PA transitions generally access the most weakly bound states with binding energies on the order of a few hundred GHz, which is small compared to the total depth around $0.03 \text{ a.u.} = 2 \times 10^5 \text{ GHz}$. To better illustrate the qualitatively different shape of the long-range part of potential energy curves, the insets of the respective plots in Fig. 7.4 (a),(b) show an enlarged view for large internuclear separations.

To obtain the wave functions and the binding energies of the $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ states, the radial Schrödinger equation is numerically solved for the respective internuclear potentials $V(R)$. Selection rules on the total angular momentum, apart from spin, restrict these transitions to $\Delta J = \pm 1$ (Herzberg, 1950). Elastic scattering of the ground-state atoms at ultracold temperatures predominantly occurs via s -wave collisions, such that only bound states with $J = 1$ are considered.

The numerical solution is based on an algorithm that employs a Fourier grid method (Marston and Balint-Kurti, 1989) and is available as a *Mathematica* library (Hansen, 1996). To verify its applicability to the long-range molecular states, it is first used for the $A^1\Sigma_u^+$ and the $1^3\Sigma_g^+$ potentials of the $2S$ - $2P$ asymptote. The binding energies determined in this way are in very good agreement with PA spectroscopy data obtained by Abraham et al. (1995b), which are given in Table 7.3 for the most weakly bound states. However, this only confirms the suitability of the algorithm for these long-range states, because the considered potential energy curves are partially based on the respective PA spectroscopy data sets.

Binding energies and wave functions of the molecular states correlated to the $2S$ - $3P$ asymptote are determined based on potential energy curves derived from *ab initio* calculations (Jasik and Sienkiewicz, 2006). The obtained binding energies of the twelve most weakly bound vibrational states of the relevant singlet and triplet potentials are given in Table 7.2. A total of 100 (67) bound states are found for the singlet (triplet) potential, and the convention is that the energetically lowest state corresponds to $\nu = 0$. It is worth noting that the energy spacing between adjacent vibrational states close to the dissociation limit is significantly larger as

compared to the one of bound states of the $2S$ - $2P$ potentials.

Selected radial wave functions of bound states correlated to the $\{A^1\Sigma_u^+, 1^3\Sigma_g^+\}$ and $\{3^1\Sigma_u^+, 3^3\Sigma_g^+\}$ potentials are shown in Fig. 7.4 and illustrate the different spatial extent of the various molecular states. In addition, the continuum radial wave function of the ground-state atoms colliding in the corresponding singlet or triplet potential are provided in order to illustrate the spatial overlap. The scattering states are evaluated for a collisional energy of 1 mK, similar to the temperature of the atomic cloud in the MOT. For the $\nu = 97$ state of the $3^1\Sigma_u^+$ potential shown in Fig 7.4 (e), the last lobe of the radial wave function of the bound state is near a node of the continuum wave function, which generally leads to a small overlap integral and a weak PA transition strength.

7.4. Calculation of dipole matrix elements and transition rates

Dipole matrix element - collisional energy The solutions of the radial Schrödinger equation for the ground- and excited-state potentials can now be used to calculate the dipole matrix element $|\langle u_{\nu,J'} | D(R) | u_{E,J} \rangle|^2$ in Eq. (7.12) for different PA transitions. These values are obtained by numerically integrating the obtained expressions for all bound states and a wide range of collisional energies of the ground-state atoms. For the $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ potentials, these matrix elements are shown in Fig. 7.5 as a function of the kinetic energy of the scattering state. For this, only the states with binding energies exceeding 10 GHz are considered (see Table 7.2). These results show that the transition dipole matrix element for the triplet transition peaks at a low kinetic energy, corresponding to a temperature of about $3\ \mu\text{K}$ of the atomic ensemble. The maximum values for the singlet transition are reached at much higher collisional energies, which are not relevant for experiments with cold and ultracold atoms.

Similar figures are shown in Appendix B.2 for PA transitions to states of the $2S$ - $2P$ asymptote of $^6\text{Li}_2$ and $^7\text{Li}_2$. For $^7\text{Li}_2$, the selected bound states and collisional energies allow for a direct comparison to results obtained by Côté and Dalgarno (1998), which are in very good agreement with the current calculation. This comparison is crucial because it confirms the validity of the calculation presented thus far.

Dipole matrix element - vibrational state In most PA spectroscopy measurements, only the weakly bound long-range states of the internuclear potential can be accessed. The reason for

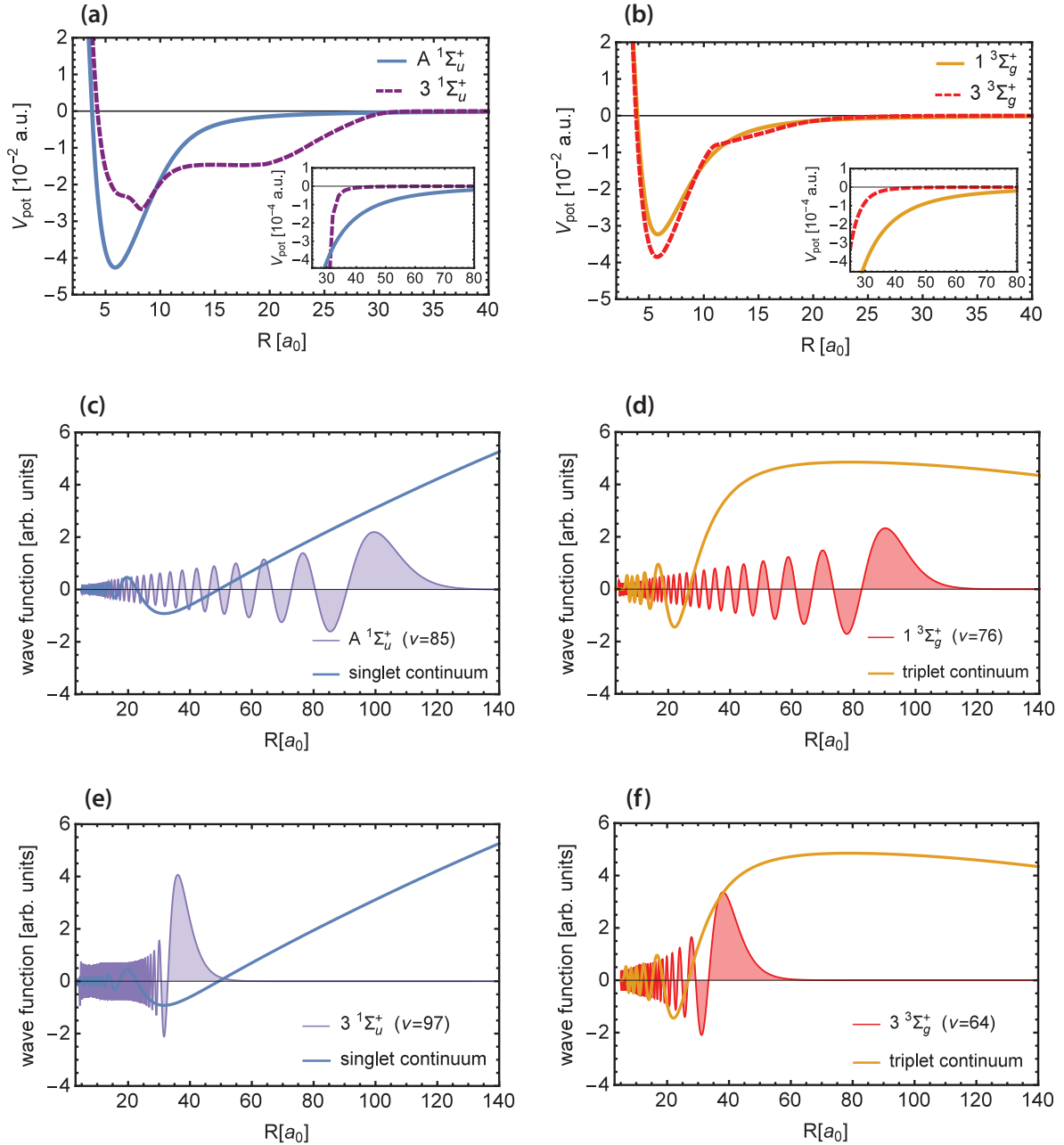


Figure 7.4.: Molecular potentials and bound states of ${}^6\text{Li}$ dimer. (a),(b) Internuclear potential energy curve with $1\Sigma_u^+$ and $3\Sigma_u^+$ symmetry of the $2S-2P$ (solid line) and of the $2S-3P$ asymptote (dashed line). The insets show an enlarged view of the long-range part of the potential (see text for references). (c)-(f) Continuum wave functions at a collisional energy of 4×10^{-9} a.u. (~ 1 mK) for the singlet and triplet ground-state potentials, as indicated in the figures. Selected bound states of $2S-2P$ (c),(d) and $2S-3P$ asymptote (e),(f). See Table 7.2 and 7.3 for corresponding binding energies.

this is the reduced transition strength to more deeply bound states, which is predominantly because of the reduced spatial extent of these vibrational states. For the PA transitions to bound states of the potentials approaching the $2S-3P$ asymptote, the dipole matrix element was calculated for all molecular states with a fixed collisional energy of the ground state and is shown in Fig 7.6. For the triplet state, the dipole matrix element has a pronounced local

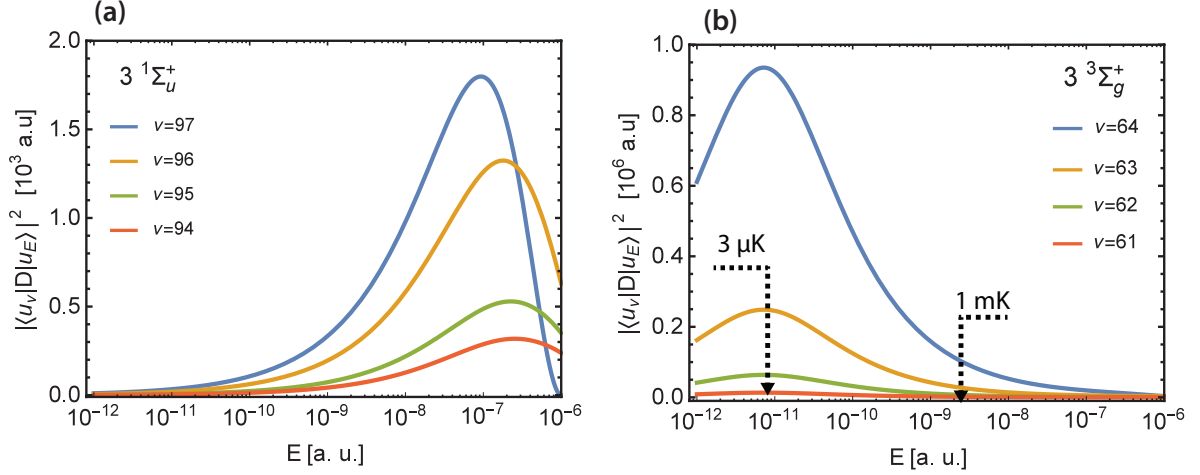


Figure 7.5.: Dipole matrix elements for PA transitions to $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ states. The matrix elements $|\langle u_{\nu,J'} | D(R) | u_{E,J} \rangle|^2$ of singlet (a) and triplet (b) transitions to $2S$ - $3P$ states are shown as a function of the collisional energy of the ^6Li atoms. The binding energies of the states shown in the figure are given in Table 7.2. The highlighted collisional energies correspond to the approximate temperature of the atoms in a MOT (1 mK) and a typically achievable temperature in an optical dipole trap ($3 \mu\text{K}$).

minimum. This occurs when the position of the last lobe of the bound state coincides with a node of the scattering wave function. For the singlet potential, however, the location of last lobe for the $\nu = 97$ state is already within the range where the radial wave function of the continuum state rapidly oscillates, as shown in Fig. 7.4 (e). The absolute value of the dipole matrix element is therefore much smaller than the one of the triplet transition. For comparison, the corresponding plots for the PA transitions to potentials approaching the $2S$ - $2P$ potential are shown in Appendix B.3.

PA transition rate coefficient With the knowledge of the dipole matrix element for the considered transitions, the PA rate coefficient given in Eq. (7.12) can be calculated. For this, the quantity is converted to SI units according to

$$K_{\text{PA}}(T, I) \approx \frac{2\pi}{3} \frac{1}{\hbar} \frac{\pi I}{Q_T \epsilon_0 c} \omega_0 e^{-1/2} |\langle u_{\nu,1} | D(R) | u(k_B T/2, 0) \rangle|^2 C_{\text{SI}}, \quad (7.18)$$

where ϵ_0 is the vacuum permittivity and $C_{\text{SI}} = e^2 a_0^2 / E_h$ is the conversion factor for the dipole matrix element, with the fundamental constants given in Table B.1. It is important to note that the unit of the squared matrix element $|\langle u_{\nu,J'} | D(R) | u_{E,J} \rangle|^2$ coincides with the unit of the term $e^2 a_0^2 / E_h$ because the continuum wave function is energy normalized. The PA rate coefficient is evaluated for a laser intensity of 1 W/cm^2 and for a collisional

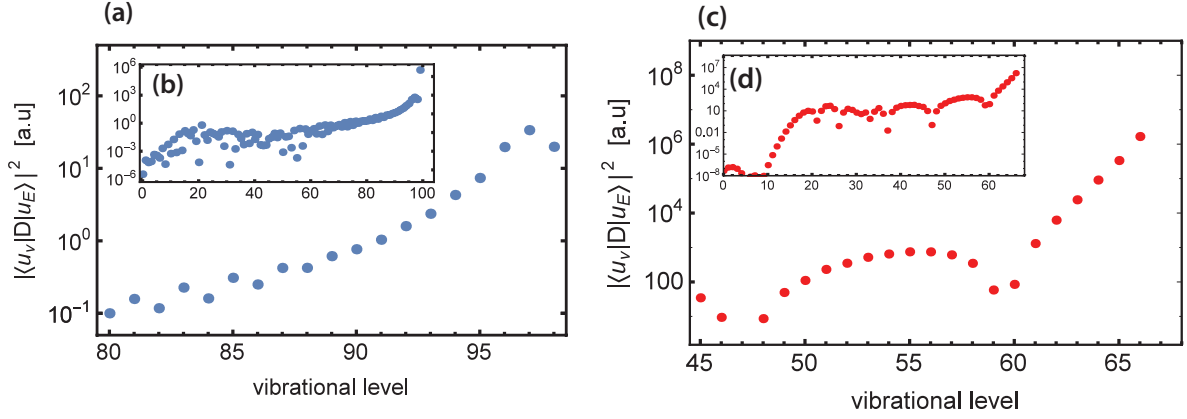


Figure 7.6.: Transition dipole matrix element as function of the vibrational level ν . Shown are the values for singlet (a) and triplet (c) transitions to a selected range of bound states. The insets show the full range of vibrational states for the respective transition. A temperature of 1 mK is assumed for the atomic ensemble.

energy corresponding to an ensemble temperature of 1 mK. The calculated values are given in standard units of cm^3/s and are summarized in Table 7.2 for transitions to states of the $\{3^1\Sigma_u^+, 3^3\Sigma_g^+\}$ potentials. The corresponding values for the $\{A^1\Sigma_u^+, 1^3\Sigma_g^+\}$ potentials are provided in Table 7.3. For the $2S-3P$ potentials, these values confirm the previous observation that the singlet transitions are much weaker than the triplet transitions. Furthermore, this calculation allows us to quantitatively compare the association rates to potentials correlated to the $2S-3P$ asymptote with the rates to the well investigated states of the $2S-2P$ potential. Considering only states with binding energies exceeding 10 GHz, one finds a reduction on the order of 10^3 in the transition rate for the weakly bound states.

PA transition rate The actual photoassociation rate per volume element is found by multiplying the rate coefficient with the squared number density n of the atomic cloud, therefore $R_{\text{PA}} = n^2 K_{\text{PA}}$ (Côté and Dalgarno, 1998). This quantity is calculated with experimental parameters for the atomic density of $1 \times 10^{10} \text{ cm}^{-3}$ and an average laser intensity of 7.5 W/cm for the PA probe beam.¹ For the transition to the $\nu = 64$ state of the $3^3\Sigma_g^+$ potential, according to Table 7.2 the strongest transition within the considered frequency range, an association rate of $2.8 \times 10^8 \text{ cm}^{-3}/\text{s}$ is found. Off-resonant atomic excitations are evaluated using Eq. (4.1) for the photon scattering rate at a detuning of 45 GHz. Furthermore, the atoms are assumed to be evenly distributed among all hyperfine states of the ground-state manifold, as described

¹For the density of the CMOT in Chapter 4, a density of $6.4 \times 10^{-10} \text{ cm}^{-3}$ is stated. However, different parameters for the CMOT were used for the PA measurement, in order to obtain a sufficiently long lifetime of the atomic sample. The value stated here is an estimate.

in Section 3.5 on absorption imaging. With the same experimental parameters used for the PA rate, an off-resonant atomic excitation rate of $5 \times 10^8 \text{ cm}^{-3}/\text{s}$ is found.

Based on the radius of the PA probe beam and the overlap with the 532-nm ionization beam, the addressed volume is estimated to be on the order of $3 \times 10^{-4} \text{ cm}^3$ and leads to a calculated molecule formation rate of $84\,000 \text{ s}^{-1}$, which has to be compared with the off-resonant excitation rate of $150\,000 \text{ s}^{-1}$. It is to note here, that for these values the duty cycle of 30 % of the PA probe light was not taken into account (Section 6.2.2). Additional factors that reduce the production and detection rate of ions that result from this process are the ionization probability ($\sim 5\%$, Section 6.2.1) and the finite collection and detection efficiencies of the CEM. However, these considerations similarly apply to both the atomic and molecular signal.

Relation to experimental observations Based on this calculation, the molecular excitation rate is estimated to be smaller than the off-resonant atomic excitation rate. This does not exclude the observation of the molecular transition with the considered experimental parameters but would require a substantially increased signal-to-noise ratio for the off-resonant excitations, as compared to the one achieved in the measurement presented in Section 6.4. However, considering all experimental measures that were required to suppress background counts, which do compromise the density in the MOT, it seems more appropriate to change the experimental approach. Specifically, this suggests to perform this measurement in an optical dipole trap in order to benefit from the different scaling of the molecular ($\propto n^2$) and the atomic ($\propto n$) excitation rates with the atomic density n . In an ODT these densities are on the order of 10^{13} cm^{-3} , as it was discussed in Section 5.2.2.

While many experimental factors, such as imperfect overlap of UV probe beam and ionization beam for example, can reduce the effective ion production rate, the obtained values in the previous paragraph suggest a rather low overall detection efficiency. Considering an experimentally observed count rate of about 20 s^{-1} compared with the calculated off-resonant excitation rate results in a detection efficiency of $\sim 1\%$. However, this value can only be regarded as a rough estimate of the detection efficiency.

$3^1\Sigma_u^+$			$3^3\Sigma_g^+$		
ν	E_B	K_{PA}	ν	E_B	K_{PA}
	[GHz]	[cm ³ /s]		[GHz]	[cm ³ /s]
88	-8846.3	1.1 [-17]	55	-4520.0	3.2 [-15]
89	-7579.6	1.5 [-17]	56	-3643.3	3.1 [-15]
90	-6336.4	1.9 [-17]	57	-2850.8	2.6 [-15]
91	-5124.1	2.6 [-17]	58	-2154.1	1.5 [-15]
92	-3955.0	4.0 [-17]	59	-1552.1	2.5 [-16]
93	-2852.7	5.9 [-17]	60	-1050.0	3.6 [-16]
94	-1851.2	1.1 [-16]	61	-646.0	5.5 [-15]
95	-983.6	1.8 [-16]	62	-345.4	2.6 [-14]
96	-335.1	4.9 [-16]	63	-147.3	1.0 [-13]
97	-69.5	8.4 [-16]	64	-44.3	3.8 [-13]
98	-8.7	5.1 [-16]	65	-7.03	1.4 [-12]
99	-0.2	8.0 [-13]	66	-0.2	8.5 [-12]

Table 7.2.: Photoassociation rate coefficient and binding energy for target vibrational state ν of $3^1\Sigma_u^+/3^3\Sigma_g^+$ potentials (2S-3P). The rate coefficients are calculated for an optical intensity of 1 W/cm² and an ensemble temperature of 1 mK. Uncertainties in the binding energies are dominated by the accuracy of the *ab initio* potentials and are not estimated here. States with detunings less than 10 GHz are excluded and are shown grayed out (see text). Numbers in brackets represent powers of ten.

$A^1\Sigma_u^+$			$1^3\Sigma_g^+$		
ν	E_B	K_{PA}	ν	E_B	K_{PA}
	[GHz]	[cm ³ /s]		[GHz]	[cm ³ /s]
78	-273.9	3.4 [-13]	70	-286.1	1.0 [-10]
79	-223.7	6.4 [-13]	71	-234.2	1.2 [-10]
80	-181.3	1.1 [-12]	72	-190	1.3 [-10]
81	-145.6	1.8 [-12]	73	-153	1.5 [-10]
82	-115.8	2.9 [-12]	74	-122.0	1.6 [-10]
83	-91.1	4.5 [-12]	75	-96.2	1.8 [-10]
84	-70.7	6.9 [-12]	76	-74.9	2.1 [-10]
85	-54.1	1.1 [-11]	77	-57.4	2.3 [-10]
86	-40.7	1.6 [-11]	78	-43.2	2.6 [-10]
87	-29.9	2.5 [-11]	79	-31.8	3.0 [-10]
88	-21.5	3.9 [-11]	80	-22.8	3.4 [-10]
...	...	...	...	...	...

Table 7.3.: Corresponding PA rate coefficients and binding energies (Abraham et al., 1995b) for target vibrational states of $A^1\Sigma_u^+/1^3\Sigma_g^+$ potentials (2S-2P). Only states with binding energies exceeding 20 GHz are shown. Numbers in brackets represent powers of ten.

7.5. Summary and outlook

In summary, photoassociation rates to states of the $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$ potentials of $^6\text{Li}_2$ were calculated. For this, the radial Schrödinger equation was numerically solved in order to determine the radial wave functions of the continuum and molecular bound states of the respective internuclear potentials. For PA transitions to states correlated to the $2S$ - $2P$ asymptote, accurate expressions for the potential energy curves are available that are based on experimental observations. However, the employed potentials for the $2S$ - $3P$ asymptote are based on *ab initio* calculations. Therefore, the derived quantities for states of the $2S$ - $3P$ asymptote should be regarded as an estimate only, in particular the values for the binding energies.

However, the calculation shows that PA transitions to states correlated to the $2S$ - $3P$ asymptote are difficult to observe in a magneto-optical trap. This is because attainable densities in lithium MOTs are comparatively low, and because an involved experimental sequence is required to suppress background ionization channels. In order to observe these weak PA transitions, the measurement could be performed in an optical dipole trap to benefit from an improved ratio of PA transitions to off-resonant atomic excitations. In addition to an enhanced atomic density, it is possible to tune the shape of the ground-state scattering wave function by applying a magnetic field to access a Feshbach resonance. This can greatly alter the PA association rate because of the changed overlap integral and was discussed in several articles (Courteille et al., 1998; Gacesa and Côté, 2014; Junker et al., 2008; Krzyzewski et al., 2015; Partridge et al., 2005; Pellegrini et al., 2008; Semczuk et al., 2013).

8. Conclusion and outlook

In this thesis we have described our apparatus and refined experimental scheme for the production of a fermionic lithium quantum gas. In Chapter 4 we have investigated laser cooling on the $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition, which was first demonstrated by [Duarte et al. \(2011\)](#), and have obtained an atomic cloud with a phase-space density of up to 3×10^{-4} at a temperature of $\sim 50 \mu\text{K}$. To obtain an unrestricted optical access to the atomic cloud, we move the atoms into a small glass cell that is attached to the main vacuum chamber. Generally, the optical transport of atoms is realized by loading the atoms into a tightly focused single ODT beam to provide a sufficient axial confinement. In most of these experimental schemes the ODT is optimized for the transport itself such that multiple optical traps are required during the experimental sequence. Here we have demonstrated a simple modification of this method by using a small-angle crossed ODT for a long-distance transport. This allows us, as described in Chapter 5, to use the same trapping confinement for loading, transport and for evaporative cooling to quantum degenerate temperatures.

The modular design of the experimental setup offers an inherent flexibility and a platform to investigate the strongly interacting Fermi gas. The excellent optical access allows the study of the quantum gas in reduced dimensions. Of particular interest is the interacting two-dimensional system, related to high-temperature superconductivity ([Lee et al., 2006](#)). Recently the quasi-2D BEC-BCS crossover was experimentally realized by [Ries et al. \(2015\)](#) and the corresponding thermodynamic equation of state was investigated [Boettcher et al. \(2016\)](#).

We have attempted to experimentally investigate photoassociation transitions to weakly bound states of the $2S$ - $3P$ asymptote, which have not been observed so far. For this, an ion detection system was installed and the experimental scheme was verified on the atomic $2^2S_{1/2} \rightarrow 3^2P_{3/2}$ transition, as described in Chapter 6. However, within the scope of this

work no spectroscopic features were observed, which we attribute to the weak free-bound transition strength to these states. This is supported by a calculation of the transition rates based on *ab initio* potential energy curves and was presented in Chapter 7. The results of this study suggest that in order to detect such excitations of molecular states below the $2S\text{-}3P$ asymptote, the experiment should be performed in an optical dipole trap due to the higher atomic density. This approach additionally offers the possibility to enhance the transition rate by tuning the *s*-wave scattering length near a Feshbach resonance. This alters the shape of the ground-state scattering wave function and can significantly enhance the photoassociation transition strength (Courteille et al., 1998; Gacesa and Côté, 2014; Semczuk et al., 2013).

Bibliography

- E. R. I. Abraham, W. I. McAlexander, C. A. Sackett, and Randall G. Hulet. Spectroscopic determination of the s -wave scattering length of lithium. *Phys. Rev. Lett.*, 74(8):1315–1318, February 1995a. doi:[10.1103/PhysRevLett.74.1315](https://doi.org/10.1103/PhysRevLett.74.1315).
- E. R. I. Abraham, N. W. M. Ritchie, W. I. McAlexander, and R. G. Hulet. Photoassociative spectroscopy of long-range states of ultracold ${}^6\text{Li}_2$ and ${}^7\text{Li}_2$. *J. Chem. Phys.*, 103(18):7773–7778, November 1995b. doi:[10.1063/1.470296](https://doi.org/10.1063/1.470296).
- E. R. I. Abraham, W. I. McAlexander, J. M. Gerton, R. G. Hulet, R. Côté, and A. Dalgarno. Singlet s -wave scattering lengths of ${}^6\text{Li}$ and ${}^7\text{Li}$. *Phys. Rev. A*, 53(6):R3713–R3715, June 1996. doi:[10.1103/PhysRevA.53.R3713](https://doi.org/10.1103/PhysRevA.53.R3713).
- E. R. I. Abraham, W. I. McAlexander, J. M. Gerton, R. G. Hulet, R. Côté, and A. Dalgarno. Triplet s -wave resonance in ${}^6\text{Li}$ collisions and scattering lengths of ${}^6\text{Li}$ and ${}^7\text{Li}$. *Phys. Rev. A*, 55(5):R3299–R3302, May 1997. doi:[10.1103/PhysRevA.55.R3299](https://doi.org/10.1103/PhysRevA.55.R3299).
- C. B. Alcock, V. P. Itkin, and M. K. Horrigan. Vapour pressure equations for the metallic elements: 2982500 K. *Can. Metall. Q.*, 23(3):309, 1984.
- M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell. Observation of Bose-Einstein condensation in a dilute atomic vapor. *Science*, 269(5221):198–201, 1995. ISSN 0036-8075. doi:[10.1126/science.269.5221.198](https://doi.org/10.1126/science.269.5221.198).
- P. W. Anderson. Ten years of superconductivity: 1980/1990, chapter The Resonating Valence Bond State in La_2CuO_4 and Superconductivity, pages 278–280. Springer Netherlands, Dordrecht, 1993. ISBN 978-94-011-1622-0. doi:[10.1007/978-94-011-1622-0_35](https://doi.org/10.1007/978-94-011-1622-0_35).
- E. Arimondo, M. Inguscio, and P. Violino. Experimental determinations of the hyperfine structure in the alkali atoms. *Rev. Mod. Phys.*, 49(1):31–75, January 1977. doi:[10.1103/RevModPhys.49.31](https://doi.org/10.1103/RevModPhys.49.31).
- Vanderlei Bagnato, David E. Pritchard, and Daniel Kleppner. Bose-Einstein condensation in an external potential. *Phys. Rev. A*, 35:4354–4358, May 1987. doi:[10.1103/PhysRevA.35.4354](https://doi.org/10.1103/PhysRevA.35.4354).
- Waseem S. Bakr, Jonathon I. Gillen, Amy Peng, Simon Fölling, and Markus Greiner. A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice. *Nature*, 462(7269):74–77, November 2009. ISSN 0028-0836. doi:[10.1038/nature08482](https://doi.org/10.1038/nature08482).
- B. Barakat, R. Bacis, F. Carrot, S. Churassy, P. Crozet, F. Martin, and J. Verges. Extensive analysis of the $X^1\Sigma_g^+$ ground state of ${}^7\text{Li}_2$ by laser-induced fluorescence Fourier transform spectrometry. *Chem. Phys.*, 102(12):215–227, February 1986. ISSN 0301-0104. doi:[10.1016/0301-0104\(86\)85133-3](https://doi.org/10.1016/0301-0104(86)85133-3).
- J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of superconductivity. *Phys. Rev.*, 108:1175–1204, Dec 1957. doi:[10.1103/PhysRev.108.1175](https://doi.org/10.1103/PhysRev.108.1175).

- M. D. Barrett, J. A. Sauer, and M. S. Chapman. All-optical formation of an atomic Bose-Einstein condensate. *Phys. Rev. Lett.*, 87:010404, Jun 2001. doi:[10.1103/PhysRevLett.87.010404](https://doi.org/10.1103/PhysRevLett.87.010404).
- Thomas E. Barrett, Samuel W. Dapore-Schwartz, Mark D. Ray, and Gregory P. Lafyatis. Slowing atoms with σ^- polarized light. *Phys. Rev. Lett.*, 67:3483–3486, Dec 1991. doi:[10.1103/PhysRevLett.67.3483](https://doi.org/10.1103/PhysRevLett.67.3483).
- M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. Hecker Denschlag, and R. Grimm. Crossover from a molecular Bose-Einstein condensate to a degenerate Fermi gas. *Phys. Rev. Lett.*, 92:120401, Mar 2004. doi:[10.1103/PhysRevLett.92.120401](https://doi.org/10.1103/PhysRevLett.92.120401).
- Hans A. Bethe and Edwin E. Salpeter. Quantum mechanics of one- and two-electron atoms. Dover Publications, 2008. doi:[10.1007/978-1-4613-4104-8](https://doi.org/10.1007/978-1-4613-4104-8).
- G. C. Bjorklund, M. D. Levenson, W. Lenth, and C. Ortiz. Frequency modulation (FM) spectroscopy. *Appl. Phys. B*, 32(3):145–152, 1983. ISSN 1432-0649. doi:[10.1007/BF00688820](https://doi.org/10.1007/BF00688820).
- Eric D. Black. An introduction to Pound-Drever-Hall laser frequency stabilization. *Am. J. Phys.*, 69:79, 2001. doi:[10.1119/1.1286663](https://doi.org/10.1119/1.1286663).
- Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, 80(3):885–964, July 2008. doi:[10.1103/RevModPhys.80.885](https://doi.org/10.1103/RevModPhys.80.885).
- I. Boettcher, L. Bayha, D. Kedar, P. A. Murthy, M. Neidig, M. G. Ries, A. N. Wenz, G. Zürn, S. Jochim, and T. Enss. Equation of state of ultracold fermions in the 2D BEC-BCS crossover region. *Phys. Rev. Lett.*, 116:045303, Jan 2016. doi:[10.1103/PhysRevLett.116.045303](https://doi.org/10.1103/PhysRevLett.116.045303).
- D. Boiron, A. Michaud, P. Lemonde, Y. Castin, C. Salomon, S. Weyers, K. Szymaniec, L. Cognet, and A. Clairon. Laser cooling of cesium atoms in gray optical molasses down to 1.1 μK . *Phys. Rev. A*, 53(6):R3734–R3737, June 1996. doi:[10.1103/PhysRevA.53.R3734](https://doi.org/10.1103/PhysRevA.53.R3734).
- Nadia Bouloufa, Anne Crubellier, and Olivier Dulieu. Photoassociative molecular spectroscopy for atomic radiative lifetimes. *Phys. Scr.*, 2009(T134):014014, 2009. doi:[10.1088/0031-8949/2009/T134/014014](https://doi.org/10.1088/0031-8949/2009/T134/014014).
- T. Bourdel, J. Cubizolles, L. Khaykovich, K. M. F. Magalhães, S. J. J. M. F. Kokkelmans, G. V. Shlyapnikov, and C. Salomon. Measurement of the interaction energy near a Feshbach resonance in a ^6Li Fermi gas. *Phys. Rev. Lett.*, 91:020402, Jul 2003. doi:[10.1103/PhysRevLett.91.020402](https://doi.org/10.1103/PhysRevLett.91.020402).
- T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. J. J. M. F. Kokkelmans, and C. Salomon. Experimental study of the BEC-BCS crossover region in lithium 6. *Phys. Rev. Lett.*, 93(5):050401–, July 2004. doi:[10.1103/PhysRevLett.93.050401](https://doi.org/10.1103/PhysRevLett.93.050401).
- M. John Brown and Alan Carrington. Rotational spectroscopy of diatomic molecules. Cambridge University Press, 2003.
- A. Burchianti, G. Valtolina, J. A. Seman, E. Pace, M. De Pas, M. Inguscio, M. Zaccanti, and G. Roati. Efficient all-optical production of large ^6Li quantum gases using D_1 gray-molasses cooling. *Phys. Rev. A*, 90:043408, Oct 2014. doi:[10.1103/PhysRevA.90.043408](https://doi.org/10.1103/PhysRevA.90.043408).
- Philip George Burke. R-Matrix theory of atomic collisions. Springer, 2011. doi:[10.1007/978-3-642-15931-2](https://doi.org/10.1007/978-3-642-15931-2).

- D. A. Butts and D. S. Rokhsar. Trapped Fermi gases. *Phys. Rev. A*, 55(6):4346–4350, June 1997. doi:[10.1103/PhysRevA.55.4346](https://doi.org/10.1103/PhysRevA.55.4346).
- J. Carlson, Stefano Gandolfi, Kevin E. Schmidt, and Shiwei Zhang. Auxiliary-field quantum Monte Carlo method for strongly paired fermions. *Phys. Rev. A*, 84:061602, Dec 2011. doi:[10.1103/PhysRevA.84.061602](https://doi.org/10.1103/PhysRevA.84.061602).
- Y. Castin and R. Dum. Bose-Einstein condensates in time dependent traps. *Phys. Rev. Lett.*, 77:5315–5319, Dec 1996. doi:[10.1103/PhysRevLett.77.5315](https://doi.org/10.1103/PhysRevLett.77.5315).
- T. Chanelière, L. He, R. Kaiser, and D. Wilkowski. Three dimensional cooling and trapping with a narrow line. *Eur. Phys. J. D*, 46:507–515, 2008. doi:[10.1140/epjd/e2007-00329-8](https://doi.org/10.1140/epjd/e2007-00329-8).
- L. W. Cheuk, M. A. Nichols, K.R. Lawrence, M. Okan, H. Zhang, E. Khatami, N. Trivedi, T. Paiva, M. Rigol, and M. W. Zwierlein. Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model. arXiv:1606.04089, 2016.
- Ananth P. Chikkatur. Colliding and moving Bose-Einstein condensates: Studies of superfluidity and optical tweezers for condensate transport. PhD thesis, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, 2002.
- Cheng Chin and Rudolf Grimm. Thermal equilibrium and efficient evaporation of an ultracold atom-molecule mixture. *Phys. Rev. A*, 69(3):033612–, March 2004. doi:[10.1103/PhysRevA.69.033612](https://doi.org/10.1103/PhysRevA.69.033612).
- Cheng Chin, Rudolf Grimm, Paul Julienne, and Eite Tiesinga. Feshbach resonances in ultracold gases. *Rev. Mod. Phys.*, 82:1225–1286, Apr 2010. doi:[10.1103/RevModPhys.82.1225](https://doi.org/10.1103/RevModPhys.82.1225).
- M. L. Chiofalo, S. J. J. M. F. Kokkelmans, J. N. Milstein, and M. J. Holland. Signatures of resonance superfluidity in a quantum Fermi gas. *Phys. Rev. Lett.*, 88:090402, Feb 2002. doi:[10.1103/PhysRevLett.88.090402](https://doi.org/10.1103/PhysRevLett.88.090402).
- Steven Chu, L. Hollberg, J. E. Bjorkholm, Alex Cable, and A. Ashkin. Three-dimensional viscous confinement and cooling of atoms by resonance radiation pressure. *Phys. Rev. Lett.*, 55(1):48–51, July 1985. doi:[10.1103/PhysRevLett.55.48](https://doi.org/10.1103/PhysRevLett.55.48).
- C. Cohen-Tannoudji and D. Guéry-Odelin. Advances in atomic physics. World Scientific, 2011.
- Louis Costa. An interacting Fermi-Fermi mixture at the crossover of a narrow Feshbach resonance. PhD thesis, Ludwig-Maximilians-Universität München, 2011.
- Joseph Noël Robin Côté. Ultra-cold collisions of identical atoms. PhD thesis, Massachusetts Institute of Technology, 1995.
- R. Côté and A. Dalgarno. Photoassociation intensities and radiative trap loss in lithium. *Phys. Rev. A*, 58:498–508, Jul 1998. doi:[10.1103/PhysRevA.58.498](https://doi.org/10.1103/PhysRevA.58.498).
- R. Côté, A. Dalgarno, and M. J. Jamieson. Elastic scattering of two ^7Li atoms. *Phys. Rev. A*, 50:399–404, Jul 1994. doi:[10.1103/PhysRevA.50.399](https://doi.org/10.1103/PhysRevA.50.399).
- Ph. Courteille, R. S. Freeland, D. J. Heinzen, F. A. van Abeelen, and B. J. Verhaar. Observation of a Feshbach resonance in cold atom scattering. *Phys. Rev. Lett.*, 81:69–72, Jul 1998. doi:[10.1103/PhysRevLett.81.69](https://doi.org/10.1103/PhysRevLett.81.69).

- A. Couvert, T. Kawalec, G. Reinaudi, and D. Guéry-Odelin. Optimal transport of ultracold atoms in the non-adiabatic regime. *EPL (Europhysics Letters)*, 83(1):13001, 2008. doi:[10.1209/0295-5075/83/13001](https://doi.org/10.1209/0295-5075/83/13001).
- J. Cubizolles, T. Bourdel, S. J. J. M. F. Kokkelmans, G. V. Shlyapnikov, and C. Salomon. Production of long-lived ultracold Li_2 molecules from a Fermi gas. *Phys. Rev. Lett.*, 91:240401, Dec 2003. doi:[10.1103/PhysRevLett.91.240401](https://doi.org/10.1103/PhysRevLett.91.240401).
- J. Dalibard and C. Cohen-Tannoudji. Laser cooling below the Doppler limit by polarization gradients: simple theoretical models. *Journal of the Optical Society of America B*, 6:2023–2045, 1989. doi:[10.1364/JOSAB.6.002023](https://doi.org/10.1364/JOSAB.6.002023).
- Nikesh S. Dattani. Analytic potentials and vibrational energies for Li_2 states dissociating to $\text{Li}(2S) + \text{Li}(3P)$. part 1: The $2^{S+1}\Pi_{u/g}$ states. arXiv:1509.07041, September 2015.
- Nikesh S. Dattani and Robert J. LeRoy. A DPF data analysis yields accurate analytic potentials for $\text{Li}_2(A^1\Sigma_u^+)$ and $\text{Li}_2(1^3\Sigma_g^+)$ that incorporate 3-state mixing near the $\text{Li}_2(1^3\Sigma_g^+)$ state asymptote. *J. Mol. Spectrosc.*, 268:199 – 210, 2011. ISSN 0022-2852. doi:[10.1016/j.jms.2011.03.030](https://doi.org/10.1016/j.jms.2011.03.030).
- J. Deiglmayr, A. Grochola, M. Repp, K. Mörtlbauer, C. Glück, J. Lange, O. Dulieu, R. Wester, and M. Weidemüller. Formation of ultracold polar molecules in the rovibrational ground state. *Phys. Rev. Lett.*, 101:133004, Sep 2008. doi:[10.1103/PhysRevLett.101.133004](https://doi.org/10.1103/PhysRevLett.101.133004).
- B. DeMarco and D. S. Jin. Onset of Fermi degeneracy in a trapped atomic gas. *Science*, 285(5434):1703–1706, 1999. doi:[10.1126/science.285.5434.1703](https://doi.org/10.1126/science.285.5434.1703).
- Marshall T DePue, S Lukman Winoto, D.J Han, and David S Weiss. Transient compression of a MOT and high intensity fluorescent imaging of optically thick clouds of atoms. *Opt. Commun.*, 180(1-3):73 – 79, 2000. ISSN 0030-4018. doi:[10.1016/S0030-4018\(00\)00701-X](https://doi.org/10.1016/S0030-4018(00)00701-X).
- B. J. DeSalvo, M. Yan, P. G. Mickelson, Y. N. Martinez de Escobar, and T. C. Killian. Degenerate Fermi gas of ^{87}Sr . *Phys. Rev. Lett.*, 105:030402, Jul 2010. doi:[10.1103/PhysRevLett.105.030402](https://doi.org/10.1103/PhysRevLett.105.030402).
- K. Dieckmann, C. A. Stan, S. Gupta, Z. Hadzibabic, C. H. Schunck, and W. Ketterle. Decay of an ultracold fermionic lithium gas near a Feshbach resonance. *Phys. Rev. Lett.*, 89:203201, Oct 2002. doi:[10.1103/PhysRevLett.89.203201](https://doi.org/10.1103/PhysRevLett.89.203201).
- Kai Dieckmann. Bose-Einstein condensation with high atom number in a deep magnetic trap. PhD thesis, Universiteit van Amsterdam, 2001.
- R.W.P. Drever, J.L. Hall, F.V. Kowalski, J. Hough, G.M. Ford, A.J. Munley, and H. Ward. Laser phase and frequency stabilization using an optical resonator. *Appl. Phys. B*, 31(2):97–105–, 1983. ISSN 0946-2171. doi:[10.1007/BF00702605](https://doi.org/10.1007/BF00702605).
- P. M. Duarte, R. A. Hart, J. M. Hitchcock, T. A. Corcovilos, T.-L. Yang, A. Reed, and R. G. Hulet. All-optical production of a lithium quantum gas using narrow-line laser cooling. *Phys. Rev. A*, 84(6):061406–, December 2011. doi:[10.1103/PhysRevA.84.061406](https://doi.org/10.1103/PhysRevA.84.061406).
- R. A. Duine and H.T.C. Stoof. Atom-molecule coherence in Bose gases. *Phys. Rep.*, 396(3):115 – 195, 2004. ISSN 0370-1573. doi:[10.1016/j.physrep.2004.03.003](https://doi.org/10.1016/j.physrep.2004.03.003).
- K. Enomoto, K. Kasa, M. Kitagawa, and Y. Takahashi. Optical Feshbach resonance using the intercombination transition. *Phys. Rev. Lett.*, 101:203201, Nov 2008. doi:[10.1103/PhysRevLett.101.203201](https://doi.org/10.1103/PhysRevLett.101.203201).

- Tilman Esslinger. Fermi-Hubbard physics with atoms in an optical lattice. *Annu. Rev. Condens. Matter Phys.*, 1(1):129–152, July 2010. ISSN 1947-5454. doi:[10.1146/annurev-conmatphys-070909-104059](https://doi.org/10.1146/annurev-conmatphys-070909-104059).
- D. Rio Fernandes, F. Sievers, N. Kretzschmar, S. Wu, C. Salomon, and F. Chevy. Sub-Doppler laser cooling of fermionic ^{40}K atoms in three-dimensional gray optical molasses. *EPL (Europhysics Letters)*, 100(6):63001, 2012. doi:[10.1209/0295-5075/100/63001](https://doi.org/10.1209/0295-5075/100/63001).
- Christopher J. Foot. Atomic physics. Oxford University Press, 2005.
- C. Fort, A. Bambini, L. Cacciapuoti, F.S. Cataliotti, M. Prevedelli, G.M. Tino, and M. Inguscio. Cooling mechanisms in potassium magneto-optical traps. *The European Physical Journal D - Atomic, Molecular, Optical and Plasma Physics*, 3(2):113–118, 1998. ISSN 1434-6079. doi:[10.1007/s100530050154](https://doi.org/10.1007/s100530050154).
- B. Fröhlich, T. Lahaye, B. Kaltenhäuser, H. Kübler, S. Müller, T. Koch, M. Fattori, and T. Pfau. Two-frequency acousto-optic modulator driver to improve the beam pointing stability during intensity ramps. *Rev. Sci. Instrum.*, 78(4):043101, 2007. doi:[10.1063/1.2720725](https://doi.org/10.1063/1.2720725).
- Takeshi Fukuhara, Yosuke Takasu, Mitsutaka Kumakura, and Yoshiro Takahashi. Degenerate Fermi gases of ytterbium. *Phys. Rev. Lett.*, 98:030401, Jan 2007. doi:[10.1103/PhysRevLett.98.030401](https://doi.org/10.1103/PhysRevLett.98.030401).
- F. Fuso, D. Ciampini, E. Arimondo, and C. Gabbanini. Ion processes in the photoionization of laser cooled alkali atoms. *Opt. Commun.*, 173:223 – 232, 2000. ISSN 0030-4018. doi:[10.1016/S0030-4018\(99\)00609-4](https://doi.org/10.1016/S0030-4018(99)00609-4).
- Marko Gacesa and Robin Côté. Photoassociation of ultracold molecules near a Feshbach resonance as a probe of the electron-proton mass ratio variation. *J. Mol. Spectrosc.*, 300: 124–130, June 2014. ISSN 0022-2852. doi:[10.1016/j.jms.2014.03.005](https://doi.org/10.1016/j.jms.2014.03.005).
- M. E. Gehm, K. M. O’Hara, T. A. Savard, and J. E. Thomas. Dynamics of noise-induced heating in atom traps. *Phys. Rev. A*, 58(5):3914–3921, November 1998. doi:[10.1103/PhysRevA.58.3914](https://doi.org/10.1103/PhysRevA.58.3914).
- Michael Eric Gehm. Preparation of an optically-trapped degenerate Fermi gas of ^6Li : Finding the route to degeneracy. PhD thesis, Duke University, 2003.
- Stefano Giorgini, Lev P. Pitaevskii, and Sandro Stringari. Theory of ultracold atomic Fermi gases. *Rev. Mod. Phys.*, 80:1215–1274, Oct 2008. doi:[10.1103/RevModPhys.80.1215](https://doi.org/10.1103/RevModPhys.80.1215).
- Vandna Gokhroo, G Rajalakshmi, R Kollengode Easwaran, and C S Unnikrishnan. Sub-Doppler deep-cooled bosonic and fermionic isotopes of potassium in a compact 2D⁺-3D MOT set-up. *J. Phys. B: At., Mol. Opt. Phys.*, 44(11):115307, 2011. doi:[10.1088/0953-4075/44/11/115307](https://doi.org/10.1088/0953-4075/44/11/115307).
- Daniel Greif, Thomas Uehlinger, Gregor Jotzu, Leticia Tarruell, and Tilman Esslinger. Short-range quantum magnetism of ultracold fermions in an optical lattice. *Science*, 340(6138): 1307–1310, 2013. ISSN 0036-8075. doi:[10.1126/science.1236362](https://doi.org/10.1126/science.1236362).
- Daniel Greif, Gregor Jotzu, Michael Messer, Rémi Desbuquois, and Tilman Esslinger. Formation and dynamics of antiferromagnetic correlations in tunable optical lattices. *Phys. Rev. Lett.*, 115:260401, Dec 2015. doi:[10.1103/PhysRevLett.115.260401](https://doi.org/10.1103/PhysRevLett.115.260401).

- Markus Greiner, Immanuel Bloch, Theodor W. Hänsch, and Tilman Esslinger. Magnetic transport of trapped cold atoms over a large distance. *Phys. Rev. A*, 63:031401, Feb 2001. doi:[10.1103/PhysRevA.63.031401](https://doi.org/10.1103/PhysRevA.63.031401).
- Markus Greiner, Cindy A. Regal, and Deborah S. Jin. Emergence of a molecular Bose-Einstein condensate from a Fermi gas. *Nature*, 426(6966):537–540, December 2003. ISSN 0028-0836. doi:[10.1038/nature02199](https://doi.org/10.1038/nature02199).
- G. F. Gribakin and V. V. Flambaum. Calculation of the scattering length in atomic collisions using the semiclassical approximation. *Phys. Rev. A*, 48:546–553, Jul 1993. doi:[10.1103/PhysRevA.48.546](https://doi.org/10.1103/PhysRevA.48.546).
- Andrew T. Grier, Igor Ferrier-Barbut, Benno S. Rem, Marion Delehaye, Lev Khaykovich, Frédéric Chevy, and Christophe Salomon. λ -enhanced sub-Doppler cooling of lithium atoms in D_1 gray molasses. *Phys. Rev. A*, 87(6):063411–, June 2013. doi:[10.1103/PhysRevA.87.063411](https://doi.org/10.1103/PhysRevA.87.063411).
- Rudolf Grimm, Matthias Weidemüller, and Yurii B. Ovchinnikov. Optical dipole traps for neutral atoms. *Adv. At., Mol., Opt. Phys.*, Volume 42:95–170, 2000. ISSN 1049-250X. doi:[10.1016/S1049-250X\(08\)60186-X](https://doi.org/10.1016/S1049-250X(08)60186-X).
- Ch. Gross, H. C. J. Gan, and K. Dieckmann. All-optical production and transport of a large ^6Li quantum gas in a crossed optical dipole trap. *Phys. Rev. A*, 93:053424, May 2016. doi:[10.1103/PhysRevA.93.053424](https://doi.org/10.1103/PhysRevA.93.053424).
- G. Grynberg and J.-Y. Courtois. Proposal for a magneto-optical lattice for trapping atoms in nearly-dark states. *EPL (Europhysics Letters)*, 27(1):41, 1994. doi:[10.1209/0295-5075/27/1/008](https://doi.org/10.1209/0295-5075/27/1/008).
- Will Gunton, Mariusz Semczuk, Nikesh S. Dattani, and Kirk W. Madison. High-resolution photoassociation spectroscopy of the $^6\text{Li}_2\text{A}(1^1\Sigma_u^+)$ state. *Phys. Rev. A*, 88:062510, Dec 2013a. doi:[10.1103/PhysRevA.88.062510](https://doi.org/10.1103/PhysRevA.88.062510).
- Will Gunton, Mariusz Semczuk, and Kirk W. Madison. Realization of BEC-BCS-crossover physics in a compact oven-loaded magneto-optic-trap apparatus. *Phys. Rev. A*, 88:023624, Aug 2013b. doi:[10.1103/PhysRevA.88.023624](https://doi.org/10.1103/PhysRevA.88.023624).
- T. L. Gustavson, A. P. Chikkatur, A. E. Leanhardt, A. Görlitz, S. Gupta, D. E. Pritchard, and W. Ketterle. Transport of Bose-Einstein condensates with optical tweezers. *Phys. Rev. Lett.*, 88(2):020401–, December 2001. doi:[10.1103/PhysRevLett.88.020401](https://doi.org/10.1103/PhysRevLett.88.020401).
- Z. Hadzibabic, S. Gupta, C. A. Stan, C. H. Schunck, M. W. Zwierlein, K. Dieckmann, and W. Ketterle. Fiftyfold improvement in the number of quantum degenerate fermionic atoms. *Phys. Rev. Lett.*, 91:160401, Oct 2003. doi:[10.1103/PhysRevLett.91.160401](https://doi.org/10.1103/PhysRevLett.91.160401).
- T. W. Hänsch and A.L. Schawlow. Cooling of gases by laser radiation. *Opt. Commun.*, 13(1):68–69, January 1975. ISSN 0030-4018. doi:[10.1016/0030-4018\(75\)90159-5](https://doi.org/10.1016/0030-4018(75)90159-5).
- John C. Hansen. Schroedinger.m: A mathematica package for solving the time-independent Schrödinger equation. Southwest State University, Marshall, MN 56258, 1996.
- Russell A. Hart, Pedro M. Duarte, Tsung-Lin Yang, Xinxing Liu, Thereza Paiva, Ehsan Khatami, Richard T. Scalettar, Nandini Trivedi, David A. Huse, and Randall G. Hulet. Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms. *Nature*, 519(7542):211–214, March 2015. ISSN 0028-0836. doi:[10.1038/nature14223](https://doi.org/10.1038/nature14223).

- Florian Alexander Henkel. Photoionisation detection of single ^{87}Rb -atoms using channel electron multipliers. PhD thesis, Ludwig MaximiliansUniversität, 2011.
- Gerhard Herzberg. Molecular spectra and molecular structure, volume I. Spectra of Diatomic Molecules. D. Van Nostrand Company Inc., 1950.
- Tin-Lun Ho. Universal thermodynamics of degenerate quantum gases in the unitarity limit. *Phys. Rev. Lett.*, 92:090402, Mar 2004. doi:[10.1103/PhysRevLett.92.090402](https://doi.org/10.1103/PhysRevLett.92.090402).
- M. Houbiers, H. T. C. Stoof, W. I. McAlexander, and R. G. Hulet. Elastic and inelastic collisions of ^6Li atoms in magnetic and optical traps. *Phys. Rev. A*, 57(3):R1497–R1500, March 1998. doi:[10.1103/PhysRevA.57.R1497](https://doi.org/10.1103/PhysRevA.57.R1497).
- Kerson Huang. Statistical mechanics. Wiley, 1987.
- J. H. Huckans, J. R. Williams, E. L. Hazlett, R. W. Stites, and K. M. O’Hara. Three-body recombination in a three-state Fermi gas with widely tunable interactions. *Phys. Rev. Lett.*, 102:165302, Apr 2009. doi:[10.1103/PhysRevLett.102.165302](https://doi.org/10.1103/PhysRevLett.102.165302).
- Keith Hulme. Private communication. Starna Scientific Ltd, 2014.
- R. C. Isler, S. Marcus, and R. Novick. Fine structure of the 3^2P and 4^2P states of lithium. *Phys. Rev.*, 187:66–75, Nov 1969. doi:[10.1103/PhysRev.187.66](https://doi.org/10.1103/PhysRev.187.66).
- P. Jasik and J.E. Sienkiewicz. Calculation of adiabatic potentials of Li_2 . *Chem. Phys.*, 323: 563 – 573, 2006. ISSN 0301-0104. doi:[10.1016/j.chemphys.2005.10.025](https://doi.org/10.1016/j.chemphys.2005.10.025).
- Patryk Jasik and Józef Sienkiewicz. Transition dipole moments of the lithium dimer. *At. Data Nucl. Data Tables*, 99(2):115–155, March 2013. ISSN 0092-640X. doi:[10.1016/j.adt.2011.06.003](https://doi.org/10.1016/j.adt.2011.06.003).
- Jasik, P., Wilczyński, J., and Sienkiewicz, J. E. Calculation of adiabatic potentials of Li_2^+ . *Eur. Phys. J. Special Topics*, 144:85–91, 2007. doi:[10.1140/epjst/e2007-00111-2](https://doi.org/10.1140/epjst/e2007-00111-2).
- S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, C. Chin, J. Hecker Denschlag, and R. Grimm. Pure gas of optically trapped molecules created from fermionic atoms. *Phys. Rev. Lett.*, 91:240402, Dec 2003a. doi:[10.1103/PhysRevLett.91.240402](https://doi.org/10.1103/PhysRevLett.91.240402).
- S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. Hecker Denschlag, and R. Grimm. Bose-Einstein condensation of molecules. *Science*, 302(5653):2101–2103, 2003b. doi:[10.1126/science.1093280](https://doi.org/10.1126/science.1093280).
- Walter R. Johnson. Atomic structure theory. Springer, 2007.
- Kevin M. Jones, Eite Tiesinga, Paul D. Lett, and Paul S. Julienne. Ultracold photoassociation spectroscopy: Long-range molecules and atomic scattering. *Rev. Mod. Phys.*, 78(2):483–535, May 2006. doi:[10.1103/RevModPhys.78.483](https://doi.org/10.1103/RevModPhys.78.483).
- Robert Jördens, Niels Strohmaier, Kenneth Gunter, Henning Moritz, and Tilman Esslinger. A Mott insulator of fermionic atoms in an optical lattice. *Nature*, 455(7210):204–207, September 2008. ISSN 0028-0836. doi:[10.1038/nature07244](https://doi.org/10.1038/nature07244).
- Paul S. Julienne and Jeremy M. Hutson. Contrasting the wide Feshbach resonances in ^6Li and ^7Li . *Phys. Rev. A*, 89:052715, May 2014. doi:[10.1103/PhysRevA.89.052715](https://doi.org/10.1103/PhysRevA.89.052715).

- M. Junker, D. Dries, C. Welford, J. Hitchcock, Y. P. Chen, and R. G. Hulet. Photoassociation of a Bose-Einstein condensate near a Feshbach resonance. *Phys. Rev. Lett.*, 101:060406, Aug 2008. doi:[10.1103/PhysRevLett.101.060406](https://doi.org/10.1103/PhysRevLett.101.060406).
- Yu. Kagan, E. L. Surkov, and G. V. Shlyapnikov. Evolution of a Bose-condensed gas under variations of the confining potential. *Phys. Rev. A*, 54:R1753–R1756, Sep 1996. doi:[10.1103/PhysRevA.54.R1753](https://doi.org/10.1103/PhysRevA.54.R1753).
- W. Ketterle and M. W. Zwierlein. Making, probing and understanding ultracold Fermi gases, January 2008.
- W. Ketterle, D. S. Durfee, and D. M. Stamper-Kurn. Making, probing and understanding Bose-Einstein condensates, 1999.
- Joseph Kinast, Andrey Turlapov, John E. Thomas, Qijin Chen, Jelena Stajic, and Kathryn Levin. Heat capacity of a strongly interacting Fermi gas. *Science*, 307(5713):1296–1299, 2005. doi:[10.1126/science.1109220](https://doi.org/10.1126/science.1109220).
- Thorsten Köhler, Krzysztof Góral, and Paul S. Julienne. Production of cold molecules via magnetically tunable Feshbach resonances. *Rev. Mod. Phys.*, 78:1311–1361, Dec 2006. doi:[10.1103/RevModPhys.78.1311](https://doi.org/10.1103/RevModPhys.78.1311).
- Daniel D. Konowalow and Mark L. Olson. The electronic structure and spectra of the $X^1\Sigma_g^+$ and $A^1\Sigma_u^+$ states of Li_2 . *The Journal of Chemical Physics*, 71(1):450–457, 1979. doi:[10.1063/1.438090](https://doi.org/10.1063/1.438090).
- Daniel D. Konowalow, Rebecca M. Regan, and Marcy E. Rosenkrantz. The “most likely” potential energy curve for the lowest $^3\Sigma^+$ state of Li_2 . *The Journal of Chemical Physics*, 81(10):4534–4536, 1984. doi:[10.1063/1.447424](https://doi.org/10.1063/1.447424).
- A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team. Nist atomic spectra database (version 5.3), [online]. National Institute of Standards and Technology, Gaithersburg, MD., June 2016. Available: <http://physics.nist.gov/asd>.
- S. P. Krzyzewski, T. G. Akin, J. Dizikes, Michael A. Morrison, and E. R. I. Abraham. Observation of deeply bound $^{85}\text{Rb}_2$ vibrational levels using Feshbach optimized photoassociation. *Phys. Rev. A*, 92:062714, Dec 2015. doi:[10.1103/PhysRevA.92.062714](https://doi.org/10.1103/PhysRevA.92.062714).
- Mark J. H. Ku, Ariel T. Sommer, Lawrence W. Cheuk, and Martin W. Zwierlein. Revealing the superfluid lambda transition in the universal thermodynamics of a unitary Fermi gas. *Science*, 335(6068):563–567, February 2012. doi:[10.1126/science.1214987](https://doi.org/10.1126/science.1214987).
- S. J. M. Kuppens, K. L. Corwin, K. W. Miller, T. E. Chupp, and C. E. Wieman. Loading an optical dipole trap. *Phys. Rev. A*, 62(1):013406–, June 2000. doi:[10.1103/PhysRevA.62.013406](https://doi.org/10.1103/PhysRevA.62.013406).
- Jayanti Lahiri and Steven T. Manson. Radiative recombination and excited-state photoionization of lithium. *Phys. Rev. A*, 48:3674–3679, Nov 1993. doi:[10.1103/PhysRevA.48.3674](https://doi.org/10.1103/PhysRevA.48.3674).
- L. D. Landau and E. M. Lifshitz. Quantum mechanics - and non-relativistic theory. Pergamon Press, 1977.
- Patrick A. Lee, Naoto Nagaosa, and Xiao-Gang Wen. Doping a Mott insulator: Physics of high-temperature superconductivity. *Rev. Mod. Phys.*, 78:17–85, Jan 2006. doi:[10.1103/RevModPhys.78.17](https://doi.org/10.1103/RevModPhys.78.17).

- Julian Léonard, Moonjoo Lee, Andrea Morales, Thomas M Karg, Tilman Esslinger, and Tobias Donner. Optical transport and manipulation of an ultracold atomic cloud using focus-tunable lenses. *New J. Phys.*, 16(9):093028, 2014. doi:[10.1088/1367-2630/16/9/093028](https://doi.org/10.1088/1367-2630/16/9/093028).
- Robert J. LeRoy and Richard B. Bernstein. Dissociation energy and long-range potential of diatomic molecules from vibrational spacings of higher levels. *The Journal of Chemical Physics*, 52(8):3869–3879, 1970. doi:[10.1063/1.1673585](https://doi.org/10.1063/1.1673585).
- Robert J. LeRoy, Nikesh S. Dattani, John A. Coxon, Amanda J. Ross, Patrick Crozet, and Colan Linton. Accurate analytic potentials for Li_2 ($X^1\Sigma_g^+$) and Li_2 ($A^1\Sigma_u^+$) from 2 to 90 Å, and the radiative lifetime of $\text{Li}(2p)$. *The Journal of Chemical Physics*, 131(20):204309, 2009. doi:[10.1063/1.3264688](https://doi.org/10.1063/1.3264688).
- P. D. Lett, W. D. Phillips, S. L. Rolston, C. E. Tanner, R. N. Watts, and C. I. Westbrook. Optical molasses. *J. Opt. Soc. Am. B*, 6(11):2084–2107, November 1989. doi:[10.1364/JOSAB.6.002084](https://doi.org/10.1364/JOSAB.6.002084).
- P. D. Lett, K. Helmerson, W. D. Phillips, L. P. Ratliff, S. L. Rolston, and M. E. Wagshul. Spectroscopy of Na_2 by photoassociation of laser-cooled Na. *Phys. Rev. Lett.*, 71:2200–2203, Oct 1993. doi:[10.1103/PhysRevLett.71.2200](https://doi.org/10.1103/PhysRevLett.71.2200).
- Paul D. Lett, Richard N. Watts, Christoph I. Westbrook, William D. Phillips, Phillip L. Gould, and Harold J. Metcalf. Observation of atoms laser cooled below the Doppler limit. *Phys. Rev. Lett.*, 61(2):169–172, July 1988. doi:[10.1103/PhysRevLett.61.169](https://doi.org/10.1103/PhysRevLett.61.169).
- H. J. Lewandowski, D. M. Harber, D. L. Whitaker, and E. A. Cornell. Simplified system for creating a Bose–Einstein condensate. *J. Low Temp. Phys.*, 132(5):309–367, 2003. ISSN 1573-7357. doi:[10.1023/A:1024800600621](https://doi.org/10.1023/A:1024800600621).
- Y.-J. Lin, A. R. Perry, R. L. Compton, I. B. Spielman, and J. V. Porto. Rapid production of ^{87}Rb Bose-Einstein condensates in a combined magnetic and optical potential. *Phys. Rev. A*, 79(6):063631–, June 2009. doi:[10.1103/PhysRevA.79.063631](https://doi.org/10.1103/PhysRevA.79.063631).
- Zhong Lin, Kazuko Shimizu, Mingsheng Zhan, Fujio Shimizu, and Hiroshi Takuma. Laser cooling and trapping of Li. *Japanese Journal of Applied Physics*, 30:1324–1326, 1991. doi:[10.1143/JJAP.30.L1324](https://doi.org/10.1143/JJAP.30.L1324).
- C. Linton, T. L. Murphy, F. Martin, R. Bacis, and J. Verges. Fourier transform spectroscopy of the $1^3\Sigma_g^+-a^3\Sigma_u^+$ transition of $^6\text{Li}_2$ molecule. *The Journal of Chemical Physics*, 91(10):6036–6041, 1989. doi:[10.1063/1.457421](https://doi.org/10.1063/1.457421).
- C. Linton, R. Bacis, P. Crozet, F. Martin, A.J. Ross, and J. Verges. Fourier transform spectroscopy of the $1^3\Delta_g-b^3\Pi_u$ transition in $^6\text{Li}_2$. *J. Mol. Spectrosc.*, 151(1):159–177, January 1992. ISSN 0022-2852. doi:[10.1016/0022-2852\(92\)90012-D](https://doi.org/10.1016/0022-2852(92)90012-D).
- C. Linton, F. Martin, I. Russier, A.J. Ross, P. Crozet, S. Churassy, and R. Bacis. Observation and analysis of the $A^1\Sigma_u^+$ state of $^6\text{Li}_2$ from $\nu = 0$ to the dissociation limit. *J. Mol. Spectrosc.*, 175(2):340–353, 1996. ISSN 0022-2852. doi:[10.1006/jmsp.1996.0039](https://doi.org/10.1006/jmsp.1996.0039).
- O. J. Luiten, M. W. Reynolds, and J. T. M. Walraven. Kinetic theory of the evaporative cooling of a trapped gas. *Phys. Rev. A*, 53:381–389, Jan 1996. doi:[10.1103/PhysRevA.53.381](https://doi.org/10.1103/PhysRevA.53.381).
- L. Luo, B. Clancy, J. Joseph, J. Kinast, A. Turlapov, and J. E. Thomas. Evaporative cooling of unitary Fermi gas mixtures in optical traps. *New J. Phys.*, 8(9):213, 2006. doi:[10.1088/1367-2630/8/9/213](https://doi.org/10.1088/1367-2630/8/9/213).

- Louis Marchildon. Quantum mechanics. Springer Berlin Heidelberg, 2002. doi:[10.1007/978-3-662-04750-7](https://doi.org/10.1007/978-3-662-04750-7).
- M. Marinescu and A. Dalgarno. Dispersion forces and long-range electronic transition dipole moments of alkali-metal dimer excited states. *Phys. Rev. A*, 52:311–328, Jul 1995. doi:[10.1103/PhysRevA.52.311](https://doi.org/10.1103/PhysRevA.52.311).
- M. Marinescu, H. R. Sadeghpour, and A. Dalgarno. Dispersion coefficients for alkali-metal dimers. *Phys. Rev. A*, 49:982–988, Feb 1994. doi:[10.1103/PhysRevA.49.982](https://doi.org/10.1103/PhysRevA.49.982).
- C. Clay Marston and Gabriel G. Balint-Kurti. The Fourier grid hamiltonian method for bound state eigenvalues and eigenfunctions. *The Journal of Chemical Physics*, 91(6):3571–3576, 1989. doi:[10.1063/1.456888](https://doi.org/10.1063/1.456888).
- G. A. Martin and W. L. Wiese. Atomic oscillator-strength distributions in spectral series of the lithium isoelectronic sequence. *Phys. Rev. A*, 13:699–714, Feb 1976. doi:[10.1103/PhysRevA.13.699](https://doi.org/10.1103/PhysRevA.13.699).
- Kirill Martiyanov, Vasily Makhlov, and Andrey Turlapov. Observation of a two-dimensional fermi gas of atoms. *Phys. Rev. Lett.*, 105(3):030404–, July 2010. doi:[10.1103/PhysRevLett.105.030404](https://doi.org/10.1103/PhysRevLett.105.030404).
- Françoise Masnou-Seeuws and Pierre Pillet. Formation of ultracold molecules ($T \leq 200\mu\text{K}$) via photoassociation in a gas of laser-cooled atoms. In Benjamin Bederson and Herbert Walther, editors, *Advances In Atomic, Molecular, and Optical Physics*, volume 47 of *Advances In Atomic, Molecular, and Optical Physics*, pages 53 – 127. Academic Press, 2001. doi:[10.1016/S1049-250X\(01\)80055-0](https://doi.org/10.1016/S1049-250X(01)80055-0).
- W. I. McAlexander, E. R. I. Abraham, N. W. M. Ritchie, C. J. Williams, H. T. C. Stoof, and R. G. Hulet. Precise atomic radiative lifetime via photoassociative spectroscopy of ultracold lithium. *Phys. Rev. A*, 51(2):R871–R874, February 1995. doi:[10.1103/PhysRevA.51.R871](https://doi.org/10.1103/PhysRevA.51.R871).
- W. I. McAlexander, E. R. I. Abraham, and R. G. Hulet. Radiative lifetime of the $2P$ state of lithium. *Phys. Rev. A*, 54(1):R5–R8, July 1996. doi:[10.1103/PhysRevA.54.R5](https://doi.org/10.1103/PhysRevA.54.R5).
- D. J. McCarron, S. A. King, and S. L. Cornish. Modulation transfer spectroscopy in atomic rubidium. *Meas. Sci. Technol.*, 19(10):105601, 2008. doi:[10.1088/0957-0233/19/10/105601](https://doi.org/10.1088/0957-0233/19/10/105601).
- D. C. McKay, D. Jervis, D. J. Fine, J. W. Simpson-Porco, G. J. A. Edge, and J. H. Thywissen. Low-temperature high-density magneto-optical trapping of potassium using the open $4S \rightarrow 5P$ transition at 405nm. *Phys. Rev. A*, 84(6):063420–, December 2011. doi:[10.1103/PhysRevA.84.063420](https://doi.org/10.1103/PhysRevA.84.063420).
- J. Harold Metcalf and Peter van der Straten. Laser cooling and trapping. Springer, 1999.
- Thomas Middelmann, Stephan Falke, Christian Lisdat, and Uwe Sterr. Long-range transport of ultracold atoms in a far-detuned one-dimensional optical lattice. *New J. Phys.*, 14(7):073020, 2012. doi:[10.1088/1367-2630/14/7/073020](https://doi.org/10.1088/1367-2630/14/7/073020).
- J. D. Miller, R. A. Cline, and D. J. Heinzen. Photoassociation spectrum of ultracold Rb atoms. *Phys. Rev. Lett.*, 71:2204–2207, Oct 1993. doi:[10.1103/PhysRevLett.71.2204](https://doi.org/10.1103/PhysRevLett.71.2204).
- G. Modugno, C. Benkö, P. Hannaford, G. Roati, and M. Inguscio. Sub-Doppler laser cooling of fermionic ^{40}K atoms. *Phys. Rev. A*, 60(5):R3373–R3376, November 1999. doi:[10.1103/PhysRevA.60.R3373](https://doi.org/10.1103/PhysRevA.60.R3373).

- Peter J. Mohr, Barry N. Taylor, and David B. Newell. Codata recommended values of the fundamental physical constants: 2010. *Journal of Physical and Chemical Reference Data*, 41(4):043109, 2012. doi:<http://dx.doi.org/10.1063/1.4724320>.
- J. H. Moore, C. C. Davis, and M. A. Coplan. Building scientific apparatus. Cambridge University Press, 4th edition, 2009.
- A. Mosk, S. Jochim, H. Moritz, Th. Elsässer, M. Weidemüller, and R. Grimm. Resonator-enhanced optical dipole trap for fermionic lithium atoms. *Opt. Lett.*, 26(23):1837–1839, Dec 2001. doi:[10.1364/OL.26.001837](https://doi.org/10.1364/OL.26.001837).
- Torben Müller. Microscopic probing and manipulation of ultracold fermions. PhD thesis, ETH Zurich, 2011.
- Monika Musial and Stanislaw A. Kucharski. First principle calculations of the potential energy curves for electronic states of the lithium dimer. *J. Chem. Theory Comput.*, 10(3):1200–1211, March 2014. ISSN 1549-9618. doi:[10.1021/ct401076e](https://doi.org/10.1021/ct401076e).
- Reginaldo Napolitano, John Weiner, Carl J. Williams, and Paul S. Julienne. Line shapes of high resolution photoassociation spectra of optically cooled atoms. *Phys. Rev. Lett.*, 73:1352–1355, Sep 1994. doi:[10.1103/PhysRevLett.73.1352](https://doi.org/10.1103/PhysRevLett.73.1352).
- S. Nascimbène, N. Navon, K. J. Jiang, F. Chevy, and C. Salomon. Exploring the thermodynamics of a universal Fermi gas. *Nature*, 463(7284):1057–1060, February 2010. ISSN 0028-0836. doi:[10.1038/nature08814](https://doi.org/10.1038/nature08814).
- P. Nozières and S. Schmitt-Rink. Bose condensation in an attractive fermion gas: From weak to strong coupling superconductivity. *J. Low Temp. Phys.*, 59(3):195–211, 1985. ISSN 1573-7357. doi:[10.1007/BF00683774](https://doi.org/10.1007/BF00683774).
- K. M. O’Hara, M. E. Gehm, S. R. Granade, and J. E. Thomas. Scaling laws for evaporative cooling in time-dependent optical traps. *Phys. Rev. A*, 64:051403, Oct 2001a. doi:[10.1103/PhysRevA.64.051403](https://doi.org/10.1103/PhysRevA.64.051403).
- K. M. O’Hara, S. R. Granade, M. E. Gehm, and J. E. Thomas. Loading dynamics of CO₂ laser traps. *Phys. Rev. A*, 63(4):043403–, March 2001b. doi:[10.1103/PhysRevA.63.043403](https://doi.org/10.1103/PhysRevA.63.043403).
- K. M. O’Hara, S. L. Hemmer, M. E. Gehm, S. R. Granade, and J. E. Thomas. Observation of a strongly interacting degenerate Fermi gas of atoms. *Science*, 298(5601):2179–2182, 2002. doi:[10.1126/science.1079107](https://doi.org/10.1126/science.1079107).
- Ahmed Omran, Martin Boll, Timon A. Hilker, Katharina Kleinlein, Guillaume Salomon, Immanuel Bloch, and Christian Gross. Microscopic observation of Pauli blocking in degenerate fermionic lattice gases. *Phys. Rev. Lett.*, 115:263001, Dec 2015. doi:[10.1103/PhysRevLett.115.263001](https://doi.org/10.1103/PhysRevLett.115.263001).
- Sambit Bikas Pal. Molecular spectroscopy of ultracold ⁶Li - ⁴⁰K molecules: Towards STIRAP transfer to absolute ground state. PhD thesis, National University of Singapore, 2016.
- M. F. Parsons, A. Mazurenko, C. S. Chiu, D. Ji, D. Greif, and M. Greiner. Site-resolved observations of antiferromagnetic correlations in the Hubbard model. arXiv:1605.02704, 2016.
- G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, and R. G. Hulet. Molecular probe of pairing in the BEC-BCS crossover. *Phys. Rev. Lett.*, 95(2):020404–, July 2005. doi:[10.1103/PhysRevLett.95.020404](https://doi.org/10.1103/PhysRevLett.95.020404).

- Philippe Pellegrini, Marko Gacesa, and Robin Côté. Giant formation rates of ultracold molecules via Feshbach-optimized photoassociation. *Phys. Rev. Lett.*, 101:053201, Aug 2008. doi:[10.1103/PhysRevLett.101.053201](https://doi.org/10.1103/PhysRevLett.101.053201).
- C. J. Pethick and H. Smith. Bose-Einstein condensation in dilute gases. Cambridge University Press, 2008.
- D. S. Petrov. Three-body problem in Fermi gases with short-range interparticle interaction. *Phys. Rev. A*, 67:010703, Jan 2003. doi:[10.1103/PhysRevA.67.010703](https://doi.org/10.1103/PhysRevA.67.010703).
- D. S. Petrov, C. Salomon, and G. V. Shlyapnikov. Weakly bound dimers of fermionic atoms. *Phys. Rev. Lett.*, 93:090404, Aug 2004. doi:[10.1103/PhysRevLett.93.090404](https://doi.org/10.1103/PhysRevLett.93.090404).
- William D. Phillips and Harold Metcalf. Laser deceleration of an atomic beam. *Phys. Rev. Lett.*, 48(9):596–599, March 1982. doi:[10.1103/PhysRevLett.48.596](https://doi.org/10.1103/PhysRevLett.48.596).
- Marin Pichler, Jianbing Qi, William C. Stwalley, Robert Beuc, and Goran Pichler. Observation of blue satellite bands and photoassociation at ultracold temperatures. *Phys. Rev. A*, 73:021403, Feb 2006. doi:[10.1103/PhysRevA.73.021403](https://doi.org/10.1103/PhysRevA.73.021403).
- P. Pillet, A. Crubellier, A. Bleton, O. Dulieu, P. Nosbaum, I. Mourachko, and F. Masnou-Seeuws. Photoassociation in a gas of cold alkali atoms: I. perturbative quantum approach. *J. Phys. B: At., Mol. Opt. Phys.*, 30(12):2801, 1997. doi:[10.1088/0953-4075/30/12/010](https://doi.org/10.1088/0953-4075/30/12/010).
- E. L. Raab, M. Prentiss, Alex Cable, Steven Chu, and D. E. Pritchard. Trapping of neutral sodium atoms with radiation pressure. *Phys. Rev. Lett.*, 59(23):2631–2634, December 1987. doi:[10.1103/PhysRevLett.59.2631](https://doi.org/10.1103/PhysRevLett.59.2631).
- Leon J. Radziemski, Rolf Jr. Engleman, and James W. Brault. Fourier-transform-spectroscopy measurements in the spectra of neutral lithium, ^6Li I and ^7Li (Li I). *Phys. Rev. A*, 52(6):4462–4470, December 1995. doi:[10.1103/PhysRevA.52.4462](https://doi.org/10.1103/PhysRevA.52.4462).
- Lyn B. Ratcliff, James L. Fish, and Daniel D. Konowalow. Electronic transition dipole moment functions for transitions among the twenty-six lowest-lying states of Li_2 . *J. Mol. Spectrosc.*, 122(2):293–312, 1987. ISSN 0022-2852. doi:[10.1016/0022-2852\(87\)90006-3](https://doi.org/10.1016/0022-2852(87)90006-3).
- C. A. Regal and D. S. Jin. Measurement of positive and negative scattering lengths in a Fermi gas of atoms. *Phys. Rev. Lett.*, 90:230404, Jun 2003. doi:[10.1103/PhysRevLett.90.230404](https://doi.org/10.1103/PhysRevLett.90.230404).
- C. A. Regal, M. Greiner, and D. S. Jin. Observation of resonance condensation of fermionic atom pairs. *Phys. Rev. Lett.*, 92:040403, Jan 2004. doi:[10.1103/PhysRevLett.92.040403](https://doi.org/10.1103/PhysRevLett.92.040403).
- Cindy A. Regal, Christopher Ticknor, John L. Bohn, and Deborah S. Jin. Creation of ultracold molecules from a Fermi gas of atoms. *Nature*, 424(6944):47–50, July 2003. ISSN 0028-0836. doi:[10.1038/nature01738](https://doi.org/10.1038/nature01738).
- L. Ricci, M. Weidemüller, T. Esslinger, A. Hemmerich, C. Zimmermann, V. Vuletic, W. König, and T.W. Hänsch. A compact grating-stabilized diode laser system for atomic physics. *Opt. Commun.*, 117(5-6):541–549, June 1995. ISSN 0030-4018. doi:[10.1016/0030-4018\(95\)00146-Y](https://doi.org/10.1016/0030-4018(95)00146-Y).
- A. Ridinger, S. Chaudhuri, T. Salez, U. Eismann, D.R. Fernandes, K. Magalhães, D. Wilkowski, C. Salomon, and F. Chevy. Large atom number dual-species magneto-optical trap for fermionic ^6Li and ^{40}K atoms. *Eur. Phys. J. D*, 65(1-2):223–242, 2011. ISSN 1434-6060. doi:[10.1140/epjd/e2011-20069-4](https://doi.org/10.1140/epjd/e2011-20069-4).

- M. G. Ries, A. N. Wenz, G. Zürn, L. Bayha, I. Boettcher, D. Kedar, P. A. Murthy, M. Neidig, T. Lompe, and S. Jochim. Observation of pair condensation in the quasi-2D BEC-BCS crossover. *Phys. Rev. Lett.*, 114:230401, Jun 2015. doi:[10.1103/PhysRevLett.114.230401](https://doi.org/10.1103/PhysRevLett.114.230401).
- N. W. M. Ritchie, E. R. I. Abraham, and R. G. Hulet. Trap loss collisions of ^7Li : The role of trap depth. *Laser Phys.*, Vol. 4:1066, 1994.
- N. W. M. Ritchie, E. R. I. Abraham, Y. Y. Xiao, C. C. Bradley, R. G. Hulet, and P. S. Julienne. Trap-loss collisions of ultracold lithium atoms. *Phys. Rev. A*, 51(2):R890–R893, February 1995. doi:[10.1103/PhysRevA.51.R890](https://doi.org/10.1103/PhysRevA.51.R890).
- M. S. Safronova, U. I. Safronova, and Charles W. Clark. Magic wavelengths for optical cooling and trapping of lithium. *Phys. Rev. A*, 86(4):042505–, October 2012. doi:[10.1103/PhysRevA.86.042505](https://doi.org/10.1103/PhysRevA.86.042505).
- G. Salomon, L. Fouché, P. Wang, A. Aspect, P. Bouyer, and T. Bourdel. Gray-molasses cooling of ^{39}K to a high phase-space density. *EPL (Europhysics Letters)*, 104(6):63002, 2013. doi:[10.1209/0295-5075/104/63002](https://doi.org/10.1209/0295-5075/104/63002).
- G. Salomon, L. Fouché, S. Lepoutre, A. Aspect, and T. Bourdel. All-optical cooling of ^{39}K to Bose-Einstein condensation. *Phys. Rev. A*, 90:033405, Sep 2014. doi:[10.1103/PhysRevA.90.033405](https://doi.org/10.1103/PhysRevA.90.033405).
- Stefan Schmid, Gregor Thalhammer, Klaus Winkler, Florian Lang, and Johannes Hecker Denschlag. Long distance transport of ultracold atoms using a 1D optical lattice. *New J. Phys.*, 8(8):159, 2006. doi:[10.1088/1367-2630/8/8/159](https://doi.org/10.1088/1367-2630/8/8/159).
- U. Schneider, L. Hackermüller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, and A. Rosch. Metallic and insulating phases of repulsively interacting fermions in a 3D optical lattice. *Science*, 322(5907):1520–1525, 2008. doi:[10.1126/science.1165449](https://doi.org/10.1126/science.1165449).
- U. Schünemann, H. Engler, M. Zielonkowski, M. Weidemüller, and R. Grimm. Magneto-optic trapping of lithium using semiconductor lasers. *Opt. Commun.*, 158:263–272, December 1998. ISSN 0030-4018. doi:[10.1016/S0030-4018\(98\)00517-3](https://doi.org/10.1016/S0030-4018(98)00517-3).
- Franz Schwabl. Statistical mechanics. Springer, 2006.
- J. Sebastian, Ch. Gross, Ke Li, H. C. J. Gan, Wenhui Li, and K. Dieckmann. Two-stage magneto-optical trapping and narrow-line cooling of ^6Li atoms to high phase-space density. *Phys. Rev. A*, 90:033417, Sep 2014. doi:[10.1103/PhysRevA.90.033417](https://doi.org/10.1103/PhysRevA.90.033417).
- Mariusz Semczuk, Xuan Li, Will Gunton, Magnus Haw, Nikesh S. Dattani, Julien Witz, Arthur K. Mills, David J. Jones, and Kirk W. Madison. High-resolution photoassociation spectroscopy of the $^6\text{Li}_2\ 1^3\Sigma_g^+$ state. *Phys. Rev. A*, 87(5):052505–, May 2013. doi:[10.1103/PhysRevA.87.052505](https://doi.org/10.1103/PhysRevA.87.052505).
- Jon H. Shirley. Modulation transfer processes in optical heterodyne saturation spectroscopy. *Opt. Lett.*, 7(11):537–539, November 1982. doi:[10.1364/OL.7.000537](https://doi.org/10.1364/OL.7.000537).
- Horst Sjuts. Cem model KBL5RS/90. Dr. Sjuts Optotechnik GmbH, 2014a.
- Horst Sjuts. Private communication. Dr. Sjuts Optotechnik GmbH, 2014b.
- J. J. Snyder, R. K. Raj, D. Bloch, and M. Ducloy. High-sensitivity nonlinear spectroscopy using a frequency-offset pump. *Opt. Lett.*, 5(4):163–165, Apr 1980. doi:[10.1364/OL.5.000163](https://doi.org/10.1364/OL.5.000163).

- Jochen Steinmann. Multiphoton ionization of laser cooled lithium. PhD thesis, Ruperto-Carola University of Heidelberg, 2007.
- J. Stenger, S. Inouye, M. R. Andrews, H.-J. Miesner, D. M. Stamper-Kurn, and W. Ketterle. Strongly enhanced inelastic collisions in a Bose-Einstein condensate near Feshbach resonances. *Phys. Rev. Lett.*, 82:2422–2425, Mar 1999. doi:[10.1103/PhysRevLett.82.2422](https://doi.org/10.1103/PhysRevLett.82.2422).
- J. G. Story and T. F. Gallagher. Temporal effects in multiphoton ionization of lithium. *Phys. Rev. A*, 47:5037–5040, Jun 1993. doi:[10.1103/PhysRevA.47.5037](https://doi.org/10.1103/PhysRevA.47.5037).
- William C. Stwalley and He Wang. Photoassociation of ultracold atoms: A new spectroscopic technique. *J. Mol. Spectrosc.*, 195(2):194 – 228, 1999. ISSN 0022-2852. doi:[10.1006/jmsp.1999.7838](https://doi.org/10.1006/jmsp.1999.7838).
- Sune Svanberg. Atomic and molecular spectroscopy. Springer, 2004.
- M. Taglieber, A.-C. Voigt, F. Henkel, S. Fray, T. W. Hänsch, and K. Dieckmann. Simultaneous magneto-optical trapping of three atomic species. *Phys. Rev. A*, 73:011402, Jan 2006. doi:[10.1103/PhysRevA.73.011402](https://doi.org/10.1103/PhysRevA.73.011402).
- Matthias Taglieber. Quantum degeneracy in an atomic Fermi-Fermi-Bose mixture. PhD thesis, Ludwig-Maximilians-Universität München, 2008.
- E. Tiesinga, B. J. Verhaar, and H. T. C. Stoof. Threshold and resonance phenomena in ultracold ground-state collisions. *Phys. Rev. A*, 47(5):4114–4122, May 1993. doi:[10.1103/PhysRevA.47.4114](https://doi.org/10.1103/PhysRevA.47.4114).
- E. Torrontegui, S. Ibáñez, Xi Chen, A. Ruschhaupt, D. Guéry-Odelin, and J. G. Muga. Fast atomic transport without vibrational heating. *Phys. Rev. A*, 83:013415, Jan 2011. doi:[10.1103/PhysRevA.83.013415](https://doi.org/10.1103/PhysRevA.83.013415).
- Andrew G. Truscott, Kevin E. Strecker, William I. McAlexander, Guthrie B. Partridge, and Randall G. Hulet. Observation of Fermi pressure in a gas of trapped atoms. *Science*, 291(5513):2570–2572, 2001. ISSN 0036-8075. doi:[10.1126/science.1059318](https://doi.org/10.1126/science.1059318).
- Juris Ulmanis, Johannes Deiglmayr, Marc Repp, Roland Wester, and Matthias Weidemüller. Ultracold molecules formed by photoassociation: Heteronuclear dimers, inelastic collisions, and interactions with ultrashort laser pulses. *Chem. Rev.*, 112(9):4890–4927, 2012. doi:[10.1021/cr300215h](https://doi.org/10.1021/cr300215h). PMID: 22931226.
- P. J. Ungar, D. S. Weiss, E. Riis, and Steven Chu. Optical molasses and multilevel atoms: theory. *J. Opt. Soc. Am. B*, 6(11):2058–2071, November 1989. doi:[10.1364/JOSAB.6.002058](https://doi.org/10.1364/JOSAB.6.002058).
- J. Van Dongen, C. Zhu, D. Clement, G. Dufour, J. L. Booth, and K. W. Madison. Trap-depth determination from residual gas collisions. *Phys. Rev. A*, 84:022708, Aug 2011. doi:[10.1103/PhysRevA.84.022708](https://doi.org/10.1103/PhysRevA.84.022708).
- J.T.M. Walraven. Quantum gases - statistics and interactions, 2014.
- John Weiner, Vanderlei S. Bagnato, Sergio Zilio, and Paul S. Julienne. Experiments and theory in cold and ultracold collisions. *Rev. Mod. Phys.*, 71(1):1–85, January 1999. doi:[10.1103/RevModPhys.71.1](https://doi.org/10.1103/RevModPhys.71.1).
- David S. Weiss, Erling Riis, Yaakov Shevy, P. Jeffrey Ungar, and Steven Chu. Optical molasses and multilevel atoms: experiment. *J. Opt. Soc. Am. B*, 6(11):2072–2083, Nov 1989. doi:[10.1364/JOSAB.6.002072](https://doi.org/10.1364/JOSAB.6.002072).

- Zong-Chao Yan, James F. Babb, A. Dalgarno, and G. W. F. Drake. Variational calculations of dispersion coefficients for interactions among H, He, and Li atoms. *Phys. Rev. A*, 54: 2824–2833, Oct 1996. doi:[10.1103/PhysRevA.54.2824](https://doi.org/10.1103/PhysRevA.54.2824).
- Ren Zhang, Yanting Cheng, Hui Zhai, and Peng Zhang. Orbital Feshbach resonance in alkali-earth atoms. *Phys. Rev. Lett.*, 115:135301, Sep 2015. doi:[10.1103/PhysRevLett.115.135301](https://doi.org/10.1103/PhysRevLett.115.135301).
- B. Zimmermann, T. Müller, J. Meineke, T. Esslinger, and H. Moritz. High-resolution imaging of ultracold fermions in microscopically tailored optical potentials. *New J. Phys.*, 13(4): 043007–, 2011. ISSN 1367-2630. doi:[10.1088/1367-2630/13/4/043007](https://doi.org/10.1088/1367-2630/13/4/043007).
- Bruno Zimmermann. Microscopy of ultra-cold fermionic lithium. PhD thesis, ETH Zurich, 2010.
- G. Zürn, T. Lompe, A. N. Wenz, S. Jochim, P. S. Julienne, and J. M. Hutson. Precise characterization of ^6Li Feshbach resonances using trap-sideband-resolved RF spectroscopy of weakly bound molecules. *Phys. Rev. Lett.*, 110:135301, Mar 2013. doi:[10.1103/PhysRevLett.110.135301](https://doi.org/10.1103/PhysRevLett.110.135301).
- M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle. Observation of Bose-Einstein condensation of molecules. *Phys. Rev. Lett.*, 91(25):250401–, December 2003. doi:[10.1103/PhysRevLett.91.250401](https://doi.org/10.1103/PhysRevLett.91.250401).
- M. W. Zwierlein, J. R. Abo-Shaer, A. Schirotzek, C. H. Schunck, and W. Ketterle. Vortices and superfluidity in a strongly interacting Fermi gas. *Nature*, 435(7045):1047–1051, June 2005. ISSN 0028-0836. doi:[10.1038/nature03858](https://doi.org/10.1038/nature03858).

A. Atomic properties of ${}^6\text{Li}$

A.1. Derived quantities for the cooling transitions of ${}^6\text{Li}$

	$2^2S_{1/2} \rightarrow 2^2P_{3/2}$	$2^2S_{1/2} \rightarrow 3^2P_{3/2}$
Wavelength λ	670.977 nm	323.36 nm
Natural linewidth Γ	$(2\pi) \times 5.871$ MHz	$(2\pi) \times 0.7539$ MHz
Lifetime $\tau = \frac{1}{\Gamma}$	27.1 ns	211.1 ns
Doppler temperature $T_D = \hbar \Gamma / 2 k_B$	141 μK	18.1 μK
Recoil energy $E_{\text{rec}}/k_B = \frac{\hbar^2 k^2}{2m k_B}$	3.54 μK	15.3 μK
Recoil velocity $v_{\text{rec}} = \frac{\hbar}{m\lambda}$	0.0991 m/s	0.206 m/s
v_{rms} (at T_D) $= \sqrt{3 k_B T_D / m}$	0.77 m/s	0.27 m/s
Saturation intensity $I_{\text{sat}}^{2P/3P} = \frac{\pi \hbar c \Gamma_{2P/3P}}{3\lambda^3}$	2.51 W/cm ²	13.8 W/cm ²

Table A.1.: Atomic properties (Kramida et al., 2016) and derived quantities of ${}^6\text{Li}$.

A.2. Zeeman shift of $2^2S_{1/2}$ and $2^2P_{3/2}$ levels

The energy shifts of the Zeeman hyperfine states are calculated by diagonalizing the perturbation Hamiltonian $H_{\text{int}} = H_B + H_{\text{HFS}}$, analogous to the discussion by (Gehm, 2003). For a magnetic field strength B , the magnetic field term is given by

$$E_B = \mu_B (g_J m_J + g_I m_I) B \quad (\text{A.1})$$

where the corresponding g-factors were summarized by Arimondo et al. (1977). The projections of the total electronic angular momentum and the nuclear spin along the direction of the magnetic field are given by m_J and m_I . The expectation value of the hyperfine interaction term in the $|IJFm_F\rangle$ basis is

$$E_{\text{HFS}} = \frac{A}{2} (F(F+1) - I(I+1) - J(J+1)) , \quad (\text{A.2})$$

if the electric quadrupole interaction is neglected (Foot, 2005; Johnson, 2007). F is the total angular momentum and A the hyperfine constant (Arimondo et al., 1977).

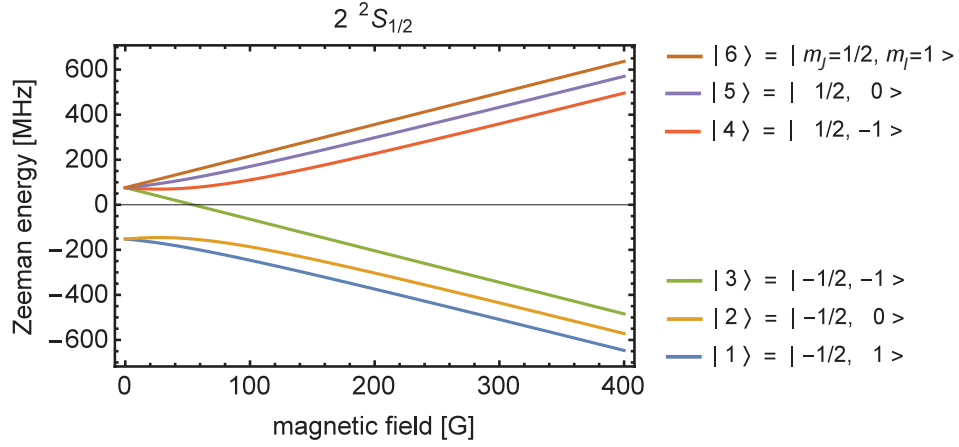


Figure A.1.: Magnetic field dependence of the Zeeman energy for the hyperfine states of the ^6Li ground state $2^2S_{1/2}$. At high magnetic fields, the nuclear and the electron spin decouple and the states are described by the quantum numbers m_j and m_i .

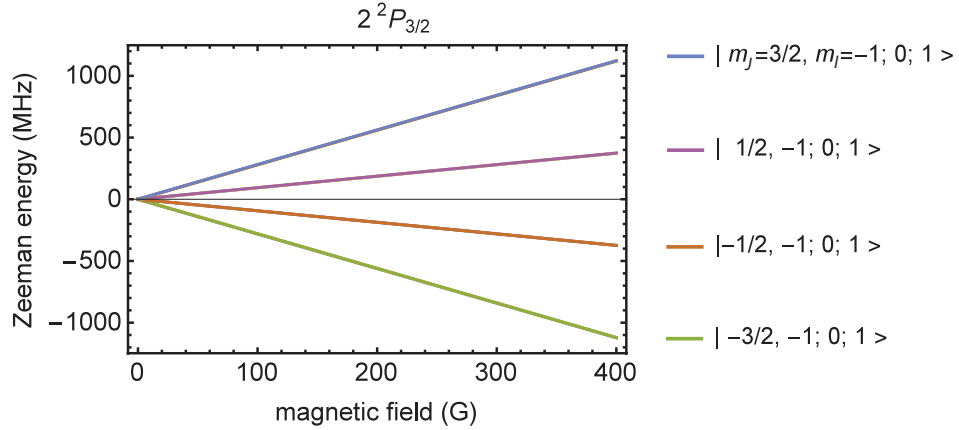


Figure A.2.: Magnetic field dependence of the Zeeman energy for the hyperfine states of excited state $2^2P_{3/2}$ of ^6Li . Due to the small hyperfine coupling constant for this state, the individual Zeeman levels are not discernible on this energy scale.

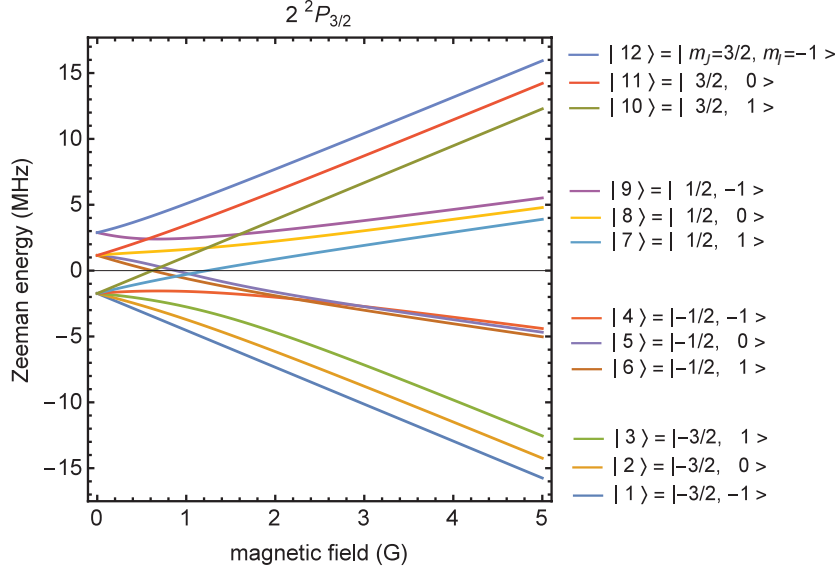


Figure A.3.: Magnetic field dependence of the Zeeman energy for the hyperfine states of excited state $2^2P_{3/2}$ of ^6Li at low magnetic field strength. The states are numbered according to the energy shift at a magnetic field of 1000 G.

A.3. s-wave scattering length of $|1\rangle$ - $|2\rangle$ mixture

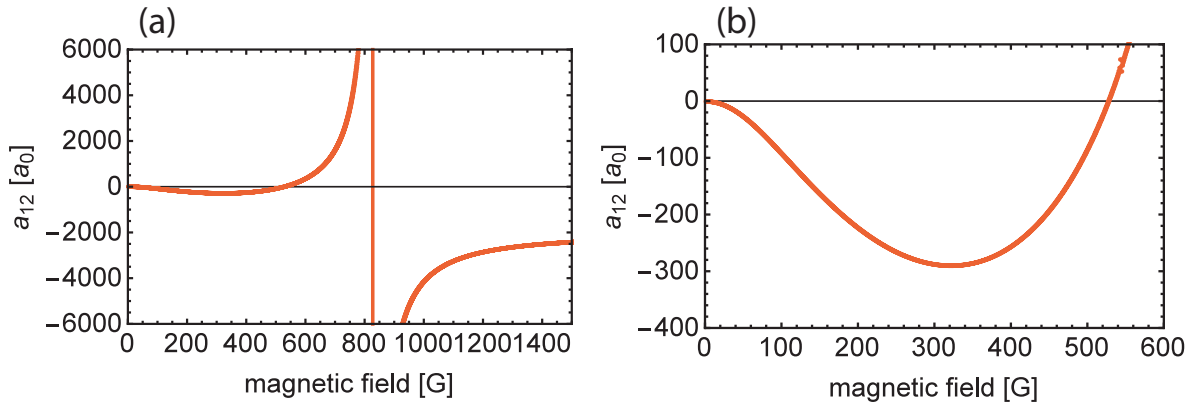


Figure A.4.: (a) s -wave scattering length a_{12} between the energetically lowest two Zeeman states $|1\rangle$ and $|2\rangle$ of the $2^2S_{1/2}$ ground state of ^6Li . The data is taken from [Zürn et al. \(2013\)](#). (b) Enlarged scale of the scattering length for magnetic fields around the local minimum at 330 G. This range is relevant for the evaporative cooling to create a weakly interacting Fermi gas.

B. Photoassociation

B.1. Atomic units

Property and symbol	Symbol	Value in SI units
Unit of length (Bohr's radius)	a_0	$0.529 \times 10^{-10} \text{ m}$
Unit of charge (charge of electron)	e	$1.60 \times 10^{-19} \text{ C}$
Unit of mass (mass of electron)	m_e	$9.11 \times 10^{-31} \text{ kg}$
Unit of energy (Hartree energy)	$E_h = \frac{e^2}{a_0}$	$4.36 \times 10^{-18} \text{ J}$
Unit of action (reduced Planck's constant)	$\hbar$	$1.05 \times 10^{-34} \text{ Js}$

Table B.1.: Atomic units (Mohr et al., 2012).

B.2. Selected dipole matrix elements for ${}^6\text{Li}_2$ and ${}^7\text{Li}_2$

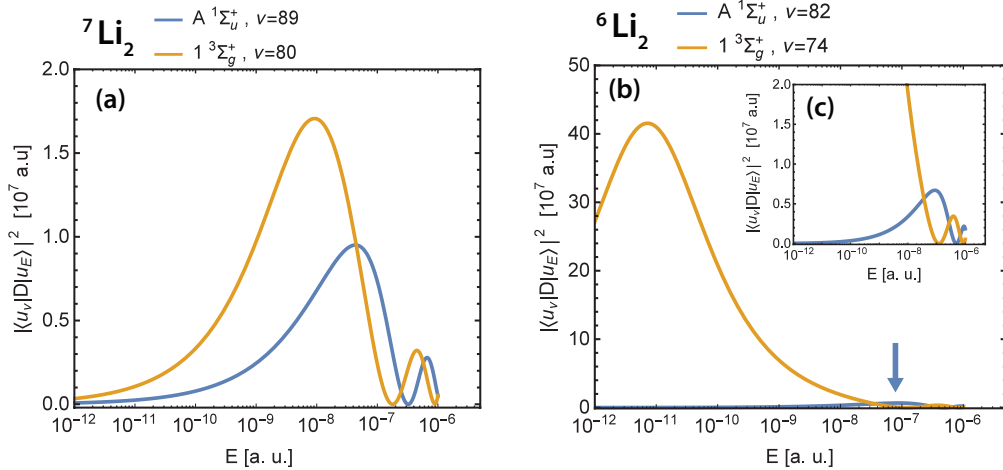


Figure B.1.: Dipole matrix element for PA transitions to $A \ ^1\Sigma_u^+$ and $1 \ ^3\Sigma_g^+$ states of lithium. (a) The vibrational levels $\nu = 89$ and $\nu = 80$ for the singlet and triplet potentials of ${}^7\text{Li}_2$ were chosen to reproduce Fig. 5 in *Physical Review A*, **58**, 498 (1998) by Côté and Dalgarno (1998). This serves as a verification for the developed numerical method and the ground-state potential energy curves that are used in Chapter 7. (b),(c) The vibrational levels $\nu = 82$ for the singlet and $\nu = 74$ for the triplet potential of ${}^6\text{Li}_2$ have similar binding energies as compared to the ones of the states shown in (a). The transition to the singlet potential (blue arrow and inset) is of similar strength as for ${}^7\text{Li}_2$ and the large value of the dipole matrix element of the triplet transition is a consequence of the large negative triplet s -wave scattering length of ${}^6\text{Li}$.

B.3. $2S$ - $2P$ photoassociation transitions of ${}^6\text{Li}_2$

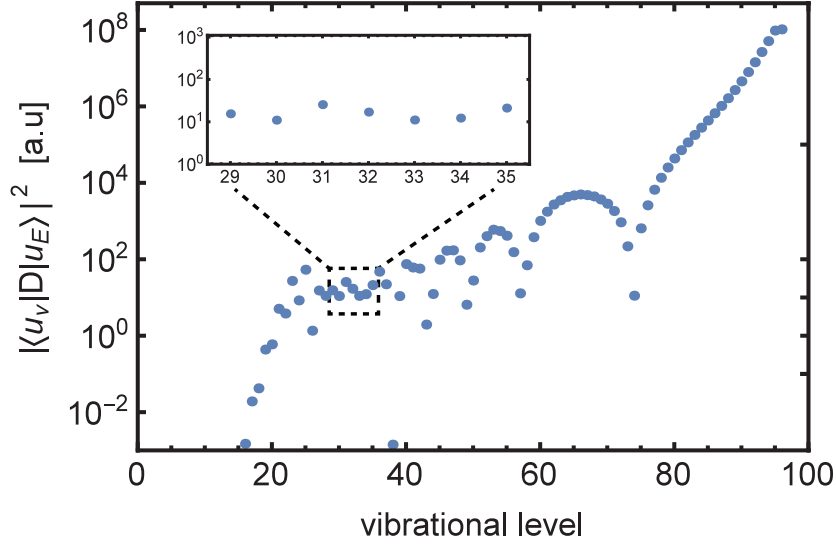


Figure B.2.: Transition dipole matrix elements to different vibrational states of the $A\ ^1\Sigma_u^+$ potential. A collisional energy of 10^{-11} is assumed for the ground-state atoms. The dashed box and the inset highlight the deeply bound levels $\nu = 29 - 35$ that were observed in a photoassociation experiment in an ultracold sample of ${}^6\text{Li}$ atoms confined in an optical dipole trap (Gunton et al., 2013a).

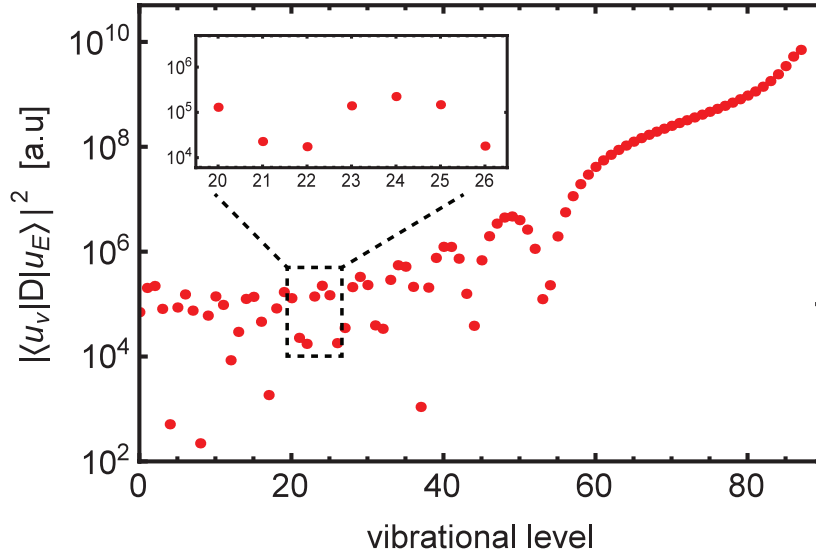


Figure B.3.: Transition dipole matrix elements to different vibrational states of the $1\ ^3\Sigma_g^+$ potential. A collisional energy of 10^{-11} is assumed for the ground-state atoms. The dashed box and the inset highlight the deeply bound levels $\nu = 20 - 26$ that were observed in a photoassociation experiment in an ultracold sample of ${}^6\text{Li}$ atoms confined in an ODT (Semczuk et al., 2013).