Calculation of Van der Waals interaction strength between rubidium atoms in the context of Rydberg blockade

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Abstract

Atoms excited to Rydberg states experience enhanced coupling to the environment. Rydberg atoms interact via dipole-dipole coupling. If the interaction strength is large enough in an ensemble of atoms it can prevent more than one atom being excited to a Rydberg state by the same laser. We calculated the interaction strength of two atoms being initially excited to s- and d-states in the Van der Waals regime. A special emphasis was put on the angular dependence of this interaction. This evaluation required calculations of radial matrix elements, the energy separation between involved interaction channels and the angular part of the Van der Waals Hamiltonian, which we explain in some detail.

samenvatting

Rubidium heeft een enkel electron in de buitenste baan. Deze atomen hebben een dipoolmoment, als gevolg van het bewegen van het buitenste electron om de nucleus. Door de baan groter te maken door het electron te exciteren naar een hoge toestand (of Rydberg toestand) wordt dit dipoolmoment groter. De interacties tussen dit soort Rydberg atomen kan de energieniveaus van de Rydberg toestand zodanig verschuiven, dat als dicht op elkaar gelegen atomen naar een Rydberg toestand worden gestuurd met een laser, slechts een enkel atoom daadwerkelijk wordt ge"exciteerd en de rest niet, omdat de energieniveaus van de anderen zijn verschoven waardoor deze niet meer in resonantie zijn met de laser. Dit heet een Rydberg blockade. Dit kan alleen als de van der Waals interactie sterk genoeg is om de het energieniveau voldoende te verschuiven. We berekenen deze van der Waals interactie voor atomen in bepaalde s- en d-toestanden en laten zien hoe deze berekeningen gedaan moeten worden. We leggen extra nadruk op de hoekafhankelijkheid van deze interactie.
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1 Introduction

Quantum information theory promises fast processing and delicate and complex quantum modelling. Over the years there have been a number of very promising experimental achievements using different set-ups.[5] With trapped ions (Blatt and Wineland, 2008) small algorithms have already been shown that yield high fidelity gates. The idea of using Rydberg states for so-called neutral atom quantum gates for quantum computing, was proposed in 2000 (Jaksch et al., 2000, Lukin et al., 2001) and has accumulated interest over the years.[5]

Rydberg atoms are atoms with highly excited valence electron states. These states have a relative long lifetime and a large orbital radii, which scales as \( n^2 \). Because of the large radius of the valence electron, the atom can have a very high, long-range dipole moment. When multiple atoms interact via dipole-dipole interaction and are being resonantly driven to a Rydberg state, the large dipole moment will shift the energy levels of the multiply-excited Rydberg state. If the interaction is strong, the energy shift can exceed the linewidth of the excitation laser and subsequently only a single atom will be excited to the Rydberg state. This effect is known as a dipole blockade. The use of blockades with Rydberg atoms is known as Rydberg blockade.[5][6]

The principle of Rydberg blockade is shown in Fig(1). Input states \( |01\rangle \) and \( |11\rangle \) are given. Quantum information is encoded on the basis states \( |1\rangle \) and \( |0\rangle \).[5]

If the initial two-atom state is \( |01\rangle \), with the control atom in the state which is not coupled to the Rydberg state, the target atom receives a \( \pi \) phase change. If the initial two-atom state is \( |11\rangle \), where both atoms are coupled to the Rydberg state, the control atom shifts the energy of the state to which the target atom couples. If this blockade shift is large enough, the excitation of the target atom is blocked and the target atom receives no phase change.[5]

In Fig(2) the atom separation dependence (R) is given for two atom interaction for single charged ions, groundstate and Rydberg neutral atoms. For groundstate atoms, the interaction is weak, which means that an array qubits can be held stable, without much interference. For the Rydberg state 100s we see that there is a resonant dipole-dipole interaction which scales as \( 1/R^3 \) at small interatomic distances and a van der Waals interaction, which scales as \( 1/R^6 \) at large interatomic distances. The cross-over distance \( R_c \) will depend on the principal quantum number \( n \). These interactions are far greater, approximately 12 orders larger, than the interactions for groundstate atoms. This means that information can be stored in an array of qubits, which is held steady in the ground-state and which can be manipulated by dipole-dipole interaction by exciting the atoms to higher states. These dipole-dipole interactions can be controlled over a vast range of
Figure 1: State $|1\rangle$ is coupled to the Rydberg state $|r\rangle$ with a Rabi-frequency $\omega_{10}$. The controlled phase gate works with three pulses: pulse 1) a $\pi$ pulse is send to the control atom, which enables the transition $|1\rangle \rightarrow |r\rangle$. pulse 2) a $2\pi$ pulse is send to the target atom in $|0\rangle$. pulse 3) a $\pi$ pulse is send to the control atom, which makes the transition $|r\rangle \rightarrow |1\rangle$. In situation a) the control atom is initially in state $|0\rangle$, so it is not excited to the Rydberg state and there is no blockade. In situation b) the control atom is initially in state $|1\rangle$ and is excited to the Rydberg state and creates a blockade for the target atom, which is then not excited to the Rydberg state and does not pick up a phase change. Source: [5].

Figure 2: interaction between two atoms, for 100s Rydberg Rb atoms, groundstate Rb atoms and ions. Source: [5].

orders. This manipulation of the large range interaction strength is the property that
makes Rydberg atoms such a promising candidate for quantum information processing.[5]

In the course of this thesis we will look more closely at the dipole-dipole interaction between atoms. A major part of this thesis is dedicated to retrieving values from the article of Saffman and Walker, cited as [6]. We will have to take a closer look at the radial wavefunction of Rydberg alkali, in our case rubidium, in order to get a quantitative hold on the interaction strength. We will see that the interaction and therefore the blockade strength will acquire an angle-dependency that has important practical consequences.

2 Theory

2.1 Rydberg atoms

2.1.1 Binding energy

Alkali metal occupy a special column in the periodic table right beneath hydrogen. Like hydrogen, the alkali metals have an outer valence electron in a s-shell. This property makes that the alkali metals are very similar to hydrogen, as you can approximate the alkali metals in many circumstances as being a hydrogen atom with a massive core. In reality, the outer valence electron is subjegated to all sorts of exchange forces form with the other electrons closer to the core and interactions with the core. The effects of these interactions obviously decrease if the distance from the valence electron to the core is enlarged.[4] It is precisely this what makes a Rydberg state so much more comparable to hydrogen than a regular state. Since the orbital of a Rydberg state has a large orbital radius, the Rydberg states satisfy exactly that criterium to make an Alkali metal seem like hydrogen, as we will soon see explicitely when we approximate its radial wavefunction by using the potential of a single proton electron as in hydrogen. The energy of an arbitrary state in hydrogen can be approximated using the Rydberg formula

\[ W = \frac{R_{\text{ryd}}}{n^2} \]  

where \( R_{\text{ryd}} \) is the Rydberg constant and \( n \) is the principal quantum number. For alkali metals the same formula can be used to calculate the binding energy of an arbitray state. The only difference is that, due to the interactions the valence electron has with the inner electrons, the principal quantum number \( n \) is replaced by an effective principal quantum number \( n^* = n - \delta_{nlj} \), where \( \delta_{nlj} \) is called the quantum defect and depends on the angular momentum \( l \), fine structure \( j \) and principal quantum number \( n \) of the state. The \( n \)-dependence is only a weak correction. The quantum defect is mainly dependent of \( l \) and \( j \). There’s a convention to what a state is called depending on the value of \( l \), which can only take integer numbers[2]

\[
\begin{align*}
  l & = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \ldots \\
  s & \quad p \quad d \quad f \quad g \quad h \quad i \quad k \quad l \ldots
\end{align*}
\]
The energy of a hydrogenic ion in the non-relativistic approximation is given by

\[ E = -\frac{m_e^4 Z^2}{2\hbar^2 n^2} \]

where \( Z \) is the charge of the nucleus and \( m_e \) is the electron mass and \( \mu = m_e M / (m_e + M) \) is the reduced mass with \( M \) the mass of nucleus.\(^2\) For alkali we can approximate the energy levels, using

\[ E_n = -\frac{m_e^4}{2\hbar^2 c} \frac{Z^2}{(n - \delta_{nlj})^2} = \frac{-R_{\text{ryd}}}{(n - \delta_{nlj})^2} \]

which is Eq (1) if we replace \( n \) with \( n^* \).\(^4\) Of these interactions of the core with the valence electron, an important one is the that states with low angular momentum \( (l \leq 3) \), the orbit of the valence electron is extremly elliptic and so the valence electron can penetrate the closed electron shell and is therefore exposed to the unscreened nuclear charge. The electrons in the inner closed shells can also be polarised by the valence electron. Both these interactions increase the binding energy of the state, as is seen by the implementation of \( n^* \) instead of \( n \) in the Rydberg formula. It also states that the quantum defect will be largest for s-states, since these have the largest core penetration.\(^4\)

The quantum defect can be empirically determined using the power series

\[ \delta_{nlj} = \delta_0 + \frac{\delta_2}{(n - \delta_0)^2} + \frac{\delta_4}{(n - \delta_0)^4} + \ldots \]

where \( \delta_0, \delta_2, \ldots \) depend on \( l \) and \( j \) and can be emperically measured, as is done for rubidium in our case of interest. These measurements have been done in a cloud of cold atoms of rubidium. For \( l > 3 \) these quantum defects quickly drop and can be approximated as being zero. These states experience a core potential that is almost perfectly a \( 1/r \) Coulomb potential like hydrogen and are therefore called hydrogenic states.\(^4\)

In this thesis we will often use the Dirac notation for describing electronic orbital eigenstates. In this notation the time-independent Schrödinger equation takes the form

\[ H_0 |nlm\rangle = E_0 |nlm\rangle \]

(3)

with \( m \) the magnetic quantum number.\(^2\) The eigenfunction in the space is then given by

\[ \psi_{nlm}(r) = \langle r |nlm\rangle = \langle r |nl\rangle \langle \hat{r} |lm\rangle \]

(4)

with \( \langle r |nl\rangle = \mathcal{R}_{nl}(r) \) which denotes the radial part which solely depends on radial coordinates, and \( \langle \hat{r} |lm\rangle = Y_l^m(\hat{r}) \) which denotes the angular part which solely depends on angular coordinates. In this notation the expectation value of an operator \( A \) for an atomic eigenstate \( |nlm\rangle \) is given by\(^2\)

\[ \langle A \rangle \equiv \langle nlm | A | nlm \rangle \]

(5)
2.1.2 Wavefunction

To calculate the radial wavefunction of the valence electron, we turn to the Schrödinger equation, which is given in atomic units (a.u.) as

\[
-\frac{1}{2\mu} \nabla^2 + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)
\]  

(6)

where \(\mu\) is again the reduced mass of the electron and \(r, \theta\) and \(\phi\) are spherical coordinates and \(V(r)\) the core potential. Since \(V(r)\) has no angular dependence, we can use separation of variables and write the wavefunction as a product of an angular and a radial part. We write \(\psi(r, \theta, \phi) = R_{nl}(r) Y_{ml}(\theta, \phi)\), using the spherical harmonics \(Y_{ml}(\theta, \phi)\) which depends on the angular momentum \(l\) of the state.[2] If we plug this in in (6), we obtain the the equation for the radial wavefunction \(R_{nl}(r)\):

\[
-\frac{1}{2\mu} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{l(l+1)}{2\mu r^2} + V(r) \right] R_{nl}(r) = E R_{nl}(r)
\]

(7)

Where the term \(l(l+1)/r^2\) denotes the centrifugal energy in the electronic motion. The orbital quantum number \(l\) denotes the orbit of the quantum state.[2]

Using quantum defect theory to approximate the energy of a state and a model potential we can approximate the radial wavefunction for a given state.

2.2 Rydberg blockade

The principle of Rydberg blockade between two atoms given in the introduction (see Fig(1)) can be extended to an ensemble qubit, where each qubit consists of \(N\) atoms. This extension relies on the collective Rydberg blockade. A single atom in the Rydberg state can shift the energy states of many surrounding atoms, which leads to a collective Rydberg blockade.[5]

We follow Safman et al. and use an \(N\) atom logical 0 defined as \(|0\rangle = \Pi_{i=1}^{N}|0\rangle\) and an \(N\) atom logical 1 defined by the symmetric state with a singly excited state \(|1\rangle = 1/\sqrt{N} \sum_{i=1}^{N}|0,...,1,...,0\rangle\). We can excite qubits to the Rydberg state \(|r\rangle\) in the logical basis \(|0\rangle,|1\rangle\). Using two photon interactions, we establish a blockade shift \(B\), see Fig(3).[5]

Provided the energy shift can exceed the linewidth of the excitation laser, the shift prevents the further excitation of qubits and the shift works as a Rydberg blockade. This establishes an effective two-level system with enhanced Rabi-frequency \(\Omega_N = \sqrt{N}\Omega\). Two-qubit gates can then be obtained in analogous fashion as for two atoms. A requirement for the blockade effect for an ensemble is that the blockade interaction is present for all atoms in the ensemble.[6]

The probability for double excitation is determined by the excitation to the blockade-shifted doubley-excited state. As given by Saffman et al., the probabillity in the limit of high, but finite blockade is given by

\[
P_2 = \frac{N - 1}{N} \frac{\Omega_N^2}{2B^2}
\]

(8)
with the collective Rabi frequency given as

$$\Omega_N = \sqrt{\sum_{\gamma k} |\Omega_{\gamma k}|^2} = \sqrt{N} \Omega_0$$

with $$\Omega_0$$ the rms single-atom Rabi frequency averaged over the Rabi frequencies of the individual atoms, $$\Omega_{\gamma k}$$ the Rabbi coupling to the state $$|\gamma k\rangle$$ and the blockade shift $$B$$ given by

$$\frac{1}{B^2} = \frac{2}{N(N-1)} \sum_{\varphi;i<j} |\kappa_{\varphi ij}|^2 \Delta_{\varphi ij}^2$$

and a frequency shift $$D$$ defined via

$$\frac{1}{D} = \frac{2}{N(N-1)} \sum_{\varphi;i<j} |\kappa_{\varphi ij}|^2 \Delta_{\varphi ij}$$

In this notation the state $$|\varphi kl\rangle$$ represents the state with both the $$k$$th and the $$l$$th atom being in the Rydberg state $$\varphi$$, which is an eigenstate of the effective Rydberg-Rydberg hamiltonian with $$\Delta_{\varphi kl}$$ as energy eigenvalue: $$H_{\text{eff}} |\varphi kl\rangle = \Delta_{\varphi kl} |\varphi kl\rangle$$.\[6\]

There are generally more than one doubly-excited states $$|\varphi\rangle$$ for an atom pair i and j, so equation (8) depends on the dipole-dipole energy shift $$\Delta_{\varphi ij}$$ of each states and the dimensionless overlapfactor $$\kappa_{\varphi ij}$$, which is a measure of the relative amplitude for exciting a given pair kl of atoms to the doubly-excited Rydberg state $$\varphi$$. This overlap factor, defined later in Eq(24), depends on the geometry of the set-up and will give rise to an angular dependence for the interaction. From Eq(10) it is obvious that the blockade shift is dominated by the weakest atom-atom interaction. In an electric circuit analogy the blockade shift can be seen as an impedance $$B^2$$, which is formed by a parallel network of
individual impedances of a size $\sim (N^2/2)|\Sigma_{i<j}|\kappa_{ij}|^2/\Delta^2_{ij}|^{-1}$. An atom pair $|\varphi\rangle$ can be excited due to a weak blockade, which is analogous to short circuiting the effectiveness blockade process. So a detailed overview of the doubly-excited states is important for an effective N-atom blockade system.[6][5]

Rydberg states have a finite lifetime due to radiative decay and black-body interaction. This means that the approach in Fig(3) only yields a fidelity that is also only finitely high. This establishes a trade-off between the lifetime of the Rydberg state, which is maximised by fast excitation (e.g. excitation to a lower Rydberg state, which takes less time to excite the ensemble), and the strength of the blockade, which is maximised by slow excitation (e.g. excitation to a higher Rydberg state). It has been shown that the error $E \sim 1/(B\tau)^{2/3}$ and that gates with an error $E \leq 0.001$ are possible.[5][6]

The blockade concept in general has a few very nice properties:

1) The gate fidelity is approximately independent of the blockade shift. The blockade shift only has to be sufficient to decouple the target atom from the Rabi frequency, but apart from that, there aren’t any restrictions on the blockade.
2) The fidelity is only weakly dependent on the atomic motion. This means that temperatures $T \sim 50\mu K$ are sufficient for high fidelity.
3) The interactions occur at high atomic distances, which allow gates between optically resolved atoms without having to move the atoms physically.[6]

### 2.3 Van der Waals interaction

If we represent the dipole-dipole interaction for the two non-overlapping atoms A and B that lie a distance $R$ apart along the $z$-axis, we can write the dipole-dipole interaction as

$$V_{dd} = \frac{e^2}{R^3} (\mathbf{a} \cdot \mathbf{b} - 3a_z b_z) = \frac{-\sqrt{6} e^2}{R^3} \sum_p C_{1p1p}^{20} a_p b_p$$

(12)

with the coefficients referring to the Clebsch-Gordon coefficients. The dipole operator in the van der Waals interaction tells us that the states with $l$ are mixed with the states with $l \pm 1$ and where $m$ can differ $\pm 1$ or $0$. The selection rules for the dipole-dipole interaction tells us that $M = m_1 + m_2$, with $m_1$ and $m_2$ the projection of the angular momentum of the initial states, is conserved. Following Saffman et al., we look at the couplings of similar initial states

$$nlj + nlj \rightarrow n_sl_sj_s + n_tt_j_t$$

(13)

where $n_s$ and $n_t$ can take arbitrary values and $l_s$, $l_t$, $j_s$ and $j_t$ are fixed. An inverse measure of the strength of these couplings is given by the energy defect, given by

$$\delta_{st} = E(n_sl_sj_s) + E(n_tlj_t) - 2E(nlj)$$

(14)
If we write the interaction in second order perturbation, we retrieve the van der Waals operator
\[ H_{vdW} = \sum_{st} \frac{-V_{dd}(st)}{\delta_{st}} \langle st | V_{dd} | st \rangle \]  
(15)
as given by Safman et al. and which works on the collection of degenerate Zeeman substates. Here s and t denote the full set of quantum numbers for the intermediate states, i.e. the states to which the initial states couple. The van der Waals operator can change \( m \pm 2 \), so different Zeeman states are coupled and so degenerate perturbation is necessary. This means that \( H_{vdW} \) has to be diagonalized in the basis of Zeeman states to derive the eigenstates and eigenvalues.[6][1]

We can split the van der Waals operator in two parts
\[ H_{vdW} = C_6 R_6 D \]  
(16)
with
\[ C_6 = \Sigma_{st} e^4 \delta_{st} \left( R_{nl}^{m_s} R_{nl}^{m_t} \right)^2 \]  
(17)
with \( R_{nl}^{m_s} \) being the matrix element between the states \(|nl⟩ \) and \(|n_l l_s⟩ \). Now \( D \) holds all the properties of the angular momentum, with \((2j+1)^2\) eigenvalues \( D_ϕ \), with \( 0 > D_ϕ > 1 \). The eigenstates of the van der Waals operator are given by
\[ H_{vdW} |ψ⟩ = C_6 R_6 D_ϕ |ψ⟩ \]  
(18)
These eigenvalues are very important for the effectivity of the blockade. To calculate the \( C_6 \) coefficient, we have to sum over all the different values for \( n_s \) and \( n_t \). In practice the values for \( C_6 \) coefficient only significantly add to the interaction for \( n_s \) and \( n_t \sim n \). It’s also important to note that the van der Waals interaction has angular dependance.[6][5]

For the intermediate states \( n_s \) and \( n_t \) can have arbitrary values, but \( l_s, l_t, j_s \) and \( j_t \) are fixed. We denote the initial two-atom states \(|nljm_Anljm_B⟩ ≡ |m_A m_B⟩ \) and the coupled, intermediate states \(|n_s l_s j_s n_t l_t j_t m_l⟩ ≡ |m_l m_l⟩ \).[6]

We use the Wigner-Eckart theorem to decompose the dipole matrix element \( V_{dd} \) in terms of the radial matrix elements and the angular momentum factors
\[ \langle n'l'j'm'|r_p|nljm⟩ = (-1)^{j'+l'} \frac{1}{\sqrt{2j'+1}} \left\{ \begin{array}{c} j \cr j' \cr l \end{array} \right\} \langle n'l'||r'||nl⟩ \]  
(19)
with the reduced matrix element given by
\[ \langle n'l'||r'||nl⟩ = \sqrt{2l+1} C_{j0l0}^{l'0} R_{nl}^{l'l'} = \sqrt{2l+1} C_{j0l0}^{l'0} \int R_{nl}^{l'l'}(r) R_{nl}(r) dr \]  
(20)
where we recognize the Wigner 3j-symbols and the Clebsch-Gordan coefficients which we can look up in the literature and depends on the \( j \) and \( m_j \) of the states.[2] \( R_{nl} \) represents the radial wavefunction of the state \(|nl⟩ \) which we can calculate using the Numerov
method and $R_{nl}^{n_i l_i}$ is the radial matrix element between the state $|n \ell \rangle$ and $|n_i \ell_i \rangle$ given as $\langle n \ell | r | n_i \ell_i \rangle$. We use the operator $M$, defined by Saffman et al., which embodies all the angular momentum properties of $V_{d\ell}$

$$
\langle m_s m_t | M | m_s m_t \rangle = (-1)^{2j+1} C_0^{j0} C_0^{j0} \sqrt{6}(2l + 1)(2j + 1) \times \left\{ \begin{array}{ccc}
\ell & 1/2 & j \\
 l_s & 1 & l_t \\
 \end{array} \right\} \sum_p C_{j_s m_s}^{p} C_{j_t m_t}^{p} C_{j_s m_s}^{p} C_{j_t m_t}^{p} \tag{21}
$$

attributed with the Wigner-3j symbols and the Clebsch-Gorden coefficients. So now the degenerate van der Waals hamiltonian can be written as:

$$
H_{vdW} = C_6 R_6 \sum_{m_s, m_t} M^\dagger |m_s m_t \rangle \langle m_s m_t | M = C_6 R_6 D \tag{22}
$$

where $C_6$ depends only on the atomic energy level structure and the radial matrix elements.

The operator $D = M^\dagger M$ contains all the angular momentum properties of the states and has $(2j+1)^2$ eigenvalues $\mathcal{D}_\varphi$ since both $m_s$ and $m_t$ range from $-j$ to $j$. The long-range energies of the two-atom eigenstates are given by multiplying by $C_6$

$$
H_{vdW} |\varphi \rangle = C_6 R_6 \mathcal{D}_\varphi |\varphi \rangle \tag{23}
$$

Rydberg mediated entanglement is only possible due to the large interatomic potential, which in turn is due to the large dipole moments attributed to Rydberg atoms. The van der Waals interaction scales as $\sim n^{11}$, except for special cases where the quantum defects yield almost zero energy defects, and the resonant dipole interaction scales as $\sim n^4$, so it is beneficial to have a $n$ as high as possible. The Zeeman degeneracy of the states at zero external field causes there to be a range of different $\mathcal{D}_\varphi$ for any given set of angular momenta and for most channels there are several states with a Förster energy eigenvalue $\mathcal{D}_\varphi$ of zero, known as 'Förster zero states'. These Förster zero states can be populated by a laser and so allow doubly excited states to be excited resonantly and diminish the efficiency of the blockade. Even in the case of multiple channels, there is always a state with an almost zero $\mathcal{D}_\varphi$ and hence result to a very weak blockade. In the figure they can be seen as the flat lines at zero. The characteristic scale $R_C$ seperates the resonant dipole regime from the van der Waals regime.

It is important to note that s-states normally do not have these Förster zero states. The excitation Rabi-frequency for these transitions although is usually much lower than
for d-states. For this, and other technical reasons, the d-states are more often used for experiments. In our calculations, we will consider both initial s- and d-states.\cite{5}

Since the interaction between the atoms happens in the interatomic basis, which is a different basis than the lab basis which is defined at the hand of the chosen quantization axis, we have to project the interaction basis to the labframe. This projection gives the interaction an angle dependence. This is shown in the dimensionless overlapfactor

$$\kappa_{\varphi,kl} = \frac{\Omega_{\gamma_k} \Omega_{\gamma_l}}{\Omega_0^2} \langle \varphi kl | \gamma_k \gamma_l \rangle$$

(24)

with $|\gamma_k \gamma_l\rangle$ the doubly-excited state, which would be populated by the laser in the absence of the blockad shift. We rotate the van der Waals eigenstates to the fixed lab frame denoted by primes through

$$\langle \varphi kl | \gamma_k \gamma_l \rangle = \sum_{m_k' m_l'} \langle \varphi kl | m_k m_l \rangle d_{m_k m_k'}^{l l'} d_{m_l m_l'}^{l l'} \langle m_k' m_l' | \gamma_k \gamma_l \rangle$$

(25)

where $d^l$ denote the \textbf{Wigner rotation matrices}.\cite{6} It are these rotation matrices that give our interaction an angular dependence.\cite{6}

For example

$$d_{1/2,1/2}^{1/2} = \cos \theta / 2$$

(26)

where $\theta$, in our case represents the angle between the two interacting atoms relative to the quantization axis.
3 Results and discussion

We look at two atoms excited to the same Rydberg state |nlj⟩. The dipole interaction causes the virtual process

\[ nlj + nlj \rightarrow n_s l_s j_s + n_t l_t j_t \]  \hspace{1cm} (27)

The Förster energy defect, or energy defect is then given as [6]

\[ \delta_{st} = E(n_s l_s j_s) + E(n_t l_t j_t) - 2E(nl) \]  \hspace{1cm} (28)

We follow Saffman et al. and look at two similar initial states. We omit the p-states given by Saffman et al. and thus we only look at the transitions of two initial d- and s-states that are allowed, given the selection rules and the fact that the projection of the combined angular momentum \( M = m_1 + m_2 \) is conserved. If we exclude the states that have only weak dipole-dipole coupling and are therefore not interesting for our ends, we find the following channels as stated by Saffman et al.[6]

For initial \( s_{1/2} \)-states

\[ \delta_1 : n s_{1/2} + n s_{1/2} \rightarrow n_s p_{3/2} + n_t p_{3/2} \]  \hspace{1cm} (29a)
\[ \delta_2 : n s_{1/2} + n s_{1/2} \rightarrow n_s p_{3/2} + n_t p_{1/2} \]  \hspace{1cm} (29b)
\[ \delta_3 : n s_{1/2} + n s_{1/2} \rightarrow n_s p_{1/2} + n_t p_{1/2} \]  \hspace{1cm} (29c)

for initial \( d_{3/2} \)-states

\[ \delta_1 : n d_{3/2} + n d_{3/2} \rightarrow n_s p_{1/2} + n_t p_{1/2} \]  \hspace{1cm} (30a)
\[ \delta_2 : n d_{3/2} + n d_{3/2} \rightarrow n_s p_{3/2} + n_t p_{1/2} \]  \hspace{1cm} (30b)
\[ \delta_3 : n d_{3/2} + n d_{3/2} \rightarrow n_s p_{3/2} + n_t p_{3/2} \]  \hspace{1cm} (30c)
\[ \delta_4 : n d_{3/2} + n d_{3/2} \rightarrow n_s p_{3/2} + n_t f_{5/2} \]  \hspace{1cm} (30d)
\[ \delta_5 : n d_{3/2} + n d_{3/2} \rightarrow n_s f_{5/2} + n_t f_{5/2} \]  \hspace{1cm} (30e)
\[ \delta_6 : n d_{3/2} + n d_{3/2} \rightarrow n_s p_{1/2} + n_t f_{5/2} \]  \hspace{1cm} (30f)

and for initial \( d_{5/2} \)-states

\[ \delta_1 : n d_{5/2} + n d_{5/2} \rightarrow n_s p_{3/2} + n_t p_{3/2} \]  \hspace{1cm} (31a)
\[ \delta_2 : n d_{5/2} + n d_{5/2} \rightarrow n_s p_{3/2} + n_t f_{7/2} \]  \hspace{1cm} (31b)
\[ \delta_3 : n d_{5/2} + n d_{5/2} \rightarrow n_s p_{3/2} + n_t f_{7/2} \]  \hspace{1cm} (31c)
\[ \delta_4 : n d_{5/2} + n d_{5/2} \rightarrow n_s f_{5/2} + n_t f_{5/2} \]  \hspace{1cm} (31d)
\[ \delta_5 : n d_{5/2} + n d_{5/2} \rightarrow n_s f_{5/2} + n_t f_{7/2} \]  \hspace{1cm} (31e)
\[ \delta_6 : n d_{5/2} + n d_{5/2} \rightarrow n_s f_{7/2} + n_t f_{7/2} \]  \hspace{1cm} (31f)

where the \( \delta_i \) denote the different channels for a given initial state, as also used by Saffman et al..
For each of these channels we have to calculate an angular part and for each set of values for $n$, $n_s$ and $n_t$, a $C_6$ coefficient. The angular parts are independent of $n$, $n_s$ and $n_t$, so for a given channel $\delta_i$ and given initial states $|nlj\rangle$ we can add all the $C_6$ coefficients with differing values of $n_s$ and $n_t$ and take this sum as being the radial part, which we then have to combine with the angular part attributed to the same channel and initial states. In theory we have to calculate the $C_6$ coefficient for all values of $n_s$ and $n_t$. We will see however, that a lot of these values are small and can be neglected, and so it is important to find dominant terms.

### 3.1 Förster energy defects

The energy defect can be calculated using equation (28). Where we calculate the energy of each state by

$$E(nlj) = -\frac{R_{\text{ryd}}}{(n - \delta_{nlj})^2}$$

where $R_{\text{ryd}}$ is the Rydberg constant and $\delta_{nlj}$ the quantum defect, which can be calculated as

$$\delta_{nlj} = \delta_0 - \frac{\delta_2}{(n - \delta_0)^2}$$

where the constants $\delta_0$ and $\delta_2$ have been measured for s-, p- and d- states by Li et al. in [8] and for f-states by Han et al. in [9] and are given in table (1). For each channel, the Förster energy defect is given for various values for $n_s$ and $n_t$, see Fig(6), Fig(8), Fig(5) and Fig(7).

<table>
<thead>
<tr>
<th></th>
<th>$\delta_0$</th>
<th>$\delta_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ns$_{1/2}$</td>
<td>3.1311804(10)</td>
<td>0.1784(6)</td>
</tr>
<tr>
<td>nd$_{3/2}$</td>
<td>1.34809171(40)</td>
<td>-0.60286(26)</td>
</tr>
<tr>
<td>nd$_{5/2}$</td>
<td>1.34646572(30)</td>
<td>-0.59600(18)</td>
</tr>
<tr>
<td>nf$_{5/2}$</td>
<td>0.0165192(9)</td>
<td>-0.085(9)</td>
</tr>
<tr>
<td>nf$_{7/2}$</td>
<td>0.0165437(7)</td>
<td>-0.086(7)</td>
</tr>
</tbody>
</table>

Since Saffman et al. use the same function to calculate the energy defect taken from quantum defect theory and the same values for the quantum defects, we yield the exact same graphs for the energy defects.

### 3.2 Radial wavefunctions and radial matrix elements

In order to calculate the radial matrix elements $\langle nlj|r|nl_ij_i\rangle$, where $i$ can be $s$ and $t$, we have to approximate the radial wavefunctions $|nlj\rangle$, which depends on the distance $r$. In order to calculate these wavefunctions, we use the numerical Numerov method.

A property of this numerical approximation:
Figure 5: Förster energy defect for the coupling $nd_{3/2,5/2} \leftrightarrow ns_{1/2,3/2} + nt_{1/2,3/2}$ in Rb

![Graph showing energy defect](image)

Figure 6: Förster energy defect for the coupling $ns_{1/2} \leftrightarrow ns_{j} + nt_{j}$ in Rb

![Graph showing energy defect](image)

it solves second order differential equations of the form: $(\partial^2 + f(x))y(x) = 0$. So the equation can not have a first order derivative. Starting with function values of two neighbouring points $x_{n-1}$ and $x_n$, we can calculate the value at point $x_{n+1}$. If $f$ is known, the
Figure 7: Förster energy defect for the coupling nd_{3/2,5/2} \leftrightarrow ns_{1/2,3/2} + nt_{5/2,7/2} in Rb

Numerov method yields:

\[ y_{n+1} = \frac{\left(2 - \frac{5h^2}{6} f_n\right) - \left(1 + \frac{h^2}{12} f_{n+1} y_{n-1}\right)}{1 + \frac{h^2}{12} f_{n+1}} + O(h^6) \]  \hspace{1cm} (33)

where \( f_n = f(x_n) \) and \( y_n = y(x_n) \) represent the values at a point \( x_n \) and \( h = x_n - x_{n-1} \) denotes the difference between two neighbouring points. In numerical context, this refers to the distance between two values if we take the space as a "grid" of quantized points in space. We take \( h \) to be 0.01 \( a_0 \). When we look at the radial Schrödinger equation and substitute \( u(r) = rR(r) \), we find:

\[ \left( \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{l(l+1)}{r^2} \right) \left( E - V(r) \right) u(r) = 0 \]  \hspace{1cm} (34)

So we see that it now qualifies for the Numerov method if we take

\[ f(x) = \frac{2\mu}{\hbar^2} \left( E - V(r) \right) - \frac{l(l+1)}{r^2} \]  \hspace{1cm} (35)

and so we can numerically approximate \( u(r) \).

We can use the Numerov algorithm only if we can specify the energy levels \( E \) and the potential \( V \) at each point on our space axis. We can use quantum defect theory to specify the energy levels, so all that is left is to specify the potential. We have to introduce a model-potential. In the literature you often find:

\[ V_C(r) = -\frac{Znl(r)}{r} - \frac{\alpha_c}{2r^4} \left(1 - e^{-r/r_c}\right)^6 \]  \hspace{1cm} (36)
Figure 8: Förster energy defect for the coupling nd₃/₂,5/₂ ↔ ns₇/₂ + nt₇/₂ in Rb where the first part is associated with the Coulomb potential, with a radial charge
\[ Z_{nl}(r) = 1 + (Z - 1)e^{-\alpha_1 r} - r(\alpha_3 + \alpha_4 r)e^{-\alpha_2 r} \] (37)

with \( \alpha_c \) a measure of the core polarisability, which increases with the number of electrons in the core and the other parts are associated with the various exchange forces. The values for the \( a_1, a_2, a_3, a_4, a_c \) and \( r_c \) parameters have been calculated by Marinescu et al.[7] This Coulomb section of the model potential is strongly dominant for our case of Rydberg atoms (\( n = 40 \) to 100), so we approximate the model potential as being purely the Coulomb \(-1/r\) potential.[7]

Using this as a model potential, we can find the radial wavefunction by numerically integrating the radial Schödinger equation. This can be simplified by using the substitution \( X(r) = r_{nl}(r)^{3/4} \) with \( x = \sqrt{r} \). With this transformation, Eq(7) converts to a form which is easily solvable using the Numerov algorithm.

The explicit code for the program Mathematica we used to calculate the radial wavefunctions is given in Fig(9), here we define a wavefunction \( \psi \) which depends on the state \( nlj \) and the appropriate quantum defect, that the code calls up as \( \delta(n,l,j) \). We also had to define a \( r\psi \) function for the calculation of the radial matrix elements. Using this code (which uses the Numerov for retrieving the radial wave functions), quantum defect theory and the values for the quantum defects we are able to calculate the radial \( C_6 \) coefficients.

The code basically performs the Numerov algorithm, using the \(-1/r\) as potential and quantum defect theory to calculate the energy levels, starting at the outer radius, where the wavefunction drops to zero, and calculating inwards.

The program we use also establishes that the wavefunction should drop at \( r \sim 0 \). If the wavefunction still increases to much at this point, the program abruptly drops
the wavefunction to zero. This normally only happens for low lying states, e.g. a value for \( n \sim 10 \) see Fig(10) and Fig(11). For our purpose, \( n \geq 40 \), the radial wavefunction approximation is sufficient.

For numerical reasons, mainly the choice of the program Mathematica, we have to define a \( r\psi \) function.

When we can approximate the radial wavefunctions \( \psi_i \), we can calculate the radial matrix elements, with

\[
R^j_i = \langle \psi_i | r | \psi_j \rangle
\]  

(38)

for states \( i \) and \( j \). The radial matrix elements for the transitions divided by \( n^2 \) are shown in Fig(17). These are shown in a similar way as by Saffman et al., to compare the values. The curves show much similarities with this paper. The small difference is due to the fact that Saffman et al. use a different method for obtaining the radial wavefunction. The fact that they all seem to become linear (or actually, parabolic) shows that for increasing \( n \), the approximation of the potential being Coulombic becomes more reliable. This also shows that our approximation that the potential is a \( 1/r \) Coulombic one is reliable.

Some of the radial matrix elements have their sign reversed. This is again to better compare our figures with those of Saffman et al.. The sign of the radial matrix elements does not have any physical meaning and for the \( C_6 \) coefficient we square the values, so this is justifiable.

![Figure 9: Explicit code used in Mathematica to retrieve the radial wavefunctions and radial matrix elements](image-url)
Figure 10: Examples of the radial wavefunctions.

Figure 11: radial wavefunction of a 10s1/2 state. it is shown that at small distance to the nucleus, the approximation fails
3.3 Interaction coefficient

To calculate the complete van der Waals Hamiltonian, we need to calculate both the \( C_6 \) coefficient and the eigenvalue \( D_\phi \) for the angular part. Calculating the \( C_6 \) is fairly straightforward. For each value of \(|nlj\rangle\) for the initial states and \(|nslj_s\rangle\) and \(|ntlj_t\rangle\) for the intermediate states, we use the equation

\[
C_6 = -9.50641 \times n^{11} \left( \frac{R_{nl}^{(l_s,l_t)}}{\delta_{st}} \right)^2 \left[ \mu m^6 / GHz \right]
\] (39)

where \( R_{nl}^{(l_s,l_t)} \), where \( i \) can be \( s \) and \( t \), are the radial matrix elements and \( \delta_{st} \) the energy defects, both of which we are now able to calculate. Here \( l_s \) and \( j_s \) have fixed values, corresponding to the angular momentum of the different channels \( \delta_i \), see Eq(31), Eq(30) and Eq(29) and \( n_s \) and \( n_t \) can have arbitrary, integer values.

This means, that in theory, all the different values for \( n_s \) and \( n_t \) will add to the interaction, by adding a different \( C_6 \) coefficient for each \( \delta_i \). The \( C_6 \) values for different \( n_s \) and \( n_t \) belonging to a given value of \(|nlj\rangle\), \( l_s \) and \( l_t \) do have the same eigenvalue for the angular part, so we can sum these different \( C_6 \) together to get the sum of \( C_6 \) coefficients for given channel \( \delta_i \), i.e. for a given value of \(|nlj\rangle\) for the initial states and \( l_s j_s \) and \( l_t j_t \) for the intermediate states.

In practice, only a few values of \( n_s \) and \( n_t \) will yield a significant \( C_6 \) coefficient and we have to determine what values of \( n_s \) and \( n_t \) will be taken into account and which not. To do so, we have to look at the equation for the \( C_6 \) coefficient. It is proportional to the radial matrix elements and inversely proportional to the energy defects. The radial matrix elements will be largest when \( n_i \) and \( n \) are close to each other depending on the angular momentum of the state. Also, the energy defects will be smallest if \( n_i \) is close to \( n \). Since the energy of a state is mainly dependent on the principal quantum number.

So we take as our rule of thumb, that the \( C_6 \) value per \( n \) is greatest if \( n_s \) and \( n_t \sim n \). We also check this explicitly for a few \( n \), by calculating the \( C_6 \) for a number of \( n_s \) and \( n_t \). It is also mentioned by Saffman et al. that the dominating \( C_6 \) coefficient occur for \( n_s \) and \( n_t \) between \( n - 3 \) and \( n + 3 \) for the explicit examples.[6]

The \( C_6 \) values are very comparable to those found by Saffman et al., see table (2).

Table 2: quantum defect measurements for ns-, nd- and nf-states, taken from [8] and [9]

<table>
<thead>
<tr>
<th>channel ( \delta_i ), state ((n,n_s,n_t))</th>
<th>values from Saffman</th>
<th>our values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta_1 ), s(70,70,69)</td>
<td>799</td>
<td>796</td>
</tr>
<tr>
<td>( \delta_2 ), s(70,70,69)</td>
<td>543</td>
<td>548</td>
</tr>
<tr>
<td>( \delta_2 ), s(70,69,70)</td>
<td>589</td>
<td>579</td>
</tr>
<tr>
<td>( \delta_3 ), s(70,70,69)</td>
<td>437</td>
<td>436</td>
</tr>
</tbody>
</table>

We calculate the \( C_6 \) coefficients for each \( n \) from \( n = 40 \) to \( n = 100 \) and for multiple values for \( n_s \) and \( n_t \). For each \( n \), we calculate the \( C_6 \) coefficient for \( n_s \) and \( n_t \) differing
\[ \pm 0, 1, 2 \text{ etc. from } n. \text{ Subsequently, we build up the matrix} \]
\[ \cdots \quad \vdots \quad \vdots \quad \vdots \quad \cdots \]
\[ \cdots C_6(n_s = n - 1, n_t = n - 1) \quad C_6(n_s = n, n_t = n - 1) \quad C_6(n_s = n + 1, n_t = n - 1) \quad \cdots \]
\[ \cdots C_6(n_s = n - 1, n_t = n) \quad C_6(n_s = n, n_t = n) \quad C_6(n_s = n + 1, n_t = n) \quad \cdots \]
\[ \cdots C_6(n_s = n - 1, n_t = n + 1) \quad C_6(n_s = n, n_t = n + 1) \quad C_6(n_s = n + 1, n_t = n + 1) \quad \cdots \]
\[ \cdots \quad \vdots \quad \vdots \quad \vdots \quad \cdots \]
\[ (40) \]

We begin by adding up the first three "layers" of this matrix (so \( n_s \) and \( n_t \) differing up to three with \( n \)), then we add a new "layer" of values (so \( n_s \) and \( n_t \) differing 4 etc) and look at the relative difference between the previous total \( C_6 \) value and the new one, so the absolute difference of the old and the new value divided by the old one. If the relative change exceeds \( 10^{-4} \), we keep adding a new layer of \( C_6 \) values. If the relative change does not exceed this limit, we stop our loop. Schematically we find:

\[
\text{condition: } \frac{|C_6(n, n_s = n \pm i, n_t = n \pm i) - C_6(n, n_s = n \pm i + 1, n_t = n \pm i + 1)|}{C_6(n, n_s = n \pm i, n_t = n \pm i)} < 10^{-4} \rightarrow i + 1, \text{otherwise: stop}.
\]

The explicit code we used is shown in the Appendix I.

With this procedure we can state that our coefficient for different values of \( n_s \) and \( n_t \) has a \( 10^{-4} \) accuracy. With this procedure we also get rid of the \( n_s \) and \( n_t \) dependence. So our radial part now only depends on the given initial state \( |nlj \rangle \) and the different channel \( \delta_i \). So, for initial \( s_{1/2} \) states we calculate three radial coefficients for each value of \( n \) (three different channels, excluding different \( n_s \) and \( n_t \) values, see Eq(29) and for initial \( d_{3/2} \) and \( d_{5/2} \) states we calculate radial six coefficients for each value of \( n \) (six different channels, excluding different \( n_s \) and \( n_t \) values, see Eq(30) and Eq(31)).

Calculating the angular part is a bit more difficult. We have to look at Eq(21), where the function \( D = \mathcal{M}^\dagger \mathcal{M} \) represents all the angular parts of the van der Waals hamiltonian.

We can calculate the eigenvalues. We look at the angular part of our van der Waals hamiltonian, particulary

\[
\langle m_s m_t | \mathcal{M} | m_A m_B \rangle = \langle 1 \rangle_{l j}^{L} \langle 0 \rangle_{ls} \langle 0 \rangle_{lt} \sum_p C_{l p m_s} C_{l p m_t} C_{j p m_A} C_{j p m_B} (41)
\]

and

\[
H_{vdW} = \frac{C_6}{R^6} \sum_{m_s, m_t} \mathcal{M} |m_s m_t \rangle \langle m_s m_t | \mathcal{M} = \frac{C_6}{R^6} D (42)
\]

When we fill in the different values for \( m_s \) and \( m_t \) we can calculate the eigenvalues of the angular part.
For each channel, we have to interchange $m_s$ and $m_t$ in Eq(41) and sum the two outcomes together. For most of the states, this does not change the value much, since interchanging the two does not change the outcome and thus only adds a factor two to the value. For "asymmetric channels", like (30b),(30d), (31b), (31c), (31e), this will definitely change the value and will not add a trivial factor two.

Important to notice is that the dimension of the matrix of the angular part dependents on the value of total projection of the angular momentum $M = m_s + m_t$. For example, for the initial s-states, $j = 1/2$ for both atoms, so $M$ can be -1, 0 or 1. The number of possibilities to obtain this value of $M$ decides the dimension of the submatrix. So for $M = 1$ and $M = -1$, there is only one possibility ($m_s = m_t = \pm 1$) so the dimension is one. For $M = 0$, there are two possibilities, so the dimension is two. The total matrix will then be four by four. See Eq(43).

\[
\begin{pmatrix}
D(M = -1) & 0 & 0 & 0 \\
0 & D(M = 0) & D(M = 0) & 0 \\
0 & D(M = 0) & D(M = 0) & 0 \\
0 & 0 & 0 & D(M = 1)
\end{pmatrix}
\]

The values obtained are the same as those from Saffman et al.

When the radial coefficients and the angular $D_\phi$ are calculated, we can determine the full hamiltonian for each initial state by adding the radial coefficients to the angular matrix and adding all these for the different channels which are affiliated to the given initial states together and diagonalizing these in a shared basis. Important to notice, s that the "different" channels now are independent of the different values of $n_s$ and $n_t$ for a given value of $n$, since we summed these different $C_6$ coefficients together. The different channels $\delta_i$ now strictly refer to the angular momentum of the initial states and that of the coupling intermediate states.

So explicitly, for a given $n$ value, we have different channels, $\delta_i$ and we find

\[
H_{vdW} = \sum_i (\text{radial part for channel } \delta_i)(\text{angular part for channel } \delta_i)
\]

When we have summed these up, we can diagonalize them in a shared basis and we have retrieved the van der Waals interaction between two atoms.

For example, we find for 70s$_{1/2}$ states, the following radial coefficients:

$\delta_1$, channel : 70s$_{1/2}$ + 70s$_{1/2}$ → $n_s$p$_{3/2}$ $+$ $n_t$p$_{3/2}$, radial coefficient: 1586

$\delta_2$, channel : 70s$_{1/2}$ + 70s$_{1/2}$ → $n_s$p$_{1/2}$ $+$ $n_t$p$_{3/2}$, radial coefficient: 1119

$\delta_3$, channel : 70s$_{1/2}$ + 70s$_{1/2}$ → $n_s$p$_{1/2}$ $+$ $n_t$p$_{1/2}$, radial coefficient: 859

and if we take our calculated angular part, we find

\[
H_{vdW} = \frac{1}{81} \begin{pmatrix}
4 & 0 & 0 & 0 \\
0 & 8 & 8 & 0 \\
0 & 0 & 8 & 0 \\
0 & 0 & 0 & 4
\end{pmatrix} \times 859 + 2 \times \frac{1}{81} \begin{pmatrix}
14 & 0 & 0 & 0 \\
0 & 10 & -8 & 0 \\
0 & -8 & 10 & 0 \\
0 & 0 & 0 & 14
\end{pmatrix} \times 1119 + \frac{1}{81} \begin{pmatrix}
22 & 0 & 0 & 0 \\
0 & 26 & 8 & 0 \\
0 & 8 & 26 & 0 \\
0 & 0 & 0 & 22
\end{pmatrix} \times 1586
\]

23
which we can diagonalize in the shared basis

\[ \left( \{-1/2, -1/2\}, \{-1/2, 1/2\}, \{1/2, -1/2\}, \{1/2, 1/2\} \right). \]

which are the possible configurations of the projection of the angular momentum (both atoms have \( j = 1/2 \), so \( m = -1/2 \) or \( 1/2 \), so we find configurations \( (-1/2, -1/2), (-1/2, 1/2), (1/2, -1/2), (1/2, 1/2) \)). Notice the factor two in front of the "asymmetric" channel, \( \delta_2 \). This factor occurs because the intermediate states can be interchanged, giving a different channel, and so both of these must be taken into account. For the \( d \)-states the same procedure is used, only with more angular matrices, some of which again 'asymmetric' and need a factor two extra.

3.4 Angular dependence

Since the interaction between the atoms happens in the interatomic basis, which is a different basis than the lab basis, we have to project the interaction basis to the lab frame. This projection gives the interaction an angular dependence. A quantitative measure of the van der Waals interaction is given by the blockade shift \( B \) and the frequency shift \( D \), given by Eq(10) and Eq(11).

We start with reproducing the angular dependence plot for \( ns_{1/2} \)-states given by Saffman et al.. This graph is shown in figure (13), also with a different example Saffman et al., for an initial \( 43d_{5/2} \).

These figures are very comparable to those from Saffman et al. and have the same shape. The values are slightly different, which is probably due to the small differences in \( C_6 \) values. One reason why our \( C_6 \) values are different is that we used a different method to calculate the radial matrix elements. Another one is that we took more channels into account when calculating the total \( C_6 \) value, so more \( C_6 \) coefficients with differing values for \( n_s \) and \( n_t \). So we can state that our interaction is more detailed than that of Saffman et al., since we look at more interacting states.

We see that the interaction for the \( s_{1/2} \) states is very isotropic, which is very good for practical use. For the \( d \)-states, there is a difference in the angle, which should be taken into account when establishing an experimental set-up. Also notable, is that (see the graphs in the appendix) the behavior of the dependence is independent of the value of \( n \), whereas the strength of the shift is of course not dependent of \( n \).

For different initial states and lab bases, we encounter strange peaks, see figure (14), for a large number of \( n \)-states for \( d_{5/2} \) and a few \( n \)-states for \( d_{3/2} \) in the lab basis \( |1/2, 1/2\rangle \). It is also strange that these peaks only arise for the frequency shift and not for the blockade shift. Usually these two behave more or less the same. The position of the peaks seem to obey the \( 2\pi \) rotation symmetry (a value at an angle \( \theta \) should have the same value at \( \theta + 2\pi \)), but the height of these points seem to differ. If this is also a numerical issue (the values are 'too high' to measure accurately and thus differ) or a
(a) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $70s_{1/2}$ in Rb with a labframe: $1/2,1/2$ and $R = 9.2 \, \mu m$

(b) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $43d_{5/2}$ in Rb and Cs with a labframe: $1/2,1/2$ and $R = 9.2 \, \mu m$. taken from Saffman et al

Figure 12: Comparison of the angle dependence of the interaction with that of Saffman et al.
(a) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $43d_{5/2}$ in Rb with a lab basis: $5/2,5/2$.

(b) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $43d_{5/2}$ in Rb and Cs with a lab basis: $5/2,5/2$. Taken from Saffman et al.

Figure 13: Comparison of the angle dependence of the interaction with that of Saffman et al.
proof that these peaks are nonsense is not entirely clear. The peaks themselves are almost certainly due to numerical issues. A lot of calculation has to be done to retrieve the $C_6$ values and the angular eigenvalues. Afterwards, different channels have to be summed and diagonalized. Then, eventually, we introduce the Wigner-rotation matrices. The program that we used, Mathematica, most probably makes strange estimates due to very small values, neglecting them or overrating them, which leads to these peaks. We were unable to obtain the exact reason for this phenomenon. In our appendix, we present a few graphs for given initial states and lab basis.

4 Conclusion

The broad range of interaction strengths make Rb a very likely candidate for quantum information processing. When these atoms are brought to a highly excited Rydberg state, the enhanced dipole-dipole coupling can block multiple excitation. We took the paper from Saffman et al. as our starting point and retrieved the values for the energy defects, the radial matrix elements, the $C_6$ coefficients and the dipole and frequency shifts for two given initial $s_{1/2}$, $d_{3/2}$ and $d_{5/2}$ states.

There were small differences in the radial matrix elements most likely because Saffman et al. used a different method for retrieving the radial wavefunctions. There were also small differences in dipole and frequency shifts. This difference could be attributed to the difference in the radial matrix elements, but most likely also to the fact that we took many different interacting states into account. These interacting states have different values for the principal quantum numbers. We took many different interacting states, starting with the dominant ones. With a more detailed interaction we conclude that our values for the dipole and frequency shifts are more accurate.

For $s_{1/2}$ states, we found that the interaction is mainly isotropic, which can be beneficial for experimental purposes. For $d_{3/2}$ and $d_{5/2}$ states, these interactions do not have a trivial angular dependence, and when setting up an experiment, this should be taken into account.

In the appendix we show a few graphs for the dipole and frequency shifts for certain lab bases and certain states. Unfortunately, for a great number of initial states for nd$_{5/2}$ and a few for nd$_{3/2}$ these graphs seem to have strange peaks that seem unrealistic. The peaks are almost certainly a numerical failure, an alligation which is strengthened by the fact that the height of these peaks disobey the $2\pi$ rotational symmetry.
(a) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $70d_{5/2}$ in Rb.

(b) Angular dependence for the dipole and frequency shift due to the van der Waals interaction for an initial state $s_{1/2}$ in Rb. Zoomed in, the angular dependence seems neglecting the peaks.

Figure 14: Our calculations seem to fail us for some examples. Beneath the peaks a more believable structure is seen.
5 References

References

[7] J.Pritchard, Cooperative optical non-linearity in a blockaded Rydberg ensemble,
(a) Radial matrix elements divided by $n^2$ for the transition $ns_{1/2} \rightarrow np_{1/2}$ for Rb

(b) Radial matrix elements divided by $n^2$ for the transition $ns_{1/2} \rightarrow np_{1/2}$ for Rb, from Saffman et al.

Figure 15: radial matrix elements for the three different channels with explicit $n_s$ and $n_t$. 

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(a) Radial matrix elements divided by $n^2$ for the transition $np_{1/2} \rightarrow nsd_{3/2}$ and $np_{3/2} \rightarrow nsd_{3/2}$ for Rb.

(b) Radial matrix elements divided by $n^2$ for the transition $np_{1/2} \rightarrow nsd_{1/2}$ for Rb, from Saffman et al.

Figure 16: radial matrix elements for the three different channels with explicit $n_s$ and $n_t$. 

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(a) Radial matrix elements divided by $n^2$ for the transition $nd_{3/2} \rightarrow n_s f_{5/2}$ and $nd_{5/2} \rightarrow n_s f_{5/2}$ and $nd_{3/2} \rightarrow n_s f_{7/2}$ for Rb

(b) Radial matrix elements divided by $n^2$ for the transition $nd_{1/2} \rightarrow n_s f_{1/2}$ for Rb, from Saffman et al.

Figure 17: radial matrix elements for the three different channels with explicit $n_s$ and $n_f$. 

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6 Appendix I

We show the Mathematica code for calculating the radial parts and the angular parts of the van der Waals hamiltonian, adding the the radial part and the angular part together and the functions that plot the angular dependence.

For calculating the $C_6$ coefficients for the coupling $nlj + nlj \rightarrow n_s l_s j_s + n_t l_t j_t$, where $nlj$, $l_s j_s$ and $l_t j_t$ are fixed for a channel and $n_s$ and $n_t$ can be arbitrary, we use the code in Fig(18). Here the parameter $a$ is a measure of $n_s$ and $n_t$, basically stating how much these differ from $n$ (±1, 2 etc).

We sum different values of $C_6$ coefficients with the different values for $n_s$ and $n_t$, together using a convergence criterium to decide when to stop adding $C_6$ coefficients. We use the code given in Fig(19). In the rest of our code it is a bit confusing that what we call the $C_6$ coefficient, which we refer to as $C6[n,l,j,l_s,j_s,l_t,j_t]$, for a channel $2|nlj\rangle \rightarrow |n_s l_s j_s\rangle + |n_t l_t j_t\rangle$, is actually the sum of different $C_6$ coefficients, using the convergence criterium shown in Fig(19). These $C_6$ coefficients are independent of $n_s$ and $n_t$ and thus only dependent on the angular part of the channel ($l_j$, $l_s j_s$ and $l_t j_t$) and the $n$ of the initial states.
We calculate different properties of the angular part, that we then call up in our code. We use the code shown in Fig(20) to import the datafiles from our directory. The properties are:

- the submatrices, belonging to a certain value of the total angular momentum projection $M$, referred to as $\text{submatrix}[l,j,ls,js,lt,jt]$,
- the base, referred to as $\text{base}[n,l,ls,js,lt,jt]$.

In the code, these properties are referred to as $\text{Importlist}[l,j,ls,js,lt,jt,’submatrices’]$ and $\text{Importlist}[l,j,ls,js,lt,jt,’Base’]$.

We use the code given in Fig(21). This code sums the different submatrices together of the different channels, each with their corresponding radial part, which is called $c_6[n,l,ls,js,lt,jt]$ (which is, again, actually the sum of different $C_6$ coefficients and depends only on $n$ and not on $n_t$ and $n_s$) and diagonalizes them. This opposed to adding the full matrices together, but adding the submatrices works better for our program. The radial part, as shown in Fig(19), is referred to as $c_6[n,l,ls,js,lt,jt]$, with the initial states $|nlj\rangle$ and the angular part of the intermediate states $|ls,js\rangle$ and $|lt,jt\rangle$. Again, this definition is a bit confusing, because this is actually the sum of different $C_6$ coefficients for different values of $n_s$ and $n_t$ for a given coupling $2|nlj\rangle \rightarrow |n_s,ls,j,s\rangle + |n_t,lt,j,t\rangle$.

We use the code shown in Fig(22) to project the interatomic basis on to the lab basis, using the overlap factor $\kappa$ which. We have to define different functions for each of the initial states ($s_{1/2}$, $d_{3/2}$ and $d_{5/2}$) to use the codes shown in Fig(21) and Fig(22) and to calculate the van der Waals hamiltonian and plot the angular dependence. For initial $s_{1/2}$-states, we use the code shown in Fig(23), for initial $d_{3/2}$-states, we use the code shown in Fig(24) and for initial $d_{5/2}$-states, we use the code shown in Fig(25).

When we have defined these functions and calculated the angular and radial parts of the hamiltonian, we can make a plot of the angular dependence via the command:

```
angulardep[n, l, j, R, {{lab basis}}], Range of angles (horizontal axis), height of plot (vertical axis)
```

for the atoms in the state $|nlj\rangle$ at a distance R (in micrometers) apart.
Figure 21: code used for adding the different angular and radial parts together and diagonalizing them in a given basis to construct the van der Waals hamiltonian
Function for projecting the interatomic base and the lab base and plotting the angular dependence

\[
\text{Overlap}[[J, \theta_m, \theta_l, \gamma_m, \gamma_l]] = WignerD[[J, \theta_m, \gamma_m], \theta] WignerD[[J, \theta_l, \gamma_l], \theta]
\]

\[
\text{CalcKappas}[[\text{LabFrame}, \text{IABase}, (\text{EigenValues}, \text{EigenVectors}), J]] :=
\text{Table}[
\sqrt{\text{Length}[[\text{LabFrame}]}}
\text{Chop}[\text{Sum}[\text{EigenVectors}[[i]][[1]] WignerD[[J, \text{IABase}][[i]][[1]],
\text{LabFrame}[[k]][[1]], \theta]]
\text{WignerD}[[J, \text{IABase}][[1]][[2]], \text{LabFrame}[[k]][[2]], \theta],
\{k, 1, \text{Length}[[\text{LabFrame}]],\}
\{j, 1, \text{Length}[[\text{EigenValues}]],\}
\}
\]

\[
\text{PlotAngDep}[[\text{LabFrame}, \text{IABase}, (\text{EigenValues}, \text{EigenVectors}), J, R, \text{range}]] :=
\text{With}[[\text{kappas} = \text{CalcKappas}[[\text{LabFrame}, \text{IABase}, (\text{EigenValues}, \text{EigenVectors}), J]],
\text{Plot}[[\text{Abs} \left( \frac{1000}{R^5} \right) \text{Sqrt} \left[ \text{Total} \left( \frac{\text{kappas}^2}{\text{EigenValues}} \right) \right]], \text{Abs} \left( \frac{1000}{R^5} \right) \text{Total} \left( \frac{\text{kappas}^2}{\text{EigenValues}} \right)],
\{\theta, \text{range}[1][1], \text{range}[1][2]\}, \text{Frame} \rightarrow \text{True},
\text{ImageSize} \rightarrow \text{Large}, \text{PlotRange} \rightarrow \text{range},
\text{FrameLabel} \rightarrow \{"\theta \text{ in radians}", "|D| \text{ (red)} \text{ and } |B| \text{ (blue) in MHz}"\}]
\]

Figure 22: code used for projecting the van der Waals hamiltonian in the interatomic base (IABase) on to the lab base
Plot function for initial $s_{1/2}$ states

\[
\text{angulardep}[n, 0, \frac{1}{2}, R, \text{LabFrame}, \text{range}] := 
\]
\[
\text{PlotAngDep}[\text{LabFrame}, \text{ImportList}[0, \frac{1}{2}, 1, \frac{1}{2}, 1, \frac{1}{2}, \text{"Base"}], 
\]
\[
\text{AddChannels}[[c6[n, 0, \frac{1}{2}, 1, \frac{1}{2}, 1, \frac{1}{2}], c6[n, 0, \frac{1}{2}, 1, \frac{1}{2}, 1, \frac{3}{2}]], 
\]
\[
\text{c6}[n, 0, \frac{1}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}], 
\]
\[
\text{ImportList}[0, 1/2, 1, 1/2, 1, 1/2, \text{"SubMatrices"}], 
2 \text{ImportList}[0, 1/2, 1, 3/2, 1, 3/2, \text{"SubMatrices"}], 
\frac{1}{2}, R, \text{range}]
\]
\[
eigensystem[n, 0, \frac{1}{2}, R, \text{LabFrame}] := \text{AddChannels}[[c6[n, 0, \frac{1}{2}, 1, \frac{1}{2}, 1, \frac{1}{2}], 
\]
\[
\text{c6}[n, 0, \frac{1}{2}, 1, \frac{1}{2}, 1, \frac{3}{2}], c6[n, 0, \frac{1}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}]], 
\]
\[
\text{ImportList}[0, 1/2, 1, 1/2, 1, 1/2, \text{"SubMatrices"}], 
2 \text{ImportList}[0, 1/2, 1, 1/2, 1, 3/2, \text{"SubMatrices"}], 
\text{ImportList}[0, 1/2, 1, 3/2, 1, 3/2, \text{"SubMatrices"}], 
\frac{1}{2}, R, \text{range}]
\]
\[
\text{BlockadeShift}[n, 0, \frac{1}{2}, R, \text{LabFrame}] := \text{With}[[\text{eigensystem} - \text{eigensystem}[n, 0, \frac{1}{2}, R, \text{LabFrame}], 
\text{IABase} = \text{ImportList}[0, 1/2, 1, 1/2, 1, 1/2, \text{"Base"}], 
\text{With}[[\text{kappas} = \text{Abs}[	ext{CalcKappas}[\text{LabFrame}, \text{IABase}, \text{eigensystem}, 1/2]]]], 
\frac{1000}{R^6} / \text{Sqrt}[\text{Total}[[\text{kappas}^2 \text{eigensystem}[[1]]]]]]
\]
\[
\text{FrequencyShift}[n, 0, \frac{1}{2}, R, \text{LabFrame}] := 
\]
\[
\text{With}[[\text{eigensystem} - \text{eigensystem}[n, 0, \frac{1}{2}, R, \text{LabFrame}], 
\text{IABase} = \text{ImportList}[0, 1/2, 1, 1/2, 1, 1/2, \text{"Base"}], 
\text{With}[[\text{kappas} = \text{Abs}[	ext{CalcKappas}[\text{LabFrame}, \text{IABase}, \text{eigensystem}, 1/2]]]], 
\frac{1000}{R^6} / \text{Total}[[\text{kappas}^2 \text{eigensystem}[[1]]]]]]
\]

Figure 23: code used for adding the channels for initial $s_{1/2}$ states, calculate the van der Waals hamiltonian, projecting this on to a given lab basis and plotting the angular dependence
Plot function for initial $d_{3/2}$ states

```
angulardep[n, 2, n, 2, 3/2, R, LabFrame, range, range] :=

PlotAnyDep[LabFrame, ImportList[2, 3/2, 1, 1/2, 1, 1/2, "Base"],
AddChannels[{c6[n, 2, 3/2, 1, 1/2, 1, 1/2], c6[n, 2, 3/2, 1, 3/2, 1, 1/2],
c6[n, 2, 3/2, 1, 1/2, 1, 3/2], c6[n, 2, 3/2, 1, 3/2, 1, 3/2],
c6[n, 2, 3/2, 3, 5/2, 3, 5/2], c6[n, 2, 3/2, 1, 1/2, 3, 5/2]}],
ImportList[2, 3/2, 1, 1/2, 1, 3/2, "SubMatrices"], 2 ImportList[2, 3/2, 1, 1/2, 1, 3/2, "SubMatrices"],
ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"], 2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"],
2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"], 2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"]], 3/2, R, range]

eigensystem[n, 2, 3/2, R, LabFrame] :=
AddChannels[{c6[n, 2, 3/2, 1, 1/2, 1, 1/2], c6[n, 2, 3/2, 1, 3/2, 1, 1/2],
c6[n, 2, 3/2, 1, 1/2, 1, 3/2], c6[n, 2, 3/2, 1, 3/2, 1, 3/2],
c6[n, 2, 3/2, 3, 5/2, 3, 5/2], c6[n, 2, 3/2, 1, 1/2, 3, 5/2]}],
ImportList[2, 3/2, 1, 1/2, 1, 3/2, "SubMatrices"], 2 ImportList[2, 3/2, 1, 1/2, 1, 3/2, "SubMatrices"],
ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"],
2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"],
2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"],
2 ImportList[2, 3/2, 1, 3/2, 1, 3/2, "SubMatrices"],
BlockageShift[n, 2, 3/2, R, LabFrame] := With[{eigensystem = eigensystem[n, 2, 3/2, R, LabFrame],
IABase = ImportList[2, 3/2, 1, 1/2, 1, 1/2, "Base"],
With[{kappas = CalcKappas[LabFrame, IABase, eigensystemv, 3/2]},
1000/\text{R}^2 / \text{Sqrt[Total[(kappas^2)/(\text{eigensystemv[[1]]})^2]]}]])
```

Figure 24: code used for adding the channels for initial $d_{3/2}$ states, calculate the van der Waals hamiltonian, projecting this on to a given lab basis and plotting the angular dependence.
Plot function for initial $d_{5/2}$ states

$$\text{angulardep} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame}, \text{range} \right] :=\,$$

PlotAngDep \left[ \text{LabFrame}, \text{ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}, \text{"Base"} \right], \right.

AddChannels \left[ \left\{ \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2} \right], \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, 3, \frac{5}{2} \right], \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, \frac{7}{2}, \frac{7}{2} \right] \right\}, \text{c6} \left[ n, 2, \frac{5}{2}, 3, \frac{5}{2}, \frac{7}{2} \right] \right],

\left\{ \text{ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}, \text{"SubMatrices"} \right], \text{2 ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 3, \frac{5}{2}, \text{"SubMatrices"} \right], \right.

\text{ImportList} \left[ 2, \frac{5}{2}, 3, \frac{7}{2}, 3, \frac{7}{2}, \text{"SubMatrices"} \right], \text{ImportList} \left[ 2, \frac{5}{2}, 3, \frac{5}{2}, \frac{7}{2}, \text{"SubMatrices"} \right], \text{ImportList} \left[ 2, \frac{5}{2}, \frac{7}{2}, \frac{7}{2}, \text{"SubMatrices"} \right] \right\}], \frac{5}{2}, R, \text{range} \right] \right]

\text{eigensystem} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame} \right] :=\,$$

AddChannels \left[ \left\{ \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2} \right], \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, 3, \frac{5}{2} \right], \text{c6} \left[ n, 2, \frac{5}{2}, 1, \frac{3}{2}, \frac{7}{2}, \frac{7}{2} \right] \right\}, \text{c6} \left[ n, 2, \frac{5}{2}, 3, \frac{5}{2}, \frac{7}{2} \right] \right],

\left\{ \text{ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}, \text{"SubMatrices"} \right], \text{2 ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 3, \frac{5}{2}, \text{"SubMatrices"} \right], \right.

\text{ImportList} \left[ 2, \frac{5}{2}, 3, \frac{7}{2}, 3, \frac{7}{2}, \text{"SubMatrices"} \right], \text{ImportList} \left[ 2, \frac{5}{2}, 3, \frac{5}{2}, \frac{7}{2}, \text{"SubMatrices"} \right], \text{ImportList} \left[ 2, \frac{5}{2}, \frac{7}{2}, \frac{7}{2}, \text{"SubMatrices"} \right] \right\}] \right]

\text{BlockadeShift} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame} \right] := \text{With} \left[ \left\{ \text{eigensystem} = \text{eigensystem} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame} \right], \right. \right.

\text{IABase} = \text{ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}, \text{"Base"} \right] \right],

\left\{ \text{c6} = \text{CaloKappas} \left[ \text{LabFrame}, \text{IABase}, \text{eigensystem}, \frac{5}{2} \right] \right\},

\frac{1000 \frac{R^2}{\sqrt{\text{Total} \left[ \frac{\text{c6}^2}{\text{eigensystem}[[1]]} \right]}}}{\text{ProximityShift} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame} \right],

\text{With} \left[ \left\{ \text{eigensystem} = \text{eigensystem} \left[ n, 2, \frac{5}{2}, R, \text{LabFrame} \right], \right. \right.

\text{IABase} = \text{ImportList} \left[ 2, \frac{5}{2}, 1, \frac{3}{2}, 1, \frac{3}{2}, \text{"Base"} \right] \right],

\text{With} \left[ \left\{ \text{c6} = \text{CaloKappas} \left[ \text{LabFrame}, \text{IABase}, \text{eigensystem}, \frac{5}{2} \right] \right\},

\frac{1000 \frac{R^2}{\sqrt{\text{Total} \left[ \frac{\text{c6}^2}{\text{eigensystem}[[1]]} \right]}}}{39}

Figure 25: code used for adding the channels for initial $d_{5/2}$ states, calculate the van der Waals hamiltonian, projecting this on to a given lab basis and plotting the angular dependence.
7 Appendix II

A few examples of the plots that we can make with our calculations. Angular dependence of the dipole and the frequency shifts for given states, distance and lab bases.

Figure 26: $85s_{1/2}$, lab basis: $1/2, 1/2$
Figure 27: 100s_{1/2}, lab basis: 1/2,1/2

Figure 28: 70d_{3/2}, lab basis: 1/2,1/2
Figure 29: $40s_{1/2}$, lab basis: $1/2,1/2$

Figure 30: $70d_{5/2}$, lab basis: $5/2,5/2$
Figure 31: 100d$_{3/2}$, lab basis: $3/2,3/2$

Figure 32: 40d$_{5/2}$, lab basis: $3/2,3/2$
Figure 33: 70s$_{1/2}$, lab basis: 1/2,1/2