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# Rydberg Atom Networks for Quantum Technologies

Philip Robert KITSON

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*Supervisor:* Prof. Luigi AMICO

*Co-Supervisor:* Prof. Antonino LA MAGNA

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*In loving memory of my grandparents, Brian, Jack and Mary*



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Rydberg atoms are poised to become strong candidates for advancing quantum technologies. Their main advantage lies in the strong dipolar interactions between multiple atoms, leading to phenomena such as the Rydberg blockade and facilitation. Alongside these notable interactions, advances in optical tweezers have established the Rydberg platform for scalable technologies due to their ability to manoeuvre individual atoms into one- and two-dimensional networks. The utility of Rydberg atoms confined in optical tweezers enables applications in the key pillars of the ongoing quantum revolution—computation, simulation, communication, and metrology.

This thesis explores theoretical simulations of Rydberg excitations. Inspired by Atomtronics, which seeks to emulate electronic devices using matter waves as the current, we propose schemes to demonstrate a novel method where the current is achieved via the propagation of Rydberg excitations through circuits composed of atoms confined in optical tweezers. The work aims to lay the groundwork for new Atomtronic devices: firstly, to develop circuitry components, and secondly, a quantum sensor for electric fields.

The premise to devise such devices lies in the strong dipolar interaction between neighbouring Rydberg atoms, leading to the Rydberg blockade—a shift in the Rydberg energy level prohibiting mutual excitations. To mitigate this, a laser detuning can be introduced to counteract the energy shift—known as the Rydberg facilitation mechanism—where both local addressability of the laser detuning and precise atom positioning using optical tweezers is essential. These proposed devices depend on both phenomena to manage excitations, enable non-reciprocal flow, and facilitate decision-making, thereby functioning as electronic components such as switches, a diode, and a universal logic gate set. Our simulations leverage realistic experimental parameters to demonstrate robustness to noise and faster operation compared to matter-propagation-based counterparts.

In the context of quantum sensing, we propose an electric-field sensor composed of a Rydberg atom network arranged in a programmable two-dimensional optical-tweezer array. The sensor leverages the Stark-shift dependence of Rydberg levels on the electric field, which effectively modifies the dipole–dipole interactions and thus the blockade radii. Our detection method relies on site-resolved Rydberg excitation measurements to determine

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the absolute value of the electric field, while two-point correlations help in measuring spatially varying fields. The scheme alternates between field-insensitive reference regions and electric-field-sensitive regions, enabling in-shot normalisation, systematic error control, and a broad dynamic range determined by the atomic species and interatomic distances. All observables are detected using standard Rydberg measurement techniques on current tweezer platforms, with clear pathways towards single-shot, multi-channel electric-field sensing with adjustable precision.

Gli atomi di Rydberg sono destinati a diventare validi candidati per il progresso delle tecnologie quantistiche. Il loro principale vantaggio risiede nelle forti interazioni dipolari tra più atomi, che portano a fenomeni come la “blockade” e la facilitazione di Rydberg. Oltre a queste notevoli interazioni, i progressi nel campo delle pinzette ottiche hanno reso la piattaforma di Rydberg ideale per tecnologie scalabili, grazie alla loro capacità di manovrare singoli atomi in reti mono e bidimensionali. L'utilità degli atomi di Rydberg confinati nelle pinzette ottiche consente la loro applicazione nei pilastri chiave dell'attuale rivoluzione quantistica: calcolo, simulazione, comunicazione e metrologia.

Questa tesi esplora simulazioni teoriche di eccitazioni di Rydberg. Ispirati dall'Atomtronica, che cerca di emulare dispositivi elettronici utilizzando correnti di onde di materia, proponiamo schemi per dimostrare un nuovo metodo in cui la corrente venga ottenuta tramite la propagazione di eccitazioni di Rydberg attraverso circuiti composti da atomi confinati in pinzette ottiche. Il lavoro mira a gettare le basi per nuovi dispositivi atomtronici: in primo luogo, per sviluppare componenti circuitali e, successivamente, un sensore quantistico per campi elettrici.

La premessa per l'ideazione di tali dispositivi risiede nella forte interazione dipolare tra atomi di Rydberg adiacenti, determinando la “Rydberg blockade”, una variazione del livello energetico di Rydberg che impedisce l'eccitazione simultanea di atomi vicini. Per mitigare questo fenomeno, è possibile introdurre un detuning laser per contrastare la variazione di energia, meccanismo noto come facilitazione di Rydberg, in cui sia il controllo locale del detuning laser, sia il posizionamento preciso degli atomi mediante pinzette ottiche sono essenziali. I dispositivi proposti dipendono da entrambi i fenomeni per gestire le eccitazioni, generarne un flusso non reciproco e facilitare il processo decisionale, funzionando così come componenti elettronici come interruttori, diodi e un set di porte logiche universali. Le nostre simulazioni sfruttano parametri sperimentali realistici per dimostrare la robustezza al rumore e un funzionamento più rapido rispetto alle controparti basate sulla propagazione di materia.

Nel contesto del rilevamento quantistico, proponiamo un sensore di campo elettrico composto da una rete di atomi di Rydberg disposti in un array bidimensionale e configurabile

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di pinzette ottiche. Il sensore sfrutta la dipendenza dello Stark-shift dei livelli di Rydberg dal campo elettrico, che modifica efficacemente le interazioni dipolo-dipolo e quindi i raggi di “blockade”. Il nostro metodo di rilevamento si basa su misure locali delle eccitazioni di Rydberg di singoli atomi, per determinare il valore assoluto del campo elettrico, mentre correlatori a due punti vengono utilizzati per misurare campi spazialmente variabili. Lo schema alterna regioni di riferimento, insensibili al campo elettrico, a regioni sensibili, consentendo la normalizzazione in-shot, il controllo sistematico degli errori e un ampio intervallo dinamico determinato dalle specie atomiche e dalle distanze interatomiche. Tutti gli osservabili vengono rilevati utilizzando tecniche di misurazione standard nelle odierne piattaforme di Rydberg basate su pinzette ottiche, che offrono prospettive concrete per una rivelazione del campo elettrico single-shot e multicanale, con precisione controllabile.

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## List of publications

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1. *“Rydberg Atomtronic Devices”*

P. Kitson, T. Haug, A. La Magna, O. Morsch and L. Amico  
Physical Review A, Phys. Rev. A **110**, 043304 (2024).

2. *“Sensing electric fields through Rydberg atom networks”*

P. Kitson, W. J. Chetcuti, G. Birkel, L. Amico and J. Polo  
arXiv:2509.01665 (2025).

3. *“Perspective on new implementations of atomtronic circuits”*

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V. Singh and L. Amico  
Quantum Science and Technology, **9**, 3 (2024).

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# CHAPTER 1

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## Introduction

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Marking a century since the pioneering work by Schrödinger and Heisenberg, fuelled by theories of Planck, Bohr, and others, modern *Quantum Physics* was born [1–6]. Such fundamental discoveries laid out the *First Quantum Revolution*: besides changing our understanding of nature [7–18], quantum physics initiated transformative technologies such as lasers [19–21], transistors [22–24], and magnetic resonance imaging [25, 26] — each recognised with Nobel Prizes in Physics – having far reaching implications in society and culminating in the current digital era. We currently find ourselves amidst what is widely regarded as the *Second Quantum Revolution*, which seeks to actively harness uniquely quantum phenomena—such as superposition and entanglement for practical applications [27]. These include quantum computing [28–34], quantum communication [35, 36], quantum sensing [37], and quantum simulation [38, 39] — fields poised to revolutionise computation, information transfer, and precision measurements [40]. Proposed physical platforms hosting such technologies span a wide range of different systems, from solid-state systems like quantum dot arrays [41–44] and superconducting circuits [45, 46] to trapped ions [47–50] and atomic systems [51–54].

The field of cold atom physics has emerged from the groundbreaking experiments, notably the creation of Bose-Einstein condensates (BECs) [55, 56], which ultimately led to the 2001 Nobel Prize in Physics “*for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates*”, and the observation of fermionic degeneracy [57]. Such milestones are realised using techniques such as Doppler [58, 59] and Sisyphus cooling [60]<sup>1</sup>, and Magneto-Optical traps. This progress marked a pathway for cold atoms as a useful platform for quantum technologies in areas such as: precision measurements, quantum simulation and exploring fundamental phenomena, like superfluidity, quantum phase transitions and exotic states

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<sup>1</sup>Both of these techniques led to the 1997 Nobel Prize in Physics “*for development of methods to cool and trap atoms with laser light*”.

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of matter, with a high controllable and flexible system's conditions [52, 61, 62]. The ongoing refinement of experimental techniques continues to drive discoveries, linking atomic physics with condensed matter [63–66].

Depending on the intended application, cold atoms can be manipulated in various ways. In this thesis, we especially refer to cold atoms trapped in optical tweezers [67, 68] - one of the three important notions of this work - which allow the crafting of quantum technologies based on trapping and controlling *individual* neutral atoms. Optical tweezers can be achieved through highly focused laser beams that exert two forces on atoms: a scattering force from the photons and a gradient force that pulls the atom towards the region of highest intensity at the centre of the beam [69] (work that lead to the 2018 Nobel Prize in Physics “*for the optical tweezers and their application to biological systems*”). Indeed, networks of tweezers with a wide range of configurations and intensities have been realized in which atom-by-atom manipulations is well developed [70]. Therefore, the creation of one-dimensional [71], two-dimensional [72–74], and three-dimensional [75–77] structures are well within the state-of-the-art of the field. The capability of atom trapping has massively developed over the past 20 years, leading from the first single atom trapped [78], to surpassing the 1000-atom threshold [79] and currently extending to 6100 atoms [80].

The second notion of the present thesis is provided by Rydberg atoms. Rydberg atoms are composed of an outer shell electron that is excited to a state with a large principal quantum number [81]. Access to these highly excited states allows the atoms to exhibit a unique scaling of their properties. Firstly, somewhat counter-intuitively, Rydberg atoms have long lifetimes [82], which are rooted in the reduction of spontaneous emission as the principal quantum number increases. Furthermore, as energy is supplied to the electron, it orbits at a much larger radius, leading to increased polarisability and electric dipole matrix elements. From this feature, it follows that Rydberg atoms experience pronounced dipolar interactions, which can be characterised by either dipole-dipole coupling or Van der Waals forces [53, 83]. A consequence of these interactions is the well known Rydberg blockade [84–87] which as the name suggests, prevents atoms located within a certain vicinity of a Rydberg atom to accessing the Rydberg state as their states are shifted from resonance. Methods have been developed that can modulate the Rydberg blockade, either by enhancing or mitigating its effects. Firstly, in the presence of a small electric field Rydberg states experience a Stark shift. For certain levels this can draw them into what is known as Förster resonance, where the pair states energy show zero energy defect [88]. In this regime, the dipole-dipole interaction is enhanced manifesting in a larger blockade radius [89]. Conversely, to counteract the Rydberg blockade, a laser detuning can be introduced and tuned to pre-emptively compensate for the energy level shift. Hence, as the interaction shifts the energy level this now brings the atoms energy level onto resonance allowing for that atom to be excited to the Rydberg state - this is known as the facilitation mechanism [90–93].

Generally, the atomic structure of Rydberg atoms consists of either one or two electrons

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in the outer shell - which are typically Alkali and Alkaline-earth atoms [94] respectively <sup>2</sup>. Since alkali and alkaline-earth atoms have different energy level structures, this permits distinct excitation techniques and various applications. For alkali atoms, a direct transition is implausible as it requires a too short wavelength laser (necessitating high-powered UV light); thus, a two-photon process is needed [97, 98]. The initial excitation involves a short-wavelength laser (infrared light) reaching a low-lying state, followed by another laser with a much longer wavelength to access the Rydberg state. Cooling the atoms reduces Doppler broadening, making the transition frequency more precise, which leads to higher excitation fidelity.

In the last decade, Rydberg atoms trapped in tweezers have been very relevant in quantum technology [53, 68, 83, 99–101]. In particular:

*Quantum Computing* - Quantum computing utilises the inherent properties of quantum mechanics, such as superposition and entanglement, to develop processors capable of solving classically difficult and intractable problems (i.e., factorisation and optimisation problems [102, 103]). In the context of Rydberg atoms, their level structure enables individual atoms to act as single qubits [72, 100, 104] with gate operations carried out via laser pulses. Moreover, through the use of the well-known Rydberg blockade [84, 85] gate operations have been demonstrated [105, 106]. Through methods such as optimal control [107] for fast single pulse operations and atomic dark states to reduce scattering [108, 109], a two-qubit gates with a fidelity  $F = 0.995$  [110] operating on up to a 60 neutral atom qubits in parallel was realised. This surpasses the surface code threshold for error correction [111, 112].

*Quantum Simulation* - Quantum simulation harness controllable physical systems to emulate complex behaviours found in otherwise inaccessible microscopic phenomena. Classically, due to the exponential growth of the Hilbert space with the increasing number of atoms, simulations become difficult on a classical computer. Therefore, the conception of quantum simulations was perceived by R. Feynman, who famously said:

“because nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy” - Richard Feynman [113] (1982).

So far, Feynman’s idea has been implemented to address many diverse problems such as certain quantum annealing (in turn equivalent to relevant optimization problem) [114–117], or finding the ground state of important models, like the Hubbard model, that are central for complex systems like high  $T_c$  superconductors [38, 118–121]. The notable properties of Rydberg atoms plus the scalability of tweezer networks provide a useful platform for both analogue and digital quantum simulation [83, 122]. For example, trapped Rydberg atoms quantum simulators have been employed to study dynamics of spin models [123–127] in a variety of different physical contexts [128–133]. As particularly relevant for the present

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<sup>2</sup>Recently, also Ytterbium atoms (alkaline-earth-like) have been use in Rydberg experiments [95, 96]

thesis, spin- $1/2$  XY model, can be realised through perturbative approaches [134] involving spin exchanges between ground and Rydberg states or naturally via the dipole-dipole interaction between Rydberg states of opposite parity [135, 136]. Due to the enduring application of Rydberg quantum simulators, future studies may explore areas such as spin liquid states [137], quantum many-body scars [138–141], lattice gauge theories [142–146], and high-energy physics [147].

Dissipative quantum physics [148] can be simulated using Rydberg atoms (a topic explored in *Chapter 3*), where coupling the system to an environment induces dissipation. Spontaneous decay of the Rydberg state can be modelled through a master equation [149], and in combination with strong dipole-dipole interactions—either producing the Rydberg blockade or facilitation—lead to highly correlated systems. Such steady-state properties have been theoretically studied through non-equilibrium phase transitions [150–152] and steady-state crystallisation [153, 154]. Pure dephasing results in an uncorrelated steady state, especially in the regime of strong dephasing, which causes kinetically restrained dynamics in soft matter systems [155]. The inclusion of both dissipative mechanisms allows for a more realistic system, resulting in more complex dynamical excitation evolutions and non-trivial steady states. These dynamical evolutions enable the simulation of excitation holes in Rydberg super-atoms [156] and directed percolation phase transitions [157–159]<sup>3</sup>, which have been observed in several experimental setups [93, 161, 162].

*Quantum Sensing* - Quantum sensing leverages quantum effects to achieve precision measurements of physical quantities beyond classical - see f.i. [37]. Due to the level structure of alkali and alkali-earth atoms they provide a powerful basis in quantum sensing. The long-lived metastable states in alkaline-earth atoms allow them to be well-suited for atomic clocks [163, 164]. Furthermore, with the abundance of Rydberg states, alkali atoms have been used for the numerous transitions with frequencies ranging from 1 MHz to 1 THz. This enables a broad spectrum of electric field sensing, spanning from microwave to terahertz electric fields [53]. Previously, various techniques and configurations of Rydberg atoms have been employed to detect DC electric fields, including field ionisation and atomic beams [165, 166] ( $\approx 100\mu\text{V}/\text{cm}$ ). A major detection technique of electric fields is Electromagnetically Induced Transparency (EIT) [167–170] in which Rydberg atoms show quantum interference effects, due to a strong coupling laser and a weak probe laser creating a transparent window in an otherwise absorbing medium through coherently driving a three level system. In the presence of an electric field, the energy levels experience a Stark shift, modifying the EIT resonance which are two distinct peaks in the transmission of the probe laser. The separation of these peaks is proportional to the applied electric field [170, 171]. This technique has been shown in ultracold and vapour cells [172] (achieving a minimum measurement of  $\pm 20\mu\text{V}/\text{cm}$  [173]), and fluorescent imaging ( $\approx 10\mu\text{V}/\text{cm}$  [174]). A similar approach has been used to detect radio frequency and far-infrared electric fields, where vapour cells serve as dielectric containers to minimise perturbations to the field. Since each atom functions as a coherent quantum interferometer, EIT can be utilised, demonstrating

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<sup>3</sup>These models also mimic disease spreading [160].

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a sensitivity of  $3\mu\text{V}/\text{cm}\sqrt{\text{Hz}}$  and an accuracy of  $\approx 1\%$  for electric fields  $\approx 1\mu\text{V}/\text{cm}$  [175]. Furthermore, efforts are underway to image THz electric fields using EIT, as the Rydberg energy manifold permits numerous dipole-allowed transitions. When these are exposed to a THz electric field, the resulting changes in Rydberg state populations can be observed and imaged [176, 177].

Relying on the fact that, atoms can be indeed trapped in a variety of different networks, with the present thesis we contribute to quantum sensing leveraged by Rydberg atoms networks. Very recently, this idea has been put forward for sensing magnetic field: cold atoms arrays can be arranged, in which single atom scanning microscopy can be performed; relying on Ramsey interferometry of two hyperfine ground states within each atom magnetic fields are then sensed. Field resolutions have been measured around  $98 \pm 29\text{nT}$ , with an estimated sensitivity of  $25\mu\text{T}/\sqrt{\text{Hz}}$  [178].

The third important ingredient of the thesis is Atomtronics. The manipulation of ultracold atomic gases in matter-wave circuits—collectively referred to as Atomtronics—emerged two decades ago, establishing a novel framework for quantum technologies [63, 179–182]. Etymologically, atomtronics embodies an atomic analogue of electronics, where neutral atoms, rather than electrons, serve as current carriers [183]. The field initially centred on realizing quantum analogues of classical electronic components, including linear and circular matter-wave guides, batteries, transistors, and diodes [183, 184]. More recently, atomtronic devices have advanced into the domain of quantum (rotation) sensing and matterwave interferometry, with ring-shaped circuits forming the basis of atomic counterparts to superconducting quantum interference devices (SQUIDs), known as AQUIDs [185]. Looking ahead, atomtronics is poised to contribute significantly to quantum simulation and the study of quantum matter both in and out of equilibrium, encompassing phenomena such as quantum transport and persistent currents [186, 187].

Atomtronic circuits have traditionally been realised using bosonic, fermionic, or mixed quantum gases. However, a recent proposal investigates the use of Rydberg atoms, where the current is not transported by propagating particles but rather by Rydberg excitations [188]: *Rydberg Atomtronics*. The core idea of using Rydberg excitations instead of atomic movement relies on the timescale of the dynamics corresponding to excitations transfer. Such time scale is in the range of  $\mu\text{sec}$  to be compared to the timescale of cold atoms motion that happens in the  $\text{msec}$  time scale. Nonetheless, the practicality of employing excitations depends on the rate at which they can propagate through an atomic system, which is inherently connected to the driving frequency (typically MHz), enabling faster atomtronic devices. In this context, a directional flow of excitation in a ring-shaped atom array is generated via a complex Rabi term, which breaks time-reversal symmetry [136, 189]. Although, in this scheme, the number of excitations was not conserved, and consequently, the flow did not persist. Protocols employing quantum optimal control [190–198] were used to engineer current states and their superpositions, creating a chiral flow of excitations. [199].

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In this thesis, we pursue Rydberg Atomtronics to conceive new devices and applications in quantum sensing. Specifically, we utilise the Rydberg blockade and facilitation mechanism to study dynamical excitation propagation through differently shaped one- and two-dimensional arrays of Rydberg atoms. Furthermore, in a different context, we examine the effects of applying an electric field on the atoms, drawing certain Rydberg levels into Förster resonance, and observing the scaling of the size of the blockade radius. In monitoring this change, we develop a system which can be utilised to detect small electric fields and show spatial fluctuations across an array of Rydberg atoms.

The thesis is organised as follows:

In *Chapter 2*, we introduce Rydberg atoms and investigate the uniqueness of their properties resulting from an electron accessing a highly excited state. To distinguish between hydrogen and alkali atoms (which are prominent species used in Rydberg experiments), we provide calculations of each wavefunction and explore their distinct features. It is shown through the calculation of the electric dipole matrix that two distinct interactions arise between Rydberg states: dipole-dipole and Van der Waals, which we associate with two Rydberg atom phenomena, the blockade and facilitation mechanisms. We also include calculations of the effects of external electric fields applied to the atoms, leading to the Rydberg energy levels experiencing a Stark Shift. The physics underlying optical tweezers is examined, with a focus on the primary trapping and repelling forces. Lastly, we discuss methods which systems can be modelled, either including or excluding noise produced via decay and dephasing. Rydberg Atomtronics as a development of standard atomtronics has been highlighted in [136, 189].

*Chapter 3* is dedicated to simulating Rydberg excitation propagation across various atom networks. We use the protocol of *Rydberg atomtronics* to demonstrate different analogous electronic devices via the Rydberg blockade and facilitation. We exemplify the limits of using the full quantum mechanical equation and a classical approximation to understand dynamics across a system of  $N = 3$  atoms, then utilise the protocol to observe the propagation of excitations in a larger system comprising of  $N = 6$  atoms. By appropriately addressing the atoms detuning, it is possible to control the flow of excitations through an array, and further, by suitably managing the atom positions, enable non-reciprocal flow of excitations. Lastly, in the high dissipative regime, classical logical decisions are exhibited through excitation propagation, illustrating the scheme for an universal logical gate. Most of the contents of this chapter were published in [200].

In *Chapter 4* we propose a method to detect spatial fluctuations in electric fields by using a two-dimensional network of atoms trapped in optical tweezers. First, the discussion begins by considering specific Rydberg energy levels that shift into a Förster resonance when exposed to a small external electric field. By utilising these states near the Förster resonance, an increased blockade radius is observed through different recordings of the fully

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excited state of  $N = 3$  atoms with equal spacing. Using this, we examine the relationship between the maximum fidelity of a system of  $N = 3$  atoms and the applied electric field for fixed atom-atom separations. The inclusion of additional atoms is also investigated due to more interactions influencing the maximum fidelity. Moreover, for larger systems, spatially varying electric fields are investigated by utilising the density-density correlator, which allows the shape of the applied electric field to be estimated. Most of the contents of this chapter were published in [201].

Finally, in *Chapter 5*, we summarise the work presented in this thesis and provide a foundation for future work to be conducted.

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## Basic Concepts: Models and Methods

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In this chapter, we examine the fundamental principles of Rydberg atoms and investigate the reasons behind the distinctive scaling of their properties. In Sec. 2.1, we provide an overview of what Rydberg atoms are and their relation to the initial work conducted by Johannes Rydberg on the hydrogen atom. Section. 2.1.1 delves deeper into alkali atoms and explores the fundamental differences that arise due to the inclusion of more electrons in the atom compared to hydrogen. Moving to Sec. 2.2, we first present the analytical solution for the hydrogen wavefunction, followed by a discussion of various numerical techniques used to determine the wavefunctions of alkali atoms. Next, in Sec. 2.3, we look at the theory of dipole coupling, beginning with Sec. 2.3.1 and calculating the electric dipole matrix elements for alkali atoms, then in Sec. 2.3.2 exploring the dipole-dipole operator for different orientations of the dipole moments, to Sec. 2.3.3 and Sec. 2.3.4 which discuss the resonant and second-order dipole-dipole interactions respectively. Sprouting from these interactions, we discuss two distinct Rydberg phenomena - the Rydberg blockade and facilitation, which underpin many areas of Rydberg physics. Subsequently, in Sec. 2.5, we discuss the Stark effect and its significant relevance to Rydberg atoms. Then, Sec. 2.6 examines how optical tweezers operate and the preparation of defect-free arrays. Lastly, in Sec. 2.7, we explore two methods to model the dynamical excitation process, both of which will be thoroughly employed throughout this thesis.

### 2.1 Rydberg Atoms

Rydberg atoms are characterised by their outermost electrons - typically alkali or alkaline-earth atoms, which have one or two electrons in their outer shell respectively - that are excited to a state with a high principal quantum number  $n$  [53, 81, 83, 90]. Even though this terminology was not coined by Johannes Rydberg himself, in the late 19<sup>th</sup> century, he developed an empirical formula to describe atomic emission spectra for all electron

transitions [202] (a generalisation of the Balmer series [203]). These electron transitions from an initial state  $n_i$  to a final state  $n_f$  are summarised by the Rydberg series,

$$\frac{1}{\lambda_{n_f, n_i}} = R_\infty \left[ \frac{1}{n_f^2} - \frac{1}{n_i^2} \right], \quad (2.1)$$

providing the associated emitted wavelength  $\lambda_{n_f, n_i}$ . Here the Rydberg constant given as,

$$R_\infty = \frac{m_e e^4}{8 \epsilon_0^2 h^2 c}, \quad (2.2)$$

with  $m_e$  representing the mass of the electron,  $e$  the charge of the electron,  $\epsilon_0$  the permittivity of free space,  $h$  as Planck's constant, and  $c$  the speed of light. It was not until 1913, when Niels Bohr introduced a theoretical model to describe the quantisation of energy levels in atoms [4], that the Rydberg series could be explained using quantised orbits of electrons, leading to an expression for the energy levels of Hydrogen,

$$\epsilon_n = -h c \frac{R_\infty}{n^2}. \quad (2.3)$$

This description, accounts for a single electron; however, for heavier atoms, an analytical solution does not exist due to the additional accountability of electron-electron inters, quantum mechanical effects, relativistic corrections and fine structure. Despite this, for certain atoms known as Hydrogen-like, which have only one valence electron (examples include alkali atoms and singly ionised alkaline-earth atoms), the screening of nuclear charges by electrons in the inner shells, allows this description to correctly predict the energy transitions of atoms if the large principal quantum number is sufficiently large - i.e., Rydberg atoms.

In the subsequent sections, we will discuss the specific properties of alkali atoms in highly excited states, such as the orbital radius, polarisability, and dipolar interactions. From this basis, we describe the protocols for exciting atoms between different states and examine methods to theoretically simulate them.

### 2.1.1 Alkali Atoms

Alkali atoms (atoms belonging to group 1 of the periodic table) are commonly used in Rydberg experiments due to the ease of trapping and the hydrogen-like structure when in a highly excited state. Recently, divalent atoms <sup>1</sup> have gained increased interest for Rydberg atom experiments [94], although the primary advantages of alkali atoms still prevail. When considering alkali atoms, we have to consider that they do not entirely follow hydrogen energy levels due to: the inner electron shells shielding the nucleus, the

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<sup>1</sup>we mention other atoms such as: Calcium, Strontium, and Ytterbium [205]; which have two electrons in their outer shell but are not alkali-earth metals.

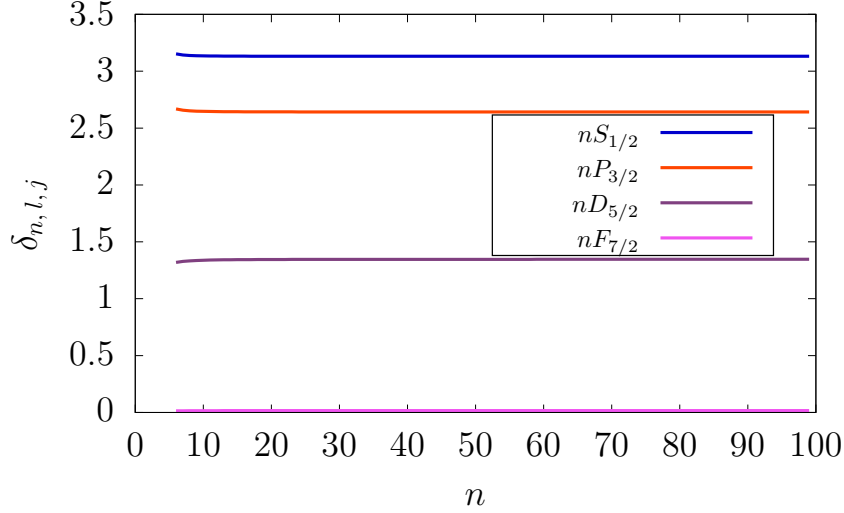


Figure 2.1: Quantum defect  $\delta_{n,l,j}$  of  $^{87}\text{Rb}$  for different angular momentum quantum numbers  $l = 0, 1, 2, 3$  for an increasing principal quantum number  $n$  and for fixed total angular momentum quantum numbers  $j$ . This data was calculated using ARC [204].

potential experienced by the valence electron is not fully Coulombic, and the electron's penetration into the inner shells is angular dependent. These consequences result in variations of energy levels compared to hydrogen, which should be considered and accounted for by quantum defect theory [206]. To incorporate these effects, we establish an effective principal quantum number  $n^* = n - \delta_{n,l,j}$ , where the quantum defect is denoted as  $\delta_{n,l,j}$ , and the subscripts  $n, l, j$  correspond to principal, angular momentum, and total angular momentum respectively. Adapting Eq. (2.3) to include such quantum defects leads to,

$$\epsilon_{n,l,j} = -\frac{R_\infty}{(n - \delta_{n,l,j})^2} = -\frac{R_\infty}{(n^*)^2}, \quad (2.4)$$

with  $\epsilon_{n,l,j}$  providing the increase in binding energy relative to the hydrogen energy levels. Since the energy defect is not strictly constant, it can be expanded as a power series,

$$\delta_{n,l,j} = \delta_0 + \frac{\delta_2}{(n^*)^2} + \frac{\delta_4}{(n^*)^4} + \dots, \quad (2.5)$$

where the higher order terms are negligible. To observe how the quantum defect is affected by the angular quantum number  $l$ , Fig. 2.1 displays  $\delta_{n,l,j}$  for the  $S, P, D$  and  $F$  orbital states of  $^{87}\text{Rb}$ <sup>2</sup>. The quantum defect is most significant for low angular momentum quantum numbers ( $l = 0, 1, 2$ ), as the electron is closer to the inner shells and penetrates deeper into the nucleus. Conversely, for  $l > 3$ , the valence electron is further away from the inner electron shells, which does not influence the nucleus, meaning the quantum defect reduces

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<sup>2</sup>This was calculated using ARC [204], which expands to  $\delta_{10}/(n^*)^{10}$ , after which the coefficients  $\delta_{12,14,\dots}$  become considerably close to zero. All the coefficients  $\delta_{0,2,\dots}$  are taken from measured energy levels.

to zero.

Alkali atoms in highly excited states exhibit unique scaling properties, making them a promising platform for quantum technologies. Table 2.1 is a concise overview of the properties of Rydberg atoms found in [83], which contains the particularly relevant ones for this thesis. The key information is rooted within the scaling of the properties, which illustrates the dependence on the principal quantum number. Through the subsequent sections, we will examine these properties further and understand where the intriguing scaling factors arise from.

| Properties                                     | Notation            | Scaling ( $n^\beta$ ) |
|------------------------------------------------|---------------------|-----------------------|
| Orbital radius                                 | $\langle r \rangle$ | 2                     |
| Polarisability                                 | $\alpha$            | 7                     |
| Resonant dipole-dipole interaction coefficient | $C_3$               | 4                     |
| Van der Waals interaction coefficient          | $C_6$               | 11                    |

Table 2.1: Tabulated properties of Rydberg atoms with the associated notation and scaling  $\beta$  with the principal quantum number  $n$ . The table includes: the orbital radius  $\langle r \rangle$ , polarisability  $\alpha$ , dipole-dipole interaction coefficient  $C_3$  and the Van der Waals interaction coefficient  $C_6$ .

## 2.2 Calculation of the Wavefunctions

### 2.2.1 Hydrogen Atoms

In atomic physics, the hydrogen atom is a model system because it has only one electron, which allows for an analytical solution to determine its wavefunction. To describe the nature of the electron's orbit, it is beneficial to express the time-independent Schrödinger equation (TISE) [207] in a spherical coordinate system,

$$\left( -\frac{\hbar^2}{2m_e} \nabla^2 + V(r) \right) \Psi(r, \theta, \phi) = \epsilon_\Psi \Psi(r, \theta, \phi), \quad (2.6)$$

where the electron provides a central potential  $V(r)$  and the energy eigenvalues  $\epsilon_\Psi$ . In this presentation, the Laplacian can be written as,

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left( \sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2}, \quad (2.7)$$

where  $r$  is the radial distance,  $\phi$  is the azimuthal angle and  $\theta$  the zenith angle. However, due to reasons presented subsequently, it is more convenient to rewrite so that the Laplacian reads:

$$\begin{aligned}
 \nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left( \sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \\
 &= \frac{1}{r^2} \left( 2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \right) + \frac{1}{r^2 \sin(\theta)} \left( \cos(\theta) \frac{\partial}{\partial \theta} + \sin(\theta) \frac{\partial^2}{\partial \theta^2} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \\
 &= \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \tan(\theta)} \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \\
 &= \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan(\theta)} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right).
 \end{aligned} \tag{2.8}$$

Substituting Eq. (2.8) into Eq. (2.6) becomes,

$$\left[ -\frac{\hbar^2}{2m_e} \left[ \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan(\theta)} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right) \right] + V(r) \right] \Psi(r, \theta, \phi) = \epsilon_\Psi(r, \theta, \phi). \tag{2.9}$$

In this form, the expression in the round brackets represents the angular momentum operator  $\hat{L}^2$  and is independent of  $r$ . Since this angular dependence is contained within  $\hat{L}^2$  and the central potential  $V(r)$  of the electron, which depends only on  $r$ , Eq. (2.9) is separable - containing an angular and a radial part. Focusing on the angular part, the eigenstates of the angular momentum operator are the spherical harmonics

$$Y_l^{(m_l)}(\theta, \phi) = (-1)^{m_l} \sqrt{\frac{(l-m_l)!}{(l+m_l)!} \frac{2l+1}{4\pi}} P_l^{(m_l)}(\cos \theta) e^{im_l \phi}, \tag{2.10}$$

where  $P_l^{(m_l)}(\cos \theta)$  are the associated Legendre polynomials, which do not encase the Condon-Shortley phase  $(-1)^{m_l}$ <sup>3</sup>. The angular  $l = 0, 1, 2, \dots$  and magnetic  $m_l = -l, \dots, l$  quantum numbers are defined, and the eigenvalues of  $\hat{L}^2$  and  $\hat{L}_z$  are  $l(l+1)$  and  $m_l$  respectively. Now, using the separation ansatz

$$\Psi(r, \theta, \phi) = R(r) Y_l^{(m_l)}(\theta, \phi), \tag{2.11}$$

where  $R(r)$  is the radial wavefunction, in conjunction with Eq. (2.6), and the eigenvalues of  $\hat{L}^2$ , yields

$$-\frac{\hbar^2}{2m_e} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} \right) + \left[ V(r) + \frac{\hbar^2}{2m_e} \frac{l(l+1)}{r^2} \right] R(r) = \epsilon_\Psi R(r). \tag{2.12}$$

Through the re-arrangement of Eq. (2.12) and the introduction of the variable:  $k(r) = 2m_e/\hbar^2[V(r) - \epsilon_\Psi]$ , this can be re-written as

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<sup>3</sup>In some representations the Condon-Shortley phase is included in the associated Legendre polynomials

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} \right) = \left( k(r) + \frac{l(l+1)}{r^2} \right) R(r). \quad (2.13)$$

Now, expanding the derivatives gives

$$\frac{\partial^2 R(r)}{\partial r^2} + \frac{2}{r} \frac{\partial R(r)}{\partial r} = \left( k(r) + \frac{l(l+1)}{r^2} \right) R(r). \quad (2.14)$$

By defining  $y_1 = R(r)$  and  $y_2 = \partial R(r)/\partial r$  the system can be expressed as two first order differential equations:

$$\begin{aligned} \frac{\partial y_1}{\partial r} &= y_2 \\ \frac{\partial y_2}{\partial r} &= \left( k(r) + \frac{l(l+1)}{r^2} \right) y_1 - \frac{2}{r} y_2. \end{aligned} \quad (2.15)$$

Resulting from hydrogen having only one proton in the nucleus, the central potential has the form of the Coulomb potential  $V(r) = -1/r$ . Using this, the radial wavefunction of the hydrogen atom can be expressed as

$$R_{n,l}(r) = \frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{(l+n)!}} \left( \frac{2r}{n} \right)^l L_{n-l-1}^{(2l+1)} \left( \frac{2r}{n} \right) e^{-r/n}, \quad (2.16)$$

where  $L_{n-l-1}^{(2l+1)}$  are the associated (generalised) Laguerre polynomials with a degree of  $n-l-1$ . The eigenenergies of the states are  $\epsilon = -1/2n^2$ . In the non-relativistic framework, the Schrödinger equation for the hydrogen atom is exact. However, with the incorporation of the coupling of the electron's spin  $s$  with its angular momentum  $l$ , this description is only an approximation. Therefore, to account for this coupling, the use of the Dirac equation is necessary, which includes the addition of the fine structure to the hydrogen level scheme.

### 2.2.2 Alkali atoms

For alkali Rydberg atoms, the energy level is given by  $\epsilon_\Psi = -h c R_\infty / (n^*)^2$  and the potential is perturbed from the Coulomb potential due to core polarisation and the spin-orbit interaction of the electron [208], which takes the form,

$$V(r) = V_p + V_c + V_{SO}. \quad (2.17)$$

The polarisation potential  $V_p$  arises from the induced core electron dipole moments (where we neglect quadrupole polarisability), and the potential has the form

$$V_p = -\frac{\alpha_c}{2r^4} \left( 1 - e^{r/\bar{r}^6} \right), \quad (2.18)$$

where  $\alpha_c$  is the static dipole polarisability of the positive-ion core,  $r$  is the radius of the electron's orbit and the cut-off radius  $\bar{r}$  removes unphysical short-range contributions close to the nucleus core. The Coulomb potential provided by the core with charge  $Z$  and the closed electron shells is given by

$$V_c = -\frac{Z_{n,l}(r)}{r} \quad (2.19)$$

where the radial charge is

$$Z_{n,l}(r) = 1 + (Z - 1)^{-a_1 r} - r(a_3 + a_4 r)e^{-a_2 r}. \quad (2.20)$$

Here, the parameters,  $a_l$  (with  $l = 1, 2, 3$ , and  $4$ ), are the multipole polarisabilities, which are obtained via a fitting procedure to experimental values [209]. The last term in Eq. (2.17) is an effective potential resulting from the spin-orbit interaction, which in relativistic form is [82]

$$V_{SO} = \frac{\bar{\alpha}^2}{2r} f(r)^2 \frac{\partial V_m(r)}{\partial r} \vec{l} \cdot \vec{s}, \quad (2.21)$$

with a fine structure constant  $\bar{\alpha}$ , the model potential  $V_m(r) = V_c(r) + V_p(r)$ ,  $\vec{l} \cdot \vec{s}$  representing the scalar product of the orbital angular momentum and the spin angular momentum of the electron and

$$f(r) = [1 + (\bar{\alpha}^2/4)(\epsilon_e - V_p - V_c)]^{-1}, \quad (2.22)$$

with  $\epsilon_e$  being the energy of the electron. Outside of the core, this simplifies to [208]

$$V_{SO} = \frac{\bar{\alpha}^2}{2r^3} \vec{l} \cdot \vec{s}, \quad (2.23)$$

where

$$\vec{l} \cdot \vec{s} = \frac{1}{2} [j(j+1) - l(l+1) - s(s+1)], \quad (2.24)$$

with  $j$  as the total angular momentum quantum number.

The additional effects of alkali atoms compared to the hydrogen atom, which influence the interaction and energy levels, implies that Eq. (2.6) cannot be solved analytically. Therefore, within the classically forbidden range from large  $r$  to 0, numerical techniques such as the Runge-Kutta method with adaptive step size (used in the Python package `rydLib` [210]) or Numerov's method with quadratic [211] or logarithmic scaling [208] (which is employed in `ARC` [204]) are utilised. To illustrate the scaling of the orbital radius

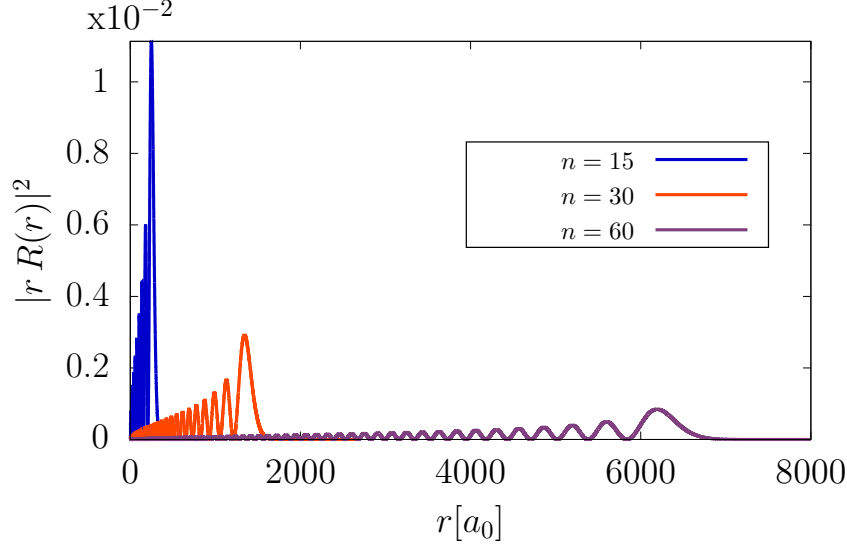


Figure 2.2: Probability distribution  $|r R(r)|^2$  for  $nS_{1/2}$  atomic wavefunction of  $^{87}\text{Rb}$ . The scaling  $r$  is expressed in units of the Bohr radius  $a_0$ .

for different principal quantum numbers, we show in Fig. 2.2 the probability distribution  $|r R(r)|^2$ .

For small principle quantum numbers  $n$ , the electron is tightly bound with a high probability, but increasing principal quantum number  $n$ , the probability distribution diminishes, but the peak shifts to larger radii. This demonstrates the scaling behaviour of the orbital radius of Rydberg atoms (see Tab. 2.1), with larger  $n$  leading to a size that can exceed  $\mu\text{m}$ .

## 2.3 Theory of Dipole-Dipole Coupling

### 2.3.1 Calculation of Electric Dipole Matrix Elements of Alkali atoms

The electric dipole matrix element of an atom describes the electric coupling between two atomic states  $|n, l, j, m_j\rangle$  and  $|n', l', j', m'_{j'}\rangle$ . For Rydberg atoms, the dipole matrix elements are significant as they encapsulate key intrinsic properties of the system (as displayed in Tab. 2.1). The electric dipole operator is defined as,  $\hat{d} = e\hat{r}$ , with  $e$  representing the elementary charge and  $\hat{r} = (x, y, z)$  as the position operator. When calculating the matrix elements, it is more practical to classify electric dipoles based on their behaviour under a coordinate system rotation. Therefore, the standard definition of a tensor in Cartesian coordinates,  $\hat{d}_{x,y,z}$ , is unsuitable, and it is more practical to define a coordinate system which under rotation act linearly. This condition is met by using spherical tensor operators,  $\hat{T}_k^{(q)}$  with the rank  $k$  having  $2k + 1$  components labelled as  $q = -k, -k + 1, \dots, k$  [212]. For the vector operator  $\hat{r}$ , this corresponds to a rank  $k = 1$  spherical tensor which has three components  $q = -1, 0, 1$ . Representing the Cartesian components in terms of a rank-1 spherical tensor can be achieved through:

$$\begin{cases} \hat{T}_1^{(+1)} = -\frac{1}{\sqrt{2}}(x + iy) \\ \hat{T}_1^{(0)} = z \\ \hat{T}_1^{(-1)} = \frac{1}{\sqrt{2}}(x - iy). \end{cases}$$

For the electric dipole operator, the appropriate choice for spherical tensors are the spherical harmonics  $Y_k^{(q)}$ , which transform analogously under a rotation of the coordinate system. The electric dipole operator can be expressed as a spherical harmonic in the following form:

$$\hat{d}_q = e\hat{r}\sqrt{\frac{4\pi}{3}}Y_1^{(q)}(\theta, \phi). \quad (2.25)$$

In a similar manner of expressing the wave function of the state  $|n, l, m_l\rangle$ , the density matrix elements can be written in two parts: radial  $R_{n,l}(r)$  and angular  $Y_1^{(q)}(\theta, \phi)$ . This representation is given as

$$\langle n, l, m_l | \hat{d}_q | n', l', m_{l'} \rangle = \langle R_{n,l} | e\hat{r} | R_{n',l'} \rangle \sqrt{\frac{4\pi}{3}} \langle Y_l^{(m_l)} | Y_1^{(q)} | Y_{l'}^{(m_{l'})} \rangle = \hat{d}_{rad} \hat{d}_{ang}. \quad (2.26)$$

Now, the matrix element is separated into two components, allowing to consider each independently. The radial component  $\hat{d}_{rad}$ , can be obtained through the numerical integration the radial wavefunction (the second part of Eq. (2.15)). Whereas the angular component  $\hat{d}_{ang}$  can be directly calculated from Eq. (2.26) using Gaunt's formula [213]. These exercises are nicely presented in [210], which as a result of the constraints for the  $3j$ - and  $6j$ - Winger symbols, produce the following selection rules:

$$|l - l'| = 1 \quad (2.27)$$

$$|j - j'| \leq 1, \text{ except } j = 0 \rightarrow j' = 0 \quad (2.28)$$

$$m_j - m_{j'} = q, \quad (2.29)$$

permitting dipole allowed transitions. Equation. (2.27), indicates that the angular momentum number must change by one, so the electron can only move between neighbouring orbitals (i.e.,  $s \leftrightarrow p$  or  $p \leftrightarrow d$ ). The rule in Eq. (2.28) says that the total angular momentum number  $j$  can change at most by one (including not changing), apart from the transition  $j = 0$  to  $j'$ . The last selection rule, Eq. (2.29), the change in the magnetic quantum number must be equal to  $q$  which is the polarization of the involved photon (here  $q = -1, 0, +1$  for left-circular, linear and right-circular respectively).

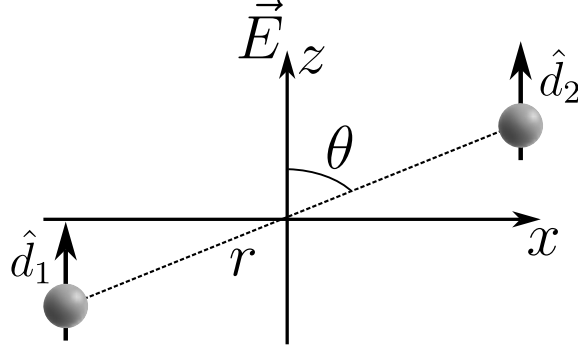


Figure 2.3: Schematic illustration of two atoms, each possessing an induced dipole moment  $\hat{d}_{1,2}$  separated by a distance  $r$ . The atoms are subject to an external electric field  $\vec{E}$  aligned with the quantisation axis  $z$ , forming an angle  $\theta$  with the unit vector  $\hat{n} = \hat{r}/r$ , which points along the line connecting the two dipoles.

### 2.3.2 The dipole-dipole operator

For two alkali atoms, as illustrated in Fig. 2.3, each with a dipole moment  $\hat{d}_1$  and  $\hat{d}_2$ , and with  $\hat{n} = \hat{r}/r$  representing the unit vector connecting the atoms separated by  $r$ , leading to the dipole-dipole operator being described as,

$$V_{dd} = \frac{\hat{d}_1 \cdot \hat{d}_2 - 3(\hat{n} \cdot \hat{d}_1)(\hat{n} \cdot \hat{d}_2)}{r^3}. \quad (2.30)$$

Here, the first term is isotropic, which is the scalar product of the two dipoles and is independent of the atom's orientation. The second term is anisotropic and depends on the projection of the dipoles along the interatomic axis; therefore, this term causes the angular dependence. The dipole moments have orientations in three dimensions, given by  $\hat{d}_i = (\hat{d}_{i,x}, \hat{d}_{i,y}, \hat{d}_{i,z})$ , with the subscript  $i$  represents the atom plus we define the quantisation axis along the  $z$ -axis and the angle between this axis and the interatomic separation,  $r$ , as  $\theta$ . Writing the dipole-dipole operator in spherical coordinates [135, 214–216],

$$V_{dd} = \frac{1}{4\pi\epsilon_0} \frac{1}{r^3} \left[ \frac{1 - 3\cos^2(\theta)}{2} (\hat{d}_{1,+} \hat{d}_{2,-} + \hat{d}_{1,-} \hat{d}_{2,+} + 2\hat{d}_{1,z} \hat{d}_{2,z}) \right. \\ \left. + \frac{3}{\sqrt{2}} \sin(\theta) \cos(\theta) (\hat{d}_{1,+} \hat{d}_{2,z} - \hat{d}_{1,-} \hat{d}_{2,z} + \hat{d}_{1,z} \hat{d}_{2,+} - \hat{d}_{1,z} \hat{d}_{2,-}) \right. \\ \left. - \frac{3}{2} \sin^2(\theta) (\hat{d}_{1,+} \hat{d}_{2,+} + \hat{d}_{1,-} \hat{d}_{2,-}) \right], \quad (2.31)$$

where  $\hat{d}_{i,\pm} = \mp(\hat{d}_{i,x} \pm i\hat{d}_{i,y})/\sqrt{2}$  are the components of the dipole operator in the spherical basis. As a result of Eq. (2.29),  $\hat{d}_z$  conserves the magnetic quantum number  $m_j$  ( $\Delta m_j = 0$ ), and  $\hat{d}_{\pm}$  altering the magnetic quantum number by one ( $\Delta m_j = \pm 1$ ).

By expressing the total magnetic quantum number as  $M = m_j^{(1)} + m_j^{(2)}$ , where the superscript indicates the atoms, and each term in Eq. (2.31) obeys  $\Delta M = 0$ ,  $\Delta M = \pm 1$ , and

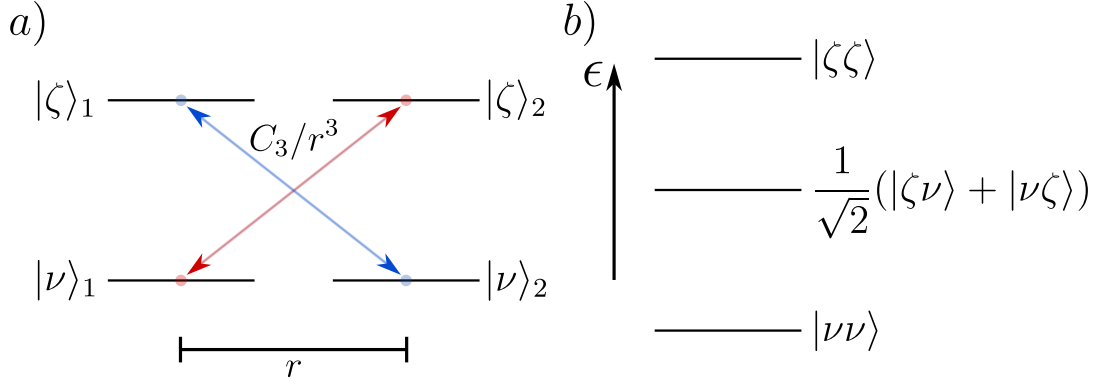


Figure 2.4: **a)** The bare states of two atoms (denoted by the subscripts: 1, 2) with the Rydberg states:  $|\zeta\rangle_{1,2}$  and  $|\nu\rangle_{1,2}$ . The atoms are separated by  $r$  and exhibit resonant dipole-dipole interactions (given from Eq. (2.35)). **b)** the energy  $\epsilon$  of the corresponding pair states.

$\Delta M = \pm 2$ , respectively. Limiting each atom to two states, results in four states in the two-atom basis. These states allow for only two types of coupling: firstly, between states close in energy, which coherently evolve by alternating states (i.e., both atoms cannot be in the same state), and secondly, between states with a sufficiently large energy difference, which can both exist in the same state. In the following sections, we will examine both types of coupling and the nature of the interactions they produce.

### 2.3.3 Resonant dipole-dipole interactions

In the two atom picture, at a separation  $r$ , the energetically similar states  $|\zeta\rangle_{1,2}$  and  $|\nu\rangle_{1,2}$  (as shown in Fig. 2.4(a) with the pair states in Fig. 2.4(b)) resonantly exchange energy, signifying that while one of the atoms is located in the state  $|\zeta\rangle$  the other must be in the state  $|\nu\rangle$ . This process mediates the coherent exchange of excitations while the involved states are of opposite parity and that the change in total magnetic quantum number is zero:  $\Delta M = 0$ , therefore, the dipole-dipole operator (Eq. (2.31)) can be simplified to

$$V_{dd} = \frac{1}{4\pi\epsilon_0} \frac{1}{r^3} \left[ \frac{1 - 3\cos^2(\theta)}{2} (\hat{d}_{1,+} \hat{d}_{2,-} + \hat{d}_{1,-} \hat{d}_{2,+} + 2\hat{d}_{1,z} \hat{d}_{2,z}) \right]. \quad (2.32)$$

Through the use of small external electric fields, the dipole moments become aligned with the quantisation axis (which we define as the  $z$ -axis), hence  $V_{dd}$  can be further simplified. This means the terms involving the  $x$ - and  $y$ -components are removed ( $\hat{d}_+$  or  $\hat{d}_-$ ). Consequently,

$$V_{dd} = \frac{1}{4\pi\epsilon_0} \frac{1}{r^3} \left[ \hat{d}_{1,z} \hat{d}_{2,z} (1 - 3\cos^2(\theta)) \right]. \quad (2.33)$$

The alignment of the unit vector  $\hat{n}$  in respect to the quantisation axis results in different angular dependencies of the dipole-dipole operator. When the unit vector is positioned

parallel to the quantisation axis, so that  $\theta = 0^\circ$  then  $(1 - 3\cos^2(\theta)) = -2$ , meaning, the operator simplifies to,

$$V_{dd} = \frac{-2}{4\pi\epsilon_0 r^3} [\hat{d}_{1,z} \hat{d}_{2,z}]. \quad (2.34)$$

This expression illustrated the attractive nature of the interactions as the dipole moments align head-to-tail along the  $z$ -axis. Conversely, when the unit vector is perpendicular to the quantisation axis,  $\theta = 90^\circ$  and  $(1 - 3\cos^2(\theta)) = 1$  which leads to,

$$V_{dd} = \frac{1}{4\pi\epsilon_0 r^3} [\hat{d}_{1,z} \hat{d}_{2,z}]. \quad (2.35)$$

Here, as the dipole moments are aligned side-by-side, they produce repulsive interactions. For atoms which are arranged perpendicular to the quantisation axis, it is common and conventional to use the notation for the dipole-dipole interaction coefficient  $C_3 = 1/4\pi\epsilon_0 [\hat{d}_{1,z} \hat{d}_{2,z}]$ . As a consequence of Eq. (2.27), the dipole moments of the Rydberg state depends on the overlap of the orbitals of  $l$  and  $l' = l \pm 1$ . For low  $l$  (generally  $l \ll n$  for Rydberg atoms <sup>4</sup>), this overlap is greatest resulting in strong dipole moments and leads to a scaling factor  $\beta = 2$  [83, 217]. Subsequently, the dipole-dipole interaction scales with a factor  $\beta = 4$  [100] - as shown in Tab. 2.1.

The modelling of the interactions between Rydberg states of opposite parity can be through the electric dipole-dipole Hamiltonian:  $V_{dd} \propto C_3/r_{i,j}^3$ . In the situations, where there is a coherent driving  $\Omega$  and a laser detuning from the atomic resonance  $\Delta$ , the Hamiltonian reads [218]

$$H = \Omega \sum_i \sigma_i^x - \Delta \sum_i \sigma_i^z + \sum_{i \neq j} \frac{C_3}{r_{ij}^3} (\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+), \quad (2.36)$$

with the final term relates the coherent ‘flip-flop’ of the internal states:  $|\zeta \nu\rangle$  and  $|\nu \zeta\rangle$  which scales with the dipole-dipole interaction, this can be computed using the python package [204] or tutorial [219]. This is indeed the XY hamiltonian, with the transverse and longitudinal fields being represented as the driving  $\Omega$  and the laser detuning  $\Delta$  respectively [218].

### 2.3.4 Second-order dipole-dipole interactions

For the second type of coupling (briefly discussed towards the end of Sec. 2.3.2), which occurs between states that are separated in energy by several tens of GHz, the excitation process connecting the states - which can be considered as the ground state  $|g\rangle$  and a

<sup>4</sup>for circular Rydberg atoms, defined by having a maximum angular momentum quantum number so that  $l = n - 1$ , this is not the case, as this condition assumes  $l \approx n$  so that the dipole moment is weaker in comparison to non-circular Rydberg atoms.

Rydberg state  $|\xi\rangle$  - occurs due to a two-photon process - as shown in Fig. 2.5(a). In the pair state basis, as seen in Fig. 2.5(b), the effects of the dipole-dipole operator are evident through the first-order expectation value:  $\langle \xi \xi | V_{dd} | \xi \xi \rangle = 0$ , because the operator only acts upon states of opposite parity. Consequently, higher-order terms must be considered, which can be physically realised by initially exciting to an intermediate state  $|k\rangle$  that has a dipolar coupling to both  $|g\rangle$  and  $|\xi\rangle$ . This energy correction can be derived via a second-order time-independent perturbation expansion

$$\epsilon^{(2)} = \sum_k \frac{|\langle k k | V_{dd} | \xi \xi \rangle|^2}{2(\epsilon_\xi - \epsilon_k)} \quad (2.37)$$

with the sum running over all possibilities of dipole allowed pair states and the energy of the pair states  $|k k\rangle$  and  $|\xi \xi\rangle$ :  $\epsilon_k$  and  $\epsilon_\xi$  respectively. As

$$\langle k k | V_{dd} | \xi \xi \rangle = \frac{1}{4\pi\epsilon_0 r^3} \langle k | \hat{d}_1 | \xi \rangle \langle k | \hat{d}_2 | \xi \rangle = \frac{C_3}{r^6}, \quad (2.38)$$

therefore,

$$\epsilon^{(2)} = \sum_k \frac{|\langle k k | V_{dd} | \xi \xi \rangle|^2}{2(\epsilon_\xi - \epsilon_k)} \propto -\frac{C_6}{r^6}. \quad (2.39)$$

Here the Van der Waals coefficient is expressed as,

$$C_6 = \sum_k \frac{|\langle k k | V_{dd} | \xi \xi \rangle|^2}{2(\epsilon_k - \epsilon_\xi)} = \frac{C_3^2}{\delta} \quad (2.40)$$

where  $\delta$  is an energy defect. As the dipole-dipole coefficient has a scaling factor  $\beta = 4$  and the energy defect  $\delta = 2(\epsilon_k - \epsilon_\xi)$  scales with  $\beta = 3$ , this leads to the Van der Waals interaction coefficient with  $\beta = 11$  - see Tab. 2.1.

In the frozen wave approximation, the description to model the dynamical process of driving an ensemble of  $N$  atoms from the ground state  $|g\rangle$  to a Rydberg state  $|\xi\rangle$ , is given via the Hamiltonian [218, 220]

$$H = \sum_i^N \Delta_i n_i + \Omega_{eff} \sum_i^N \sigma_i^x + \frac{1}{2} \sum_{i \neq j}^N \frac{C_6}{|x_i - x_j|^6} n_i n_j. \quad (2.41)$$

Here,  $\Delta$  is a laser detuning,  $n_i = \frac{1}{2}(\sigma_i^z + \mathbb{1})$  represents the number operator and  $\sigma_i^u$  (with  $u = x, y, z$ ) denote the Pauli matrices. The driving between the ground and Rydberg state is supplied by an effective Rabi frequency  $\Omega_{eff}$  provided by,

$$\Omega_{eff} = \frac{\Omega_{(\lambda_1)} \Omega_{(\lambda_2)}}{2 \Delta_k}, \quad (2.42)$$

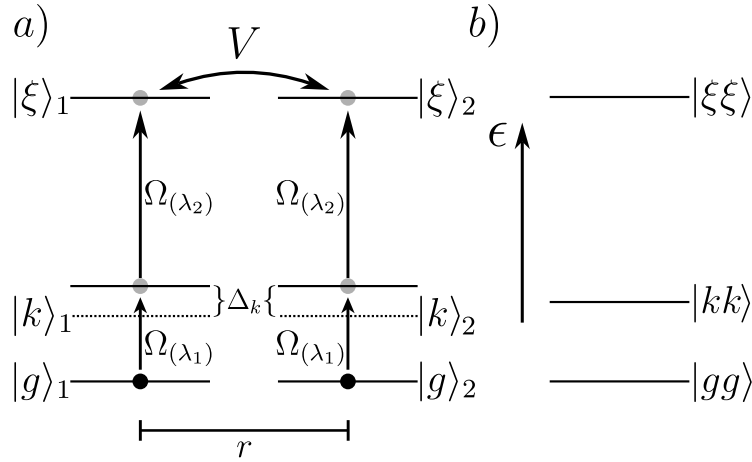


Figure 2.5: **a)** The bare states of two atoms which are separated by  $r$  and are comprised of the ground state  $|g\rangle_{1,2}$ , an intermediate state:  $|k\rangle_{1,2}$  which is detuned by  $\Delta_k$  and the Rydberg state  $|\xi\rangle_{1,2}$ . The two-photon process is depicted by two lasers with drivings  $\Omega_{(\lambda_1)}$  (the ground to intermediate state) and  $\Omega_{(\lambda_2)}$  (the intermediate state to the Rydberg state). **b)** the energy levels of the pair states.

with Rabi frequency  $\Omega$  each with a subscripts  $(\lambda_1)$  and  $(\lambda_2)$  denoting the wavelength of each laser and  $\Delta_k$  being the detuning of the intermediate state  $|k\rangle$ . The effective Rabi frequency acts globally on all of the  $N$  atoms, and the Van der Waals coefficient  $C_6$  is the strength at which two Rydberg states interact. Equation. (2.41) has the form of a quantum Ising model [128, 130, 221, 222]<sup>5</sup> where the transverse and longitudinal magnetic fields correspond to  $\Omega$  and  $\Delta$  respectively and the Ising coupling decays with  $1/r^6$ .

## 2.4 Rydberg Phenomena

### 2.4.1 Rydberg Blockade

The previous sections discussed the strong dipole matrix elements that lead to two distinct types of interactions. A particular interesting consequence of these interactions is the phenomenon known as the Rydberg blockade [84–87]. It is instructive to first consider the Rydberg blockade between two atoms driven from the ground state to the Rydberg state with a frequency  $\Omega_{eff}$ . Supposing both atoms are excited to the Rydberg state, their mutual interaction would cause an energy shift that prevents the initial excitation—thus blocking such process. In order to avoid resonance effects caused by laser detuning, the blockade is most prominent when  $\Delta = 0$ . To observe the blockade, the energy shift must exceed the laser linewidth; otherwise, mutual excitations can still occur. Therefore, in defining a boundary at which the blockade becomes effective, the interaction and the driving frequency must satisfy the condition  $C_k/r^k = \Omega_{eff}$  where  $r^k = |x_i - x_j|^k$ . This occurs within a specific region, known as the blockade radius  $r_b = (C_k/\Omega_{eff})^{1/k}$ , with  $k = 3$  for dipole-dipole interactions and  $k = 6$  for Van der Waals interactions.

<sup>5</sup>Eq. 2.41 is the same form as  $H_{Ising} = \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z + \sum_i (h_i^x \sigma_i^x + h_i^z \sigma_i^z)$  [223]

In the case of a larger system comprised of  $N$  atoms, which can either be contained within a magneto-optical trap or in optical tweezers, the blockade radius can encompass multiple atoms - defining a Rydberg superatom [98, 100, 224, 225]. By considering that the entire ensemble can be encapsulated by a single blockade radius, the Rydberg superatom, is a collection of all the atoms in the ground state with a single Rydberg atom at its epicentre. In this description, the system has a ground state  $|G\rangle = |g_1, \dots, g_N\rangle$  and a symmetric singly-excited state represented by the W state:  $|W\rangle = 1/\sqrt{N} \sum_{i=1}^N |g_1, \dots, \xi_i, \dots, g_N\rangle$  (with  $|\xi\rangle$  being the Rydberg state) where both states can be coupled through an enhanced Rabi frequency  $\Omega_N = \sqrt{N} \Omega_{eff}$ . However, further transitions to higher excited states are blocked.

The blockade has been demonstrated in both gas clouds [226] and with individually trapped atoms [105, 227–229].

### 2.4.2 Rydberg Facilitation

To counteract the Rydberg blockade, a method involving laser detuning that compensates the energy shift is used - this is known as the Rydberg facilitation mechanism [91, 92]. In the two-atom picture, the technique involves an energy level offset created through laser detuning; therefore, when the shift occurs, it brings the atoms' energy levels into resonance, allowing both atoms to be driven to the Rydberg state. To satisfy this criterion, two conditions must be met: the laser detuning must greatly exceed the driving strength,  $|\Delta| \gg \Omega_{eff}$  and the detuning must be equal in magnitude but opposite in sign to the interaction,  $\Delta_f = -C_6/r^6$ . When these conditions are fulfilled, at the precise perimeter, known as the facilitation radius  $r_f = (C_6/\Delta)^{1/6}$ , the atoms need to be positioned for both to be excited.

In larger ensembles, the facilitation condition can be achieved when each atom experiences a laser detuning proportional to the interaction and distance from the initial excitation. Therefore, if multiple atoms lie upon the facilitation radius with the correct detuning each atom's energy shift is compensated for and all can be excited.

## 2.5 The Stark Effect

The Stark effect [230] is the shifting or splitting of energy levels caused by an external electric field <sup>6</sup>. For Rydberg atoms, the Stark effect is particularly pronounced due to their spatially large electron wavefunctions, allowing small electric fields to significantly perturb the loosely bound electron.

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<sup>6</sup>This is analogous to the Zeeman splitting with magnetic fields, which we will not investigate in this thesis.

Owing to the selection rules of the dipole operator (Eq. 2.27), the coupling between states with the same angular momentum  $l$  is forbidden because of the equal parity; therefore, second-order perturbation theory is required for Rydberg states with  $l < 4$  in the presence of a small electric field  $\vec{E}$ <sup>7</sup>. This results in a quadratic Stark effect:

$$\Delta\epsilon_S = \sum_{k \neq i} \frac{|\langle \psi_k | \hat{d} \cdot \vec{E} | \psi_i \rangle|^2}{\epsilon_k - \epsilon_i} = -\frac{1}{2} \alpha |\vec{E}|^2, \quad (2.43)$$

where the subscript  $i$  denotes the initial state, and the sum runs over all states  $k$ . Although all states  $k$  contribute in principle, only a few have significant impact due to the small energy differences  $(\epsilon_k - \epsilon_i)$ , which dominates the  $1/(\epsilon_k - \epsilon_i)$  dependence. Additionally, contributions are further restricted by the selection rules related to the absolute value of the projection of the magnetic quantum number for total angular momentum  $|m_j|$ . The quadratic Stark shift, is particularly notable for Rydberg states due to the fierce polarisability, inducing a dipole moment. The effect is the atom's response to external electric fields and has a scaling factor  $\beta = 7$ .

For Rydberg states with high angular momenta  $l > 4$ , there are no quantum defects, and degenerate states of opposite parity appear. This allows the mixing of states and the formation of eigenstates with a permanent electric dipole moment. Consequently, a linear Stark effect occurs in first-order perturbation theory.

For electric fields where the Stark shift  $\Delta\epsilon_S$  is on the order of the energy difference to the next dipole coupled states, the Stark effect cannot be treated perturbatively. For this reasons, the Stark shifts are calculated by diagonalising the Hamiltonian

$$H = H_0 + H_E \quad (2.44)$$

where  $H_0$  represents the eigenenergies at zero electric field, and  $H_E = \hat{d} \cdot \vec{E}$  is the Hamiltonian for the electric field. The matrix elements of  $H_E$  can be found using Eq. (2.26). Since this is a non-perturbative approach, all possible states  $|n, l, s, j, m_j\rangle$  must be considered. However, due to the selection rules for electric dipole transitions, there are sub-spaces of states that are not coupled and can therefore be treated independently. Because the radial electric dipole coupling  $\hat{d}_{rad}$  decreases significantly as  $|n_i - n_k|$  increases, it is sufficient to restrict the basis to states with  $n \pm 5$  [210]. Furthermore, the calculation can be limited to states with the same  $m_j$  ( $\Delta m_j = 0$ ) as a consequence of Eq. (2.29).

## 2.6 Optical Tweezers

Optical tweezers are a sophisticated tool that uses focused light to trap and manipulate particles. They have a wide-range of uses spanning for direct use in physics of trapping

<sup>7</sup>For the following description, we assume the electric field is aligned with the quantisation axis.

atoms and quantum dots ( $\approx 0.1 - 10$  nm), to biological with virus and bacteria ( $\approx 10 - 100$  nm) and chemistry with synthetic colloids ( $\approx 100$  nm -  $10\mu\text{m}$ ) applications [231]. They can be utilised for many different particles from the nanometer (atoms), micrometer (cells and viruses) and millimeter (dielectric beads) scales [231]. The technique relies on the radiation pressure of light exerting piconewton-scaled forces in order to trap the particle in the light beam. Using a highly focused beam, as shown in Fig. 2.6, a particle experiences a forces due to the interaction with the light's electric field. The interaction is composed of two components: gradient force and a scattering force <sup>8</sup>.

The gradient force is a stable trapping force exert upon the particle toward the region of highest intensity - the focus of the beam. As a result of the electric field, the particle behaves as a dipole, therefore drawing it close toward the center of the light beam. On the other hand, the scattering force, is caused by momentum transfer of the photons on to the particle due to scattering and/or absorption. This is an unstable force as it is acting to move the particle away from the trap and is directed parallel to the propagation of the light beam.

From this description above, there are three different regimes which are dependent on the size of particle compared to the wavelength of the laser used for the optical tweezer. These regimes are known as:

1. Rayleigh Regime ( $r \ll \lambda$ ) [232]
2. Mie Regime ( $r \approx \lambda$ ) [233]
3. Geometric Tay Optics model ( $r \gg \lambda$ ) [234].

For this discussion, we will consider the trapping of atoms whose ground-state size is much smaller than the wavelength of the laser. Consequently, the following analysis will focus on the Rayleigh regime.

### 2.6.1 Gradient Force

In the Rayleigh regime, due to the atoms size across the dielectric the electric field  $\vec{E}(\vec{r}, t)$  can be considered to be uniform. A result of this allows the treatment of the atoms to act as induce point dipoles

$$\hat{d}(\vec{r}, t) = \alpha \vec{E}(\vec{r}, t), \quad (2.45)$$

which is portrayed with polarisibility  $\alpha$ . The force gradient expressed as

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<sup>8</sup>The particle experiences more forces such as a gravitational force, but in this description we only consider the forces due to the laser light.

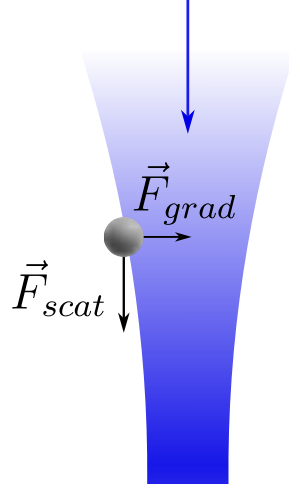


Figure 2.6: The forces which an atom experiences due to an optical tweezer.  $\vec{F}_{grad}$  is the gradient force drawing the atom to the region of higher intensity and the scattering force  $\vec{F}_{scat}$  provided by the scattering/absorption of the photon momentum in the propagation of the light (symbolised by the downward facing arrow).

$$\vec{F}_{grad}(\vec{r}, t) = [\hat{d}(\vec{r}, t) \nabla] \vec{E}(\vec{r}, t), \quad (2.46)$$

and by using the identity  $\nabla^2 = 2(\vec{E} \cdot \nabla) \vec{E} + 2\vec{E} \times (\nabla \times \vec{E})$  and assuming the electromagnetic field is constant, Faraday's law:  $\nabla \times \vec{E} = -\partial \vec{B} / \partial t = 0$ , it becomes

$$\vec{F}_{grad} = \frac{1}{2} \alpha \nabla \vec{E}^2(\vec{r}, t). \quad (2.47)$$

The gradient force which the atom experiences is time-averaged, so  $\langle \vec{E}^2(\vec{r}, t) \rangle_t = \frac{1}{2} |\vec{E}(r)|^2$  which yields:

$$\vec{F}_{grad}(r) = \langle \vec{F}_{grad}(\vec{r}, t) \rangle_t = \frac{1}{2} \alpha \nabla \langle \vec{E}^2(\vec{r}, t) \rangle_t = \frac{1}{4} \alpha \nabla |\vec{E}(\vec{r})|^2. \quad (2.48)$$

The intensity of the light beam is given as [232]

$$I(\vec{r}) = \frac{n_a \epsilon_0 c}{2} |\vec{E}(\vec{r})|^2, \quad (2.49)$$

where  $n_a$  is the refractive index of the atom,  $\epsilon_0$  the permittivity of free space and  $c$  the speed of light. By substituting into Eq. (2.48) gives,

$$\vec{F}_{grad}(\vec{r}) = \frac{1}{2n_a \epsilon_0 c} \alpha \nabla I(\vec{r}). \quad (2.50)$$

This expression indicates that at higher light beam intensity, the gradient force becomes stronger, thereby drawing the atom towards the focus point of the beam.

### 2.6.2 Scattering Force

The scattering force is proportional to the energy flux and is direction along the propagation of the light, represented by [235, 236]

$$\vec{F}_{scat} = n_m \frac{\sigma \langle S \rangle}{c}, \quad (2.51)$$

where  $n_m$  is the refractive index of the medium,  $\langle S \rangle$  is the Poynting vector and  $\sigma$  is the scattering cross section of a Rayleigh sphere of radius  $r$ , which is given as [237]

$$\sigma = \frac{8}{3} \pi (k r)^4 r^2 \left( \frac{m^2 - 1}{m^2 + 2} \right)^2, \quad (2.52)$$

with  $m = n_a/n_m$  being the relative refractive index and  $k = 2\pi n_m/\lambda$  as the wave vector associated to the laser light of wavelength  $\lambda$ .

To efficiently trap atoms in optical tweezers, either  $\vec{F}_{scat}$  needs to be small or  $\vec{F}_{grad}$  needs to be large-which can be achieved in two ways. By observing Eq. (2.51),  $\vec{F}_{scat}$  can be reduced if the refractive index of the medium is small compared to the refractive index of the atoms (so  $n_a > n_m$ ). On the other hand, from Eq. (2.50)  $\vec{F}_{grad}$  can be increased by having a lens with a high numerical aperture, as this decreases the focal point size therefore increasing the intensity of the beam.

### 2.6.3 Loading of the Optical Tweezers

Loading the tweezers is crucial for creating atom arrays. This process begins with the generation of a magneto-optical trap (MOT) that confines a gas cloud of atoms and cools them to suitable temperatures. The tweezers are overlapped with the MOT, where nearby atoms are drawn into the regions of high intensity, trapping some atoms in the optical tweezers. Once this process is complete, the MOT is turned off and the tweezers are loaded. However, due to light-assisted collisions, if two atoms enter a trap, they repel each other, leaving the tweezer empty. As a result, stochastic loading occurs, with each tweezer either trapping a single atom or none at all. This phenomenon, known as the collisional blockade mechanism, and results in a loading probability of roughly 50% for the entire tweezer array [68].

With half the tweezers filled and half empty, constructing useful arrays for computation and simulation requires a technique called atom-by-atom assembly. Typically, the process begins with an array containing more than twice as many tweezers as the number of atoms needed. After loading, a short image pulse is used to detect the atoms via fluorescence, and a camera records the population in each tweezer. Once the atom positions are known, a classical algorithm is employed to re-arrange the tweezers to form the desired atom array. Using equipment such as spatial light modulators (SLMs), the atoms can be adiabatically

rearranged <sup>9</sup>. This technique is generally used to create defect-free arrays in one, two, and three dimensions.

## 2.7 Modelling State Dynamics

As this thesis pertains to the simulation of Rydberg excitations, the following section discusses two ways in which to model time evolutions of density matrices: systems which are closed to any environmental noise and systems are exposed to the environment (the atoms are susceptible to dissipation in the form of decay and dephasing).

### 2.7.1 Closed Systems

In an idealised setting, where a system is completely isolated from the environment (with no sources of dissipation), the ability to describe how a quantum state (whether mixed or pure) evolves over time is given by the Liouville-von Neumann equation [238]. By considering  $N$  systems with a state  $|\Psi\rangle$  in an ensemble, each with a probability  $p_i$ , the mixed state density matrix can be expressed as,

$$\rho^{mix} = \sum_i p_i \rho_i^{pure} = \sum_i p_i |\Psi_i\rangle \langle \Psi_i|. \quad (2.53)$$

This density matrix has two properties: firstly, it is always positive  $\rho^{mix} > 0$ , and secondly, its trace is equal to one,  $\text{Tr}[\rho^{mix}] = 1$ . To observe the evolution of the density matrix over time, differentiating Eq. (2.53) with respect to time yields,

$$\frac{\partial \rho^{mix}}{\partial t} = \sum_i p_i \left( \left( \frac{\partial}{\partial t} |\Psi_i\rangle \right) \langle \Psi_i| + |\Psi_i\rangle \left( \frac{\partial}{\partial t} \langle \Psi_i| \right) \right). \quad (2.54)$$

By recognising the time-dependent Schrödinger equation  $i\hbar \partial/\partial t |\Psi\rangle = H |\Psi\rangle$  and its Hermitian conjugate, it allows us to re-write Eq. (2.54) as,

$$i\hbar \frac{\partial \rho^{mix}}{\partial t} = i\hbar \sum_i p_i \left( \frac{-i}{\hbar} H |\Psi_i\rangle \langle \Psi_i| + \frac{i}{\hbar} |\Psi_i\rangle \langle \Psi_i| H \right). \quad (2.55)$$

Re-writing in terms of the density matrix of the pure state leads to the Liouville-von Neumann equation in its final form,

$$i\hbar \frac{\partial \rho^{mix}}{\partial t} = \sum_i p_i (H \rho_i^{pure} - \rho_i^{pure} H) = [H, \rho^{mix}]. \quad (2.56)$$

This equation describes the evolution of a mixed state over time; in the case of pure states, the equation reduces to the Schrödinger equation.

<sup>9</sup>The adiabatic movement is to prevent heating of the atoms, which could lead to atom loss.

### 2.7.2 Open Systems

In reality, no such system can be completely shielded from environmental effects, this creates the pathway for Open Quantum Theory [239, 240]. The modelling of a “total system”, one which considers a environment coupled to a quantum system, such that

$$\mathcal{H}_{tot} = \mathcal{H}_s \otimes \mathcal{H}_e \quad (2.57)$$

with  $\mathcal{H}_s$  and  $\mathcal{H}_e$  being the Hilbert spaces of the quantum system and the environment respectively. The total system evolves unitarily under the Schrödinger equation governed by a total Hamiltonian:

$$H_{tot} = H_s \otimes I_e + I_s \otimes H_e + H_{int}. \quad (2.58)$$

Here,  $H_s$  and  $H_e$  are the Hamiltonians of the system and environment, with  $I_{e,s}$  representing the identity matrices, and  $H_{int}$  denotes their interaction. The entire setup is described by the total density matrix  $\rho_{tot}$ , but since only the system is of interest, the environment is traced out to obtain the reduced density matrix of the system:

$$\rho_s = \text{Tr}_e [\rho_{tot}] \quad (2.59)$$

This tracing introduces non-unitary effect such as dissipation, decoherence and noise. A particular case of an open system, is while the system is connected by either several baths/drains which model a Markovian interaction. In this situation, most quantum mechanical models are evaluated via the Lindblad equation (also known as Gorini-Kossakowski-Sudarshan-Lindblad equation) [241, 242].

In [149], provides a nice derivation of the Lindblad equation, resulting in the final form:

$$\partial_t \rho_s = -i[H, \rho_s] + \sum_k \sum_{v=s,d} \left( \mathcal{L}_v^k \rho_s \mathcal{L}_v^{k\dagger} - 1/2 \{ \mathcal{L}_v^{k\dagger} \mathcal{L}_v^k, \rho_s \} \right). \quad (2.60)$$

which offers the time evolution of the density matrix  $\rho_s$ , here the first term corresponds to the unitary dynamics, and the second term accounts for the dissipative processes. In the case of Rydberg atoms, the Lindblad jump operators correspond to two dissipative processes: spontaneous decay ( $v = s$ ) and dephasing ( $v = d$ ) acting on the atom  $k$ . The decay rate of the Rydberg state is given by  $\kappa$  represented as  $\mathcal{L}_s^k = \sqrt{\kappa} \sigma_k^-$ . The rate of dephasing  $\gamma$  is present in the Lindblad operators as  $\mathcal{L}_d^k = \sqrt{\gamma} n_k$ , and denotes the loss of coherence (the dephasing of a superposition of states into pure states) caused by the environment.



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## Excitation Propagation through Networks of Rydberg Atoms

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The field of *Atomtronics* harnesses the properties of ultracold atoms manipulated by laser fields of varying shapes and intensities to construct atomic circuits, enabling the development of devices analogous to their electronic counterparts [179, 180, 183, 188]. In particular, atomic devices such as atomtronic transistors and switches for cold atoms have been proposed [243–245] and realised [246]. Another essential component for performing classical analogue or digital computation is the diode. Similar to electronics, the atomtronic diode has been proposed by combining doped conducting cold atom systems together [179, 184, 247]. Recently, a proposal used Rydberg excitations as the “current carriers” in circuits of ring-shaped arrangements [136, 189]. The concept of using Rydberg excitation relies in the propagation through arrays of atoms can be on the order of  $\mu\text{sec}$  compared to matter-wave currents timescales ( $\approx \text{msec}$ ). Despite their long-life times, Rydberg atoms are open to dissipation such as decay and dephasing, therefore the notion of the moving the atoms fails as they de-excite to the ground state quicker compared to their movement. Consequently, the platform realises circuits with trapped atoms in specific designs.

In this chapter, we explore the dynamics of Rydberg excitations in differently shaped atom networks, which mimic electronic switches, diodes, and universal classical logic gates. The fundamental physics of Rydberg atoms and the extensive expertise in coherent manipulations [70, 71, 73] of networks comprising various sizes of Rydberg atoms [79, 80] offer a rich and adaptable toolkit for quantum simulators and, more broadly, quantum technologies [53, 83, 91, 130, 135, 140, 218, 248–250]. Rydberg networks also offer a promising foundation for quantum information processors [84, 100, 251].

The chapter structure is as follows: in Sec. 3.1, the platform and the excitation process scheme are discussed, where we explicitly mention suitable experimental parameters on which we base the simulations. In the limit of strong dephasing, we compare the Lindblad

master equation and classical approximation for  $N = 3$  atoms. Section. 3.2 is dedicated to excitation propagation over  $N = 6$  atoms by utilising the facilitation mechanism with different dissipation conditions. Later, in Sec. 3.3, the protocol for controlling the flow of excitations is presented by using local detuning addressing. Section. 3.5 explores a two-dimensional atom array whereby classical logical decisions can be computed in a highly dissipative regime through the dynamics of excitations. Lastly, Sec. 3.6 summarises the presented work and offers ideas for future development.

The results presented in the following are based on our work published in “Phys. Rev. A **110**, 043304” [200].

### 3.1 Scheme & Parameters

The experimental procedure to excite atoms from a ground to Rydberg states of the same parity [252] is carried out through a two-photon transition. For  $^{87}\text{Rb}$  atoms this procedure is detailed in [91], where the use of an intermediate state separates the two transitions. Initially, the transition from the ground  $|5S_{1/2}\rangle$  to the Rydberg state  $|70S_{1/2}\rangle$ , is achieved by the laser driving  $\Omega_{420}$  from the ground to the intermediate state  $|6P_{3/2}\rangle$ . Once the atoms are in this state, a second laser drives the atoms to the Rydberg state with a driving  $\Omega_{1013}$ . Although, this can be modelled as a two-level system for a theoretical description, we have an effective Rabi frequency given by Eq. (2.42),

$$\Omega = \frac{\Omega_{420}\Omega_{1013}}{2\Delta_{6P}}. \quad (3.1)$$

where the subscripts 420 and 1013 denote the wavelength of each laser. For the simulations presented within this thesis, we choose parameter values in close alignment with experimental work conducted on Rubidium atoms [91, 253]. The dimensionfull parameters are: the Rabi frequency  $\tilde{\Omega}/(2\pi) = 0.51 \text{ MHz}$  [86], the decay rate  $\tilde{\kappa}/(2\pi) = 12.5 \text{ kHz}$ , the dephasing rate  $\tilde{\gamma}/(2\pi) = 0.7 \text{ MHz}$  and the Van der Waal interaction coefficient  $\tilde{C}_6/(2\pi) = 1337 \text{ GHz}\mu\text{m}^6$ . For ease, we convert these values to be in units of the driving frequency  $\Omega = 1$ , therefore,  $\gamma = \tilde{\gamma}/\tilde{\Omega} = 1.4$ ,  $\kappa = \tilde{\kappa}/\tilde{\Omega} = 0.02$  and by defining a facilitation radius  $\tilde{r}_f = 7.1\mu\text{m}$ , then  $C_6 = \tilde{C}_6/(\tilde{\Omega}\tilde{r}_f) = 20$ . For our systems, we consider detuning localised at each site, allowing for different atoms to have local addressing (see Fig. 3.1). In practice, such conditions can be implemented by suitably shifting the excitation laser frequency (for example through an acousto-optic modulator) and then by exciting specific portions of the Rydberg network with different frequencies. Note that it is possible to control  $\tilde{\kappa}$  in the experiment following the scheme presented in [254] and experimentally shown in [255] via an intermediate level coupled with the Rydberg state.

In the limit of strong dephasing  $\gamma \gg \Omega$ , the atoms rapidly dephase into mixed states [91] and quantum decoherences can be neglected. In this regime a classical master equation

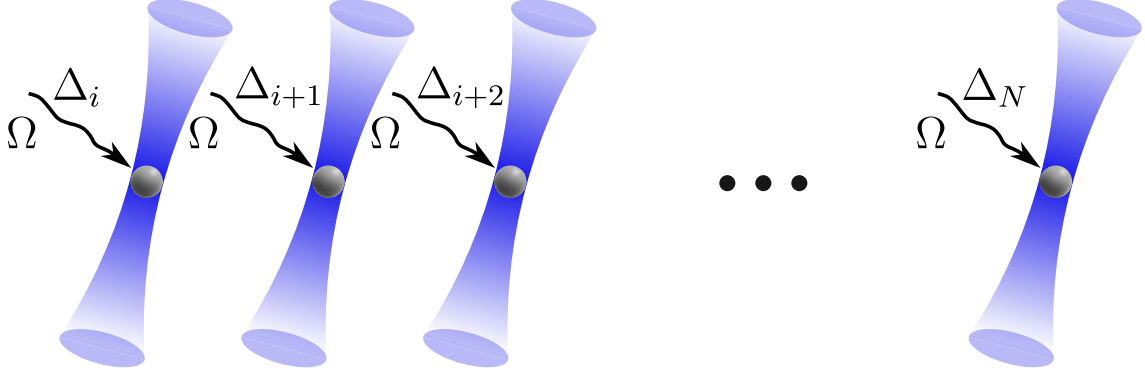


Figure 3.1: An array of  $N$  atoms trapped in optical tweezers equally separated with a constant driving  $\Omega$ . Each atom is subject to a separate laser detuning  $\Delta$ .

can be derived via second-order perturbation theory [155, 252]. The evolution of the probabilities of the basis states  $\mathbf{p} = \text{diag}(\rho)$  is given by,

$$\partial_t \mathbf{p} = \sum_i \Gamma_i [\sigma_i^+ + \sigma_i^-] \mathbf{p} + \sum_i \kappa [\sigma_i^+ - n_i] \mathbf{p} \quad (3.2)$$

where  $\sigma^\pm = 1/2(\sigma^x \pm i\sigma^y)$ ,  $n_i$  is the pre-defined number operator and the transition rate,

$$\Gamma_i = \frac{\Omega^2 \gamma}{\left(\frac{\gamma}{2}\right)^2 + \left(\Delta_i + C_6 \sum_{i \neq j} \frac{n_j}{|x_i - x_j|^6}\right)^2}. \quad (3.3)$$

A comparison can be made between the full quantum equation (Eq. (2.60)) and the classical approximation (Eq. (3.2)) for different values of the dephasing. In Fig. 3.2, a system of  $N = 3$  atoms evolve under different parameters following an initial excitation of the first atom. By recording the population of the final atom, with different values of the dephasing, we observe the limitations of the classical approximation. For small values of dephasing, where  $\gamma \ll \Omega$ , the classical approximation struggles to capture the effects of the Rabi driving, resulting in mismatched evolutions. With the addition of decay ( $\kappa = 0.02$ ), the population of the final atom decreases in the process of reaching the Rydberg state, but this has no effect when the atom is driven back to the ground state by  $\Omega$ . Furthermore, the decay becomes more pronounced over longer timescales, as the distinction between the two evolutions increases with greater driving excitation processes. As  $\gamma \approx \Omega$ , the driving effect on the system diminishes; however the classical approximation still fails to accurately describe the effects of the driving. When dephasing is further increased, such that  $\gamma \gg \Omega$ , the two evolutions align well, with the driving being dampened as the quantum coherence between the atoms grows too large for the classical approximation to fully represent the system.

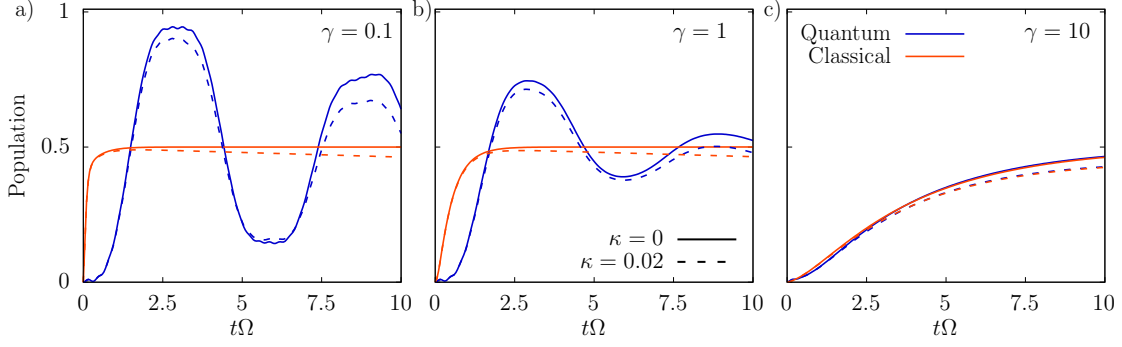


Figure 3.2: The population of the final atom in a  $N = 3$  atoms system over the time period  $t\Omega$  with  $\Omega$  as the Rabi Driving. The comparison between the full quantum simulation (Eq. (2.60)) and the classical approximation (Eq. (3.2)) is conducted for different values of the dephasing **a)**  $\gamma = 0.1$  **b)**  $\gamma = 1$  **c)**  $\gamma = 10$ . In each scenario the atoms are separated by  $r_f$  with an interaction coefficient  $C_6 = 20$ .

### 3.2 Transport

Using the scheme illustrated in Fig. 3.1, the propagation of excitations via the facilitation mechanism can be observed. To adhere to the constraints of the facilitation mechanism, the atoms are subjected to a laser detuning  $\Delta_f$  and are separated by a distance  $r_f$ . In a system comprising of  $N = 6$  atoms, the dynamics of excitations are noted over the period  $t\Omega \in (0, 10)$  when atom  $i = 1$  is initialised in the Rydberg state. We consider two scenarios: one with dissipation (the parameters used are noted above) and another without dissipation, each with three different interaction strengths. These interaction strengths correspond with different principal quantum numbers  $n$  for the  $|nS\rangle$  state. For  $n = 70$  the interaction strength between neighbouring atoms  $C_6 = 20$ : ( $\tilde{C}_6/(2\pi) = 1337$  GHz $\mu\text{m}^6$  [91, 253]), for  $n = 75$  the interaction increases to  $C_6 = 29$ : ( $\tilde{C}_6/(2\pi) = 1947$  GHz $\mu\text{m}^6$  [256]) and lastly, for  $n = 80$  the interaction yields  $C_6 = 61$ : ( $\tilde{C}_6/(2\pi) = 4000$  GHz $\mu\text{m}^6$  [257]).

In both of the scenarios we consider, due to the zero or low value of the dephasing, we simulate the dynamics of excitations using the full quantum equation (Eq. (2.60)), to observe the quantum effects of the driving present in each system. In the situation with zero dissipation (see upper panel of Fig. 3.3), the excitation initialised in atom  $i = 1$  propagates through the system due to the facilitation mechanism. As a result of the driving, atom separation, and atom detuning, each atom in the network will be sequentially driven from the ground state to the Rydberg state and then back to the ground state. The interaction strength  $C_6$  in each system, has a minimal effect on the dynamics, as this is always compensated by the detuning of each atom. However, for much larger interactions (or for larger systems not presented here) it is observed that atoms far away from the initial excitation do not reach the Rydberg state, as the influence of other atoms in the system also affects the energy level shift, impeding the excitation. It is noted that the final atom in the system is always excited, as for the atom's two neighbours, the excitation

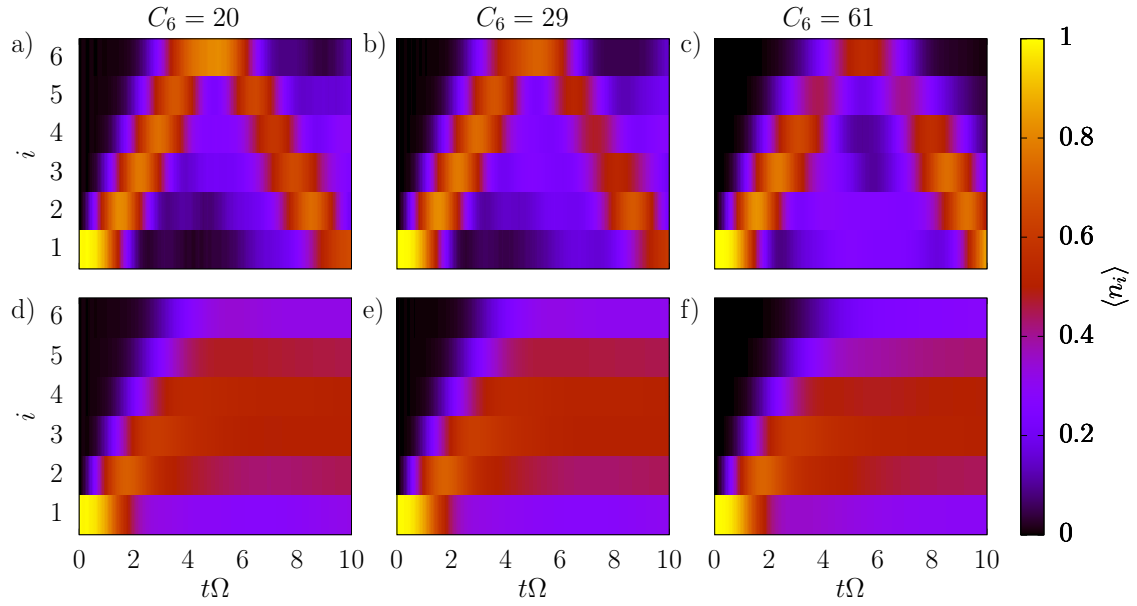


Figure 3.3: Propagation of excitations through  $N = 6$  array of atoms over the time period  $t\Omega$  which is dictated by the Rabi frequency  $\Omega$ . **Upper panel:** Zero dissipation,  $\gamma = 0$  and  $\kappa = 0$ . **Lower panel:** Dissipation,  $\gamma = 1.4$ ,  $\kappa = 0.02$ . **a). d)**  $C_6 = 20$ . **b). e)**  $C_6 = 29$ . **c). f)**  $C_6 = 61$ .

primarily propagating in one direction can also be back-reflected, ultimately accumulating in the final atom. Following this, the excitation then propagates back to the initial atom, resulting in a back reflection as well.

In the presence of dissipation (see lower panel of Fig. 3.3) the propagation of the excitation fails to reach the end of the array. Now as the dephasing is equal in magnitude to the driving, this dominates the system and causes the states to dephase into mixed states destroying the coherence of the state. To overcome the effect of dephasing, the driving needs to be increased, which will also reduce the time of propagation.

### 3.3 Excitation Control

A switch is a device that allows current to pass through when it is enabled but prevents the flow of current when it is disabled. By using atoms trapped in optical tweezers, as illustrated in Fig. 3.4(a), with appropriate detuning and atom separations, the propagation of excitations can be controlled. The proposed method involves a one-dimensional chain of  $N = 3$  atoms separated by the facilitation radius  $r_f$  and with the left- and right-hand terminals having the facilitation detuning. However, the gate atom has a detuning  $\Delta_g$  which controls whether the excitation can propagate or is blocked from reaching the right-hand terminal.

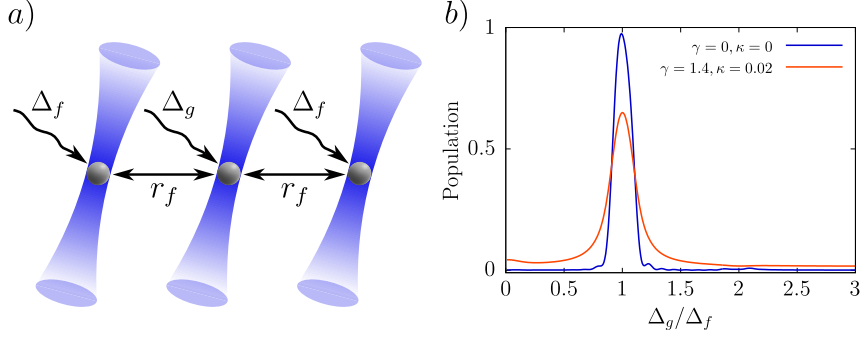


Figure 3.4: **a)** Schematic representation of  $N = 3$  atoms controlling the flow of excitations from the left- to right-hand terminals which are separated by the facilitation radius  $r_f$ . The detuning at the left- and right-hand terminals is set to the facilitation  $\Delta_f$ , while, the detuning on the gate atom is set to  $\Delta_g/\Delta_f$ . **b)** The population of the right-hand terminal for various values of  $\Delta_g/\Delta_f \in (0, 3)$  recorded at  $t\Omega = 3.05$  and  $t\Omega = 3.15$  with and without dissipation respectively.

By varying  $\Delta_g/\Delta_f$  and recording the population in the right-hand terminal, the values of the gate atoms' detuning can be noted to either enable or disable excitation flow. To observe this, the population of the right-hand terminal is recorded at  $t\Omega = 3.05$  and  $t\Omega = 3.15$  with and without dissipation respectively (which corresponds to the maximum population when all the atoms in the system have the facilitation detuning) and shown in Fig 3.4(b). In both circumstances (with and without dissipation), the flow to the right-hand terminal occurs around the facilitation detuning  $\Delta_g/\Delta_f = 1$ . As the produced facilitation radius, matches the atom separation, the excitation can be transferred along the system. However, for values of the gate atoms' detuning away from this  $\Delta_g/\Delta_f < 1$  (or  $\Delta_g/\Delta_f > 1$ ), the facilitation radius is larger (or smaller) than the atom separation. Therefore, the energy shift is not compensated for in the detuning and the excitation cannot propagate through the system.

In the presence of dissipation, around  $\Delta_g/\Delta_f = 1$ , the population of the final atom is reduced as the system begins to dephase. However, away from  $\Delta_g/\Delta_f = 1$ , the population of the dissipative system becomes larger than the non-dissipative system. This is resulted from the specific recording times of the two systems, as for the non-dissipative, the time the maximum population occurs changes away from the recording time for less incrementation of  $\Delta_g$  compared to the dissipative system.

The switch is the only device present in this thesis which can also be also proposed used  $N$  atoms trapped in a three-dimensional potential. This scheme and methods to simulate the dynamics of excitations are presented in the Appendix.

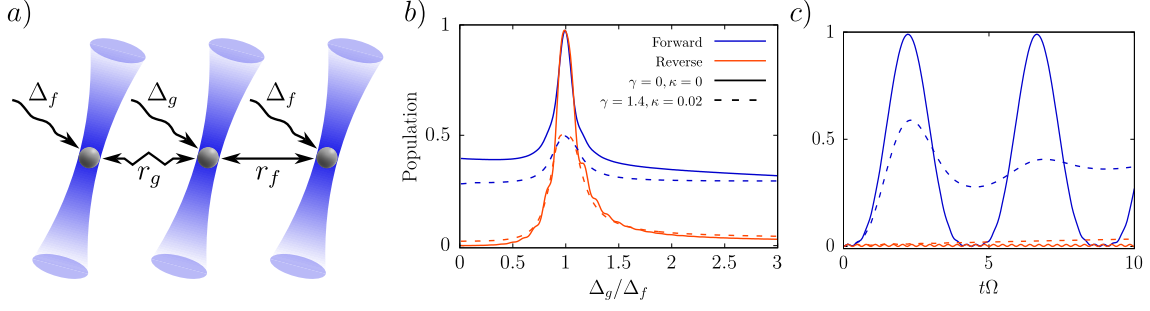


Figure 3.5: **a)** Schematic illustrating a diode composed of  $N = 3$  atoms. The gate atom has a detuning  $\Delta_g$  and is positioned  $r_g = (C_6/\Delta_g)^{1/6}$  from the left-hand terminal and  $r_f$  from the right-hand terminal. **b)** Population of the final atom recorded at  $t\Omega = 3.05$  and  $t\Omega = 3.15$  (with and without dissipation respectively) when the initial excitation is at the left-hand terminal (Forward direction) and when the excitation is initialised at the right-hand terminal (Reverse direction). **c)** The excitation dynamics of the final atom in the forward and reverse directions (with and without dissipation) for  $\Delta_g/\Delta_f = 0.01$ .

### 3.4 Non-Reciprocal Excitation Propagation

The non-reciprocal flow of excitations through a one-dimensional chain of atoms permits excitations to travel in one direction while blocking transport in the opposite direction. To achieve this, we demonstrate an arrangement of  $N = 3$  atoms in Fig. 3.5(a), in which the left-hand and right-hand atoms are subject to a facilitation detuning  $\Delta_f$  whereas the central atom has a detuning  $\Delta_g$ . The spacing between the atoms is chosen to aid and restrict the flow of excitations; therefore, the atom separation from the left-hand atom to the central atom is defined as  $r_g = (C_6/\Delta_g)^{1/6}$ . In contrast, the atom spacing from the central to the right-hand atom remains constant at  $r_f$ . As  $r_g$  depends on the detuning of the central atom, the separation can either be larger (if  $\Delta_g < \Delta_f$ ) or smaller (if  $\Delta_g > \Delta_f$ ) compared to  $r_f$ . By establishing the forward direction of the excitations from the left-hand atom to the right-hand atom, along with the chosen distances and detuning, the facilitation condition is reached. Conversely, the reverse direction is from the right-hand atom to the left-hand atom, so that now with the increased spacing and larger detuning of the gate atom, the facilitation condition will not be met, thereby blocking any transport.

To understand the system's requirements for producing non-reciprocal flow, we evolve the system (using Eq. (2.60) to observe the quantum effects) and record the population in the final atom (in the forward direction, this is the right-hand terminal and in the reverse direction, the left-hand terminal) at  $t\Omega = 3.05$  and  $t\Omega = 3.15$  (with and without dissipation, respectively) - which are summarised in Fig. 3.5(b). In the region,  $\Delta_g \approx \Delta_f$ , the separation  $r_g \approx r_f$ ; therefore, excitations can flow in both directions since these are the same dynamics discussed in Sec. 3.2. Conversely, the production of non-reciprocal flow is determined by setting the value of  $\Delta_g \neq \Delta_f$ . In this regime, the propagation in the forward direction is permitted as, for each atom separation, the position matches where the energy shift aligns with the detuning applied on each atom. However, in the reverse

direction, the position of the gate atom  $r_f$  is not aligned with the detuning  $\Delta_g$  meaning that the energy shift is not compensated, and the facilitation condition remains unmet.

To observe the desired dynamics of excitations through the system, the value  $\Delta_g/\Delta_f = 0.01$  represents the largest discrepancy between the forward and reverse directions for zero dissipation. As seen in Fig. 3.5(c), the dynamics oscillate between the ground and Rydberg state in the forward direction however, in reverse, there is a high probability of the final atom remaining in the ground state. Indeed, with the source of dissipation, the final atom quickly dephases into a mixed state so over short time-scales, we observe non-reciprocal flow.

### 3.5 Logical Decisions

The construction of classical logical gates with different atom networks can be implemented as a response from the strong Rydberg interactions causing different energy levels shifts. Logic gates return a binary outcome depending on given input bits. To define these different binary outcomes, logic 0 as an atom in the ground state, while 1 corresponds to an excited Rydberg atom.

In the highly dissipative regime, where the atoms lose coherence quickly, we propose schemes to create a universal classical logic gate based on the native excitation dynamics of the atoms. By first creating an AND gate and inverting this decision through the use of a NOT gate, this results in a universal NAND gate. To demonstrate an AND gate, two atoms are set to be the inputs and a single output atom which is illustrated in Fig. 3.6(a). To achieve the AND gate truth table, the output atom should only become excited when there is a fully initial state of the input atoms (written in the Fock basis)  $|1, 1\rangle$ . In doing so, the output atom is situated  $r_f$  away from both input atoms and is subjected to a detuning  $2\Delta_f$ . The reasoning behind the doubled facilitation detuning is that the desired energy shift needs to be doubled so that only when both input atoms are excited is this energy shift matched, allowing the output to be excited. In the other situations, when there are zero initial excitations  $|0, 0\rangle$  or only one excitation  $(|0, 1\rangle + |1, 0\rangle)/\sqrt{2}$  this energy shift does not equal the detuning, and therefore the facilitation requirement is not fulfilled.

In response to the dissipative parameters, we simulate the dynamics of excitation in the output atom using Eq. (2.60). The population of the output atom is recorded in Fig. 3.6(b), for different initial states of the input atoms ( $|0, 0\rangle$ ,  $(|0, 1\rangle + |1, 0\rangle)/\sqrt{2}$ , and  $|1, 1\rangle$ ) over the period  $t\Omega \in (0, 4)$ . When there is no excitation in the input, the population of the output remains low, as there is no excitation to propagate through the system. Similarly, with only one initial excitation, the output atom's population stays low because the energy shift does not match the detuning, preventing the excitation from reaching the output. In the circumstance when both input atoms are excited, the energy shift caused in the output atom now equals to twice the facilitation detuning ( $2\Delta_f$ ), meaning the output

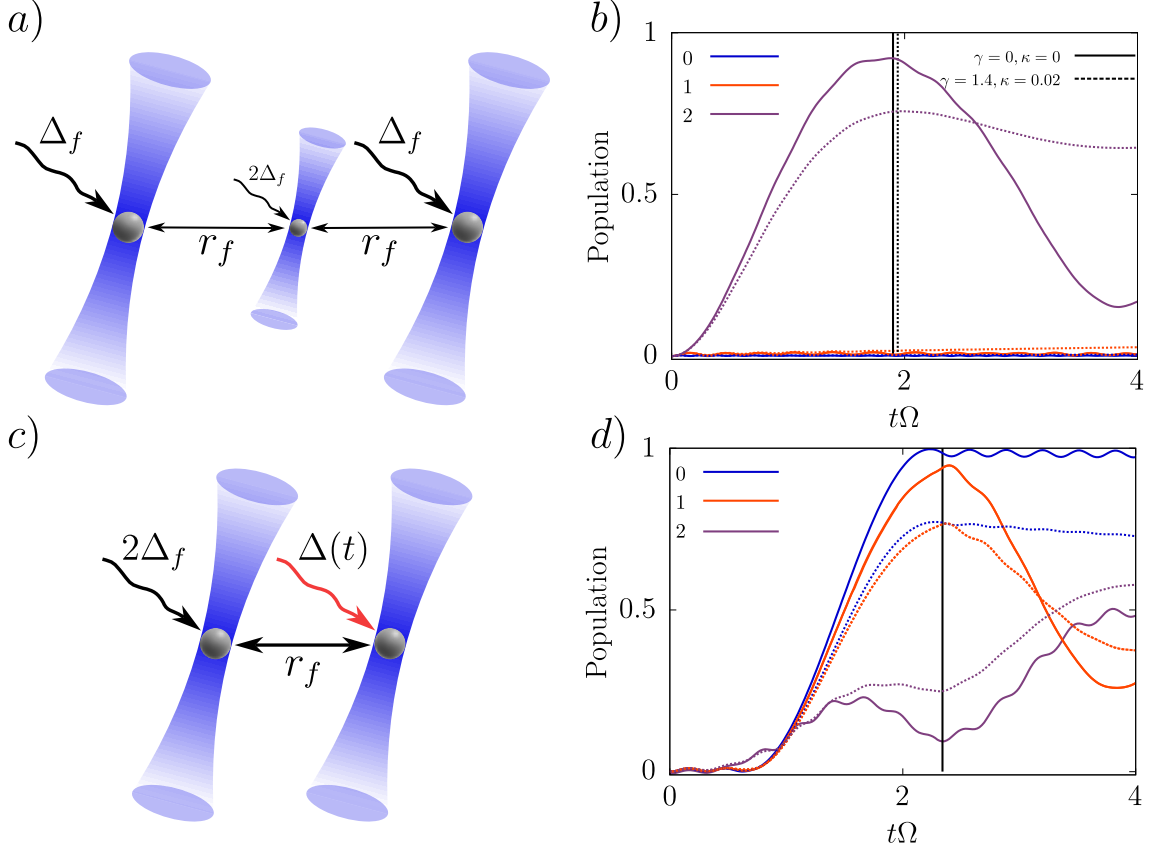


Figure 3.6: **a)** Schematic representation of an AND gate, where the left-hand and right-hand terminals are the input atoms experiencing  $\Delta_f$  and the central atom serves as the output atom which is separated from the input atoms by  $r_f$  and is subjected to  $2\Delta_f$ . **b)** The population of the output atom over the period  $t\Omega \in (0, 4)$  where the key refers to the number of excitations in the input atoms, therefore, written in the Fock basis correspond to 0:  $|0, 0\rangle$ , 1:  $(|0, 1\rangle + |1, 0\rangle)/\sqrt{2}$  and 2:  $|1, 1\rangle$ . **c)** Schematic representation of the NOT gate, where the output atom (right-hand terminal) has a variable detuning  $\Delta(t)$ . **d)** The population of the output atom for the combination of the AND and NOT gates over the period  $t\Omega \in (0, 4)$ . The vertical lines (dashed and solid line to represent with and without dissipation) represent the optimal read-out time.

atoms can be excited. This is observed for both scenarios with and without dissipation. With the additional effects of dephasing, we observe that soon after the excitation the state quickly dephases into a mixed state. The vertical lines indicate the optimal read-out time (indicated by the largest difference in population for the various input states)  $t_w\Omega = 1.94$  and  $t_w\Omega = 1.9$  with and without dissipation.

The inversion of this decision can be implemented through using a NOT gate, which transforms a 0 into a 1 and vice versa. This is achieved through a variable detuning on an additional atom (now considered the output atom), as illustrated in Fig. 3.6(c). With a spacing of  $r_f$  from the final atom in the AND gate, the NOT gate is realised by setting the detuning of the output atom to  $\Delta = 0$  for a time period  $\delta t = \pi/(2\Omega)$  centred around

$t\Omega = 1.5$ , and  $\Delta = \Delta_f$  at all other times. This detuning, in combination with the constant Rabi driving, realises a  $\pi$  pulse that excites the ground state to the Rydberg state and de-excites the Rydberg state back to the ground state.

The population of the output atom is shown in Fig. 3.6(d), where  $1.5 - \pi/2 \leq t\Omega \leq 1.5 + \pi/2$  implies that the detuning  $\Delta = 0$ . Therefore, if the result of the AND gate is a ground state atom, this inverts the result so that the output is in the Rydberg state. Conversely, if the AND gate decision is a Rydberg atom, the propagation to the output fails as the changing detuning drives the output to the ground state. These results hold true with and without dissipation, despite the effects of the dephasing turning into a mixed state. Furthermore, for the chosen parameters, the read-out times for both dissipation and no dissipation coincide at  $t_w/\Omega = 2.34$ . After this time, the detuning returns to  $\Delta_f$ , at which point the output atom's populations then change, rendering the read-out for a NAND gate invalid.

### 3.6 Conclusion

In this chapter, we examine the dynamics of Rydberg excitation across various networks of atoms. Due to the strong interactions between Rydberg atoms, energy level shifts occur, preventing simultaneous excitation to the same state - known as the Rydberg blockade. To overcome this, the energy shift can be compensated for in the laser detuning, which matches the shift and enables neighbouring atoms to be in the same Rydberg state - Rydberg facilitation. By utilising both of these phenomena, we propose different practical devices by recording the population of atoms in the network.

The real-time dynamics of arrays with  $N = 3$  and  $N = 6$  atoms have been presented using experimental parameters. Under the conditions of the facilitation mechanism, a comparison between the full quantum Lindblad master equation and a classical approximation was performed. It is verified in Fig. 3.2 that, in the limit where  $\gamma \gg \Omega$ , the classical approximation matches the Lindblad master equation. However, as  $\gamma \ll \Omega$  it cannot capture the quantum effects of the Rabi driving as these fast dynamics are neglected in the approximation. The impact of the larger principal quantum number (resulting in a increased interaction coefficient  $C_6$ ), results in a reduced  $\langle n_6 \rangle$ . This is caused from the other atoms which are remaining in the Rydberg state for longer, therefore, they slightly contribute to the energy shift of the other atoms mismatching the proposed facilitation detuning. Additionally, a back-reflection can be seen because the excitation can propagate in both directions, allowing, it to accumulate and influence the reflected excitation. In performing simulations with the effects of dephasing and decay of the Rydberg state, the observed dynamics are diminished due to these sources of dissipation. The influence of these dissipative mechanisms prevents the excitation from propagating over small array sizes, as they dephase into mixed state before reaching the end of the array.

The ability to control excitations between two terminals via a gate atom is implemented by a local addressing of the laser detuning. By fixing the atom separations to  $r_f$  and applying a specific laser detuning to the gate atoms, this allows to control if the excitations propagate through the network of atoms. For  $\Delta_f$ , this indeed matches the energy shift, and since the adjacent atom is situated at  $r_f$ , excitation can propagate through the system. However, when deviating from this detuning,  $\Delta_g < \Delta_f$  or  $\Delta_f > \Delta_f$ , the ability for the excitation to propagate diminishes, as the energy shift no longer equals the detuning, thus preventing the propagation - as shown in Fig. 3.4. In this way, the system functions as a switch, whereby changing the gate atom's detuning can enable or disable excitation flow between the terminals.

The engineering of non-reciprocal flow of excitations can be achieved through appropriate laser detuning and atom separations. Figure. 3.5 shows that by setting the detuning of the gate atom away from the facilitation such that  $\Delta_g/\Delta_f = 0.01$ , and adjusting the spacing between the left-hand terminal and the gate atom to be  $r_g = (C_6/\Delta_g)^{1/6}$ , facilitation is only realised one direction. This mechanism relies on the compensation for the energy level shifts by the laser detunings, which is only valid when the atom to be excited experiences the same detuning associated with its separation (i.e.,  $\Delta_g$  and  $r_g$ ). In the reverse direction, the detuning does not match the energy shift, preventing the excitation from propagating to the atom. The dynamics of these flows are analysed, showing that only in the forward direction can the final atom reach the Rydberg state; otherwise, it remains with high probability in the ground state.

The energy shift caused by the strong interactions is a collective effect - as shown in Sec. 2.4. In a similar manner, if multiple atoms lie on another atoms facilitation radius, they will all experience suitable energy level shift compensation if applied with the correct laser detuning. Using this effect, a classical logical decision process can be observed through the dynamics of Rydberg excitations. For two types of gates (AND and NAND gate - depicted in Fig. 3.6) the dynamics with different input excitations are studied. The inversion of the AND gate was achieved with a  $\pi$  pulse, which is implemented by shifting the atoms' detuning  $\Delta = \Delta_f \rightarrow 0$  with continuous driving. The optimal readout times for the gates are identified and are robust against dissipation.

Within our protocol, we demonstrate that networks of Rydberg atoms can serve as an alternative platform for creating atomtronic devices. Instead of matter-waves, these devices are based on a controlled flow of excitations where the matter is precisely trapped in optical tweezers. The propagation of matter-waves in typical cold atom clouds occurs on a millisecond timescale, whereas due to the Rabi driving Rydberg excitations can travel in microseconds. Therefore, Rydberg excitations have the potential to support fast atomtronic devices.



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## Sensing electric fields through Rydberg atom networks

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The dipolar interaction can be effectively scaled as either  $r^{-3}$  or  $r^{-6}$ , depending on the coupled Rydberg states involved, i.e., states with either opposite or same parity, respectively. These strong interactions can cause shifts in Rydberg energy levels, leading to an excitation blockade effect in nearby atoms when excited with narrow-band radiation [84, 85]. One way to manipulate the atom-atom interactions is by applying an electric field, which results in a differential Stark shift of the levels. For certain transitions between *pairs* of Rydberg states, each in different atoms, they can become resonant; hence, leading to an increased strength of resonant dipole-dipole interactions and in turn an enhanced blockade radius. In analogy with the energy transfer originally discussed for organic molecules [258, 259], such a regime is known as a Förster resonance [88, 260–265]. These resonances have been investigated for two atoms (two-body Förster resonances) and can also be achieved in many-body systems. Specifically, efforts have been used to explore three-body Förster resonances [266–270] with applications for three-qubit quantum gates [271] and measurements of the dipole-dipole interaction [272]. Local addressability is also possible using inhomogeneous light fields such as focused laser beams [273].

In general, the effect of external fields on atomic systems is pivotal to advanced quantum sensing applications. Quantum sensing represents one of the most significant stakes in quantum technology [37, 53]. For electric field sensors, Rydberg atoms offer an excellent platform due to their notable polarizability [37, 274, 275]. The platform has demonstrated sensitivities of several  $\mu\text{V}/\text{cm}\sqrt{\text{Hz}}$  [276, 277] and can detect fields up to the THz range [176, 278]. For scalability and decoupling from unwanted external influences, one can arrange atoms in arrays of optical tweezers generating one-, two-, and three-dimensional (1D, 2D, and 3D) networks [79, 279] of quantum sensors with selectable separations down to the single-micron range (Fig. 4.1). Recently, a 2D network of individual rubidium atoms has been used as a sensor for a spatially varying magnetic field [280].

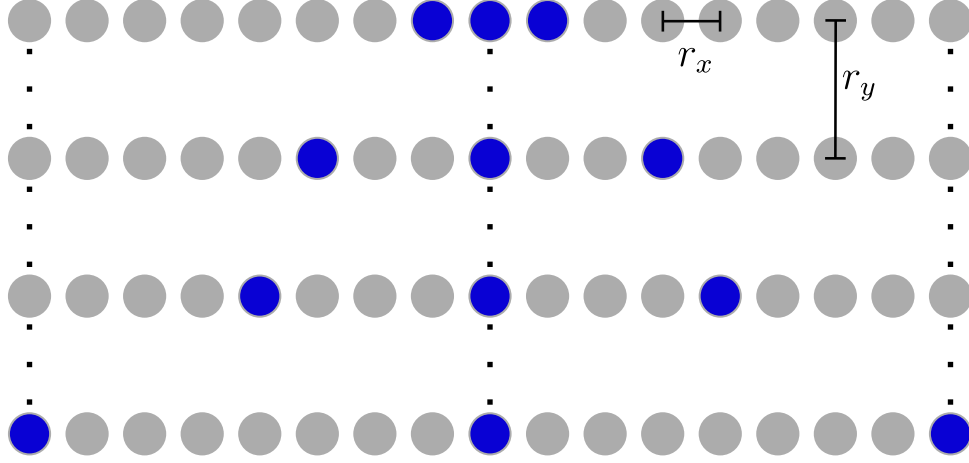


Figure 4.1: Schematic arrangement of a 2D tweezer array (grey dots) with pitch  $r_x$ . Trapped atoms, which have the possibility to be excited to a Rydberg state, are shown in blue. Each row corresponds to a different atom separation  $r$  in multiples of  $r_x$ . The separation between the rows that are used for measurements fulfils the condition  $r_y \gg r_x$  so that the interaction between atoms in different rows is suppressed. Such a network can be used to sense an electric field  $E$  (constant or spatially dependent) that is applied across the atoms (see the main text for the detailed scheme).

In the following, we present a complementary approach to gas-cell-based sensors that addresses the limitation that such sensors cannot resolve spatial variations in the electric field. The proposed design of the sensor is illustrated in Fig. 4.1 and is based on a two-dimensional network of atoms. The tweezer array features a horizontal pitch of  $r_x$ , and a separation  $r_y$  between the various rows, with  $r_y \gg r_x$  such that interactions between atoms in different rows are suppressed. The number of empty tweezers between adjacent atoms is chosen so that the atoms are regularly spaced with a distance  $r$  between them, which is independently selected for each row in the 2D array. This configuration enables simultaneous measurements across multiple interatomic spacings, providing both reference baselines—spacings at which the electric-field dependence is negligible (corresponding to small and large separations)—and rows for direct electric-field sensing where the atom-atom distance is similar to the Rydberg blockade radius. The sensitivity of these sensing rows, spanning from broad dynamic range to high precision, is determined by their pitch separation and the applied field.

In this chapter, we first investigate the working principle of the electric field sensor in a single array of Rydberg atoms in the presence of a uniform electric field. In Sec. 4.1, we examine the model extended to include an electric field and propose a protocol using a two-dimensional array of atoms to detect electric fields. Section. 4.2 explores the dependence of the Rydberg blockade on the electric field through the fidelity of the fully excited state. Furthermore, the maximum fidelity over a period is recorded for two scenarios: for constant electric fields, but after each repetition, the atom separation is increased in intermediate increments from  $r = 5\mu\text{m}$  to  $r = 40\mu\text{m}$ , and for fixed atom spacings, with

each iteration increasing the electric field from  $E = 15$  mV/cm to 29.787 mV/cm (corresponding to the Förster resonance). As the interaction is primarily governed by two-body processes, we employ the density-density correlation function in Sec. 4.3. This is calculated for systems of  $N = 3$  and  $N = 19$ , where the applied electric fields demonstrate spatial fluctuations and can exhibit different functions, such as mimicking an AC Stark shift of a laser beam. The previously discussed measurements for uniform and spatially varying electric fields (the fidelity and density-density correlator) are compiled in Sec. 4.4, which discusses their application as a quantum sensor. Finally, in Sec. 4.5, we summarise the results and explore further avenues for investigation.

The results presented in the following are found in the preprint “arXiv:2509.01665 (2025)”.

## 4.1 Model and Methods

Atoms which can be driven between a ground state  $|g\rangle$  and a specific Rydberg state  $|\xi\rangle$  by using a resonant field that couples the two states can be modelled via Eq. (2.41). Assuming a coupling strength characterised by the Rabi frequency  $\Omega_{eff}$  (Eq. (2.42)), the system undergoes Rabi oscillations between the two states [53, 94]. When multiple atoms are driven simultaneously, long-range interactions emerge due to the large dipole moment of Rydberg atoms. For  $N$  atoms, with no detuning of the Rydberg state ( $\Delta = 0$ ), the modelling of the system can conveniently be written as:

$$H = \frac{\Omega_{eff}}{2} \sum_i^N \sigma_i^x + \sum_{i \neq j}^N V_{i,j} n_i n_j. \quad (4.1)$$

The Pauli matrices are denoted by  $\sigma_i^u$  (with  $u = x, y, z$ ), and  $V_{i,j}$  for the interaction strength between Rydberg atoms  $i$  and  $j$ . The local number operator defined as  $n_i = \frac{1}{2}(\sigma_i^z + \mathbb{1})$  counts atoms in the Rydberg state. Due to the combination of zero detuning and the interaction-induced energy level shift, nearby atoms are prevented from being excited to the Rydberg state – an effect known as the Rydberg blockade [84–87].

The Hamiltonian in Eq. (4.1) describes the physics when an atom is excited to a specific Rydberg state  $|\xi\rangle$ . We now extend this description to the case where additional nearby Rydberg states are energetically accessible. Consider two identical atoms separated by a distance  $r \equiv r_{1,2}$ , each with available Rydberg states  $|\xi\rangle$ ,  $|\zeta\rangle$ , and  $|\nu\rangle$ . Whenever the pair state  $|\xi, \xi\rangle \equiv |\xi\rangle_1 \otimes |\xi\rangle_2$  is nearly degenerate with  $|\zeta, \nu\rangle$  (and  $|\nu, \zeta\rangle$ ), it can couple via the dipole–dipole interaction. In fact, due to the exchange symmetry of the dipole–dipole interaction,  $|\xi, \xi\rangle$  couples only to the symmetric superposition  $|+\rangle = (|\zeta, \nu\rangle + |\nu, \zeta\rangle)/\sqrt{2}$  [281]. Therefore, in the subspace  $\{|\xi, \xi\rangle, |+\rangle\}$ , the interaction can be described by an effective two-level Förster Hamiltonian:

$$V(\xi) = \begin{pmatrix} \delta & C_3/r^3 \\ C_3/r^3 & 0 \end{pmatrix}, \quad (4.2)$$

where we define the so-called energy defect  $\delta = 2\epsilon_\xi - \epsilon_\zeta - \epsilon_\nu$ , with  $\epsilon_\eta$  denoting the single-atom energy of state  $\eta$ . The term  $C_3/r^3$  represents the resonant dipole-dipole matrix element between the pair states, with  $C_3$  being dependent on the dipole matrix elements of the pair states. The effective interaction between two atoms is provided by the lowest energy eigenvalue of Eq. (4.2):

$$V = \frac{\delta - \sqrt{\delta^2 + 4C_3^2/r^6}}{2}, \quad (4.3)$$

whereby, the competition between  $\delta$  and  $C_3/r^3$  determines the nature of the interaction term. In the case  $\delta \gg C_3/r^3$ , Eq. (4.3) can be simplified by using a binomial expansion for small  $x = C_3/\delta r^3 \ll 1$ . Therefore,

$$\frac{4C_3^2}{r^6} = 4\delta^2 x^2 \quad \text{and} \quad \sqrt{\delta^2 + \frac{4C_3^2}{r^6}} = \delta \sqrt{1 + 4x^2}, \quad (4.4)$$

and the expansion  $\sqrt{1+x} \approx 1 + x/2 + x^2/8 + \dots$ , gives

$$\delta \sqrt{1 + 4x^2} \rightarrow \delta(1 + 2x^2) = \delta + \frac{2C_3^2}{\delta r^6}. \quad (4.5)$$

The effective interaction becomes

$$V \simeq \frac{\delta - \left(\delta + \frac{2C_3^2}{\delta r^6}\right)}{2} \simeq -\frac{C_3^2}{\delta r^6}, \quad (4.6)$$

giving rise to Van der Waals-like interactions (VdW). Conversely, if  $\delta \ll C_3/r^3$ , then

$$\delta^2 \ll \frac{C_3^2}{r^6} \quad (4.7)$$

and

$$\sqrt{\delta^2 + \frac{4C_3^2}{r^6}} \rightarrow \sqrt{\frac{4C_3^2}{r^6}} = \frac{2C_3}{r^3}. \quad (4.8)$$

Substituting this into the effective interaction leads to

$$V \simeq \left(\delta - \frac{2C_3}{r^3}\right) \rightarrow \frac{\delta}{2} - \frac{C_3}{r^3}, \quad (4.9)$$

and due to  $\delta \ll C_3/r^3$ , then the effective interaction becomes

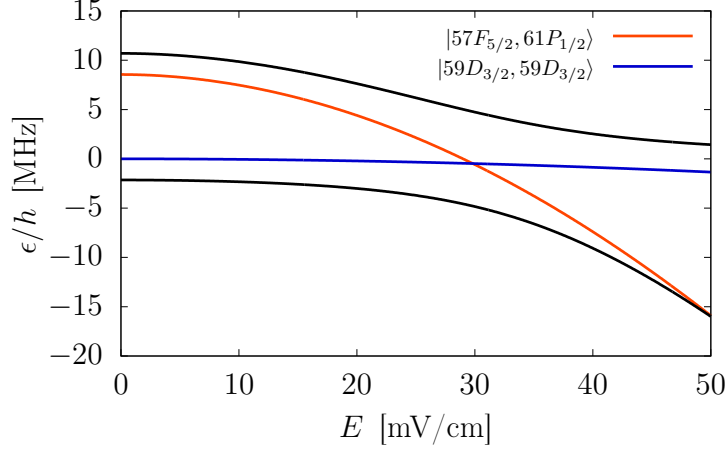


Figure 4.2: The relative energies  $\epsilon$  in units of the Planck constant  $h$  for the pair states  $|59D_{3/2}, 59D_{3/2}\rangle$  and  $|57F_{5/2}, 61P_{1/2}\rangle$  in the presence of an electric field  $E$  for a coupled (black) and uncoupled (coloured) system. The two atoms are separated by a distance  $r = 8.1\mu\text{m}$  and magnetic field  $B_z = 0$  G.

$$V \simeq -\frac{C_3}{r^3}. \quad (4.10)$$

This results in dipole-dipole interactions. When  $\delta \approx C_3/r^3$ , the system undergoes a crossover between the two types of interactions, which is denoted as

$$r_c = \left( \frac{C_3}{\hbar|\delta|} \right)^{1/3}. \quad (4.11)$$

In the presence of an electric field  $E$ , the energy levels experience a Stark shift that alters both  $\delta(E)$  and  $C_3(E)$ . Therefore, by gradually increasing the electric field towards the Förster resonance, the nature of interaction changes between VdW-like and dipole-dipole: *resulting in an enlarged blockade radius* [282]. Here, we consider states that have been previously shown to display a Förster resonance in  $^{87}\text{Rb}$ , e.g.,  $|\xi\rangle = |59D_{3/2}\rangle$ ,  $|\zeta\rangle = |61P_{1/2}\rangle$ , and  $|\nu\rangle = |57F_{5/2}\rangle$  at the electric field  $E \approx 32$  mV/cm with a magnetic field  $B_z = 3$  G [281]. For these states, we utilise the Alkali Rydberg Calculator (ARC) [204] and obtain  $C_3(E)$  and  $\delta(E)$  at zero magnetic field  $B_z = 0$  G. In doing so, the relative energy  $\epsilon$  of  $|59D_{3/2}, 59D_{3/2}\rangle$  and  $|57F_{5/2}, 61P_{1/2}\rangle$  are shown in Fig. 4.2.

Now, with the values of  $C_3$  and  $\delta$  for the selected states, we can return to look at both the crossover radius and the blockade radius. Figure 4.3(a) illustrates how the effective interaction  $V$  varies with the separation between atoms. At short distances, the interaction is strong ( $C_3 > \delta$ ), resulting in a dipole-dipole-like behaviour with  $V \propto r^{-3}$ . As the separation increases and the interaction strength becomes weaker than the energy defect ( $C_3 < \delta$ ), the interaction crosses over to a van der Waals regime, scaling as  $r^{-6}$ . The point at which this transition occurs is identified as the crossover radius, which depends on the applied electric field. The largest value of the crossover radius is observed at the Förster

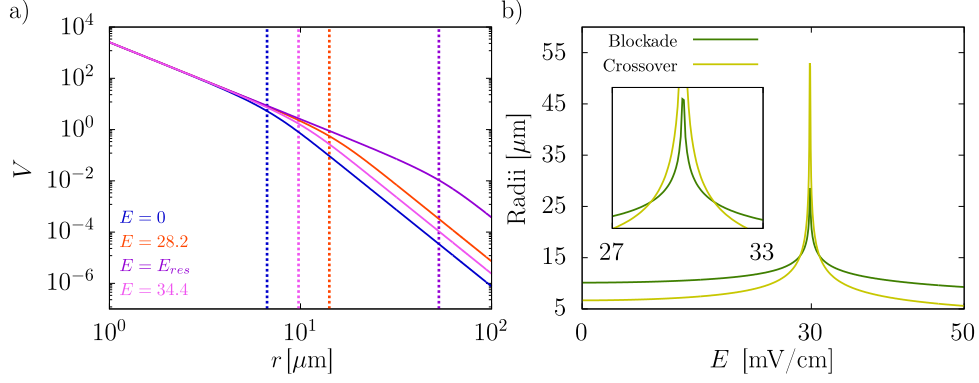


Figure 4.3: **a)** Effective interaction  $V$  between two Rydberg atoms separated by a distance  $r$  when subjected to an electric field  $E = 0$  mV/cm ( $r_c = 6.68 \mu\text{m}$ ),  $E = 28.2$  mV/cm ( $r_c = 14.15 \mu\text{m}$ ),  $E = 29$  mV/cm ( $r_c = 52.95 \mu\text{m}$ ) and  $E = 34.4$  mV/cm ( $r_c = 9.76 \mu\text{m}$ ). The change of behaviour between the dipole-dipole and Van der Waals interaction is recorded as  $r_c$ . **b)** The blockade radius (as defined in Eq. (4.12)) and the interaction crossover radius,  $r_c$  for different electric fields. The insert zooms into the region between  $E = 27 - 33$  mV/cm.

resonance,  $E = E_{\text{res}}$  mV/cm. This trend is further highlighted in Fig. 4.3(b), where the crossover radius is plotted as a function of the electric field, showing a pronounced peak at the Förster resonance. For comparison, we also overlay the blockade radius [283], defined as

$$r_b = \left( \frac{C_6}{\Omega} \right)^{1/6} = \left( \frac{C_3^2}{\hbar|\delta|\Omega} \right)^{1/6}, \quad (4.12)$$

where the angular component of the interaction is set to 1. Since the blockade radius depends on the energy defect  $\delta$ , it varies with the electric field. As the field approaches the Förster resonance ( $E = E_{\text{res}}$  mV/cm),  $\delta \rightarrow 0$  and the blockade radius reaches its maximum value. The nature of the interaction governing this phenomenon can be inferred by comparing it to the crossover radius. When the crossover radius is smaller than the blockade radius ( $r_b > r_c$ ), the interaction follows a van der Waals scaling,  $V \propto r^{-6}$ . Conversely, when the crossover radius is larger than the blockade radius ( $r_b < r_c$ ), the interaction is in the resonant regime and scales as  $V \propto r^{-3}$ —a situation that occurs predominantly near the Förster resonance.

In the following sections, we mainly investigate the time dynamics of different states while the atoms are subjected to various constant and spatially varying electric fields. The inclusion of the influence of the electric field is accounted for through the effective interactions Eq. (4.3) in Eq. (4.1).

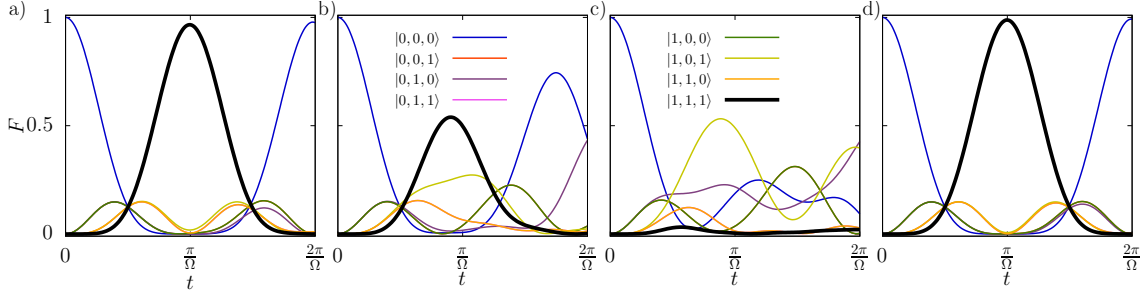


Figure 4.4: The fidelity  $F$  of the basis states for three interacting atoms having a separation  $r = 15 \mu\text{m}$  over a Rabi period,  $t \in (0, \tau = 2\pi/\Omega)$  for different electric fields  $E$  with  $\Omega$  corresponding to the Rabi frequency. **a)**  $E = 0 \text{ mV/cm}$  with  $F_{\text{max}} = 0.938$  being the maximum projection over the fully excited state (see Eq. (4.13)). **b)**  $E = 25 \text{ mV/cm}$  with  $F_{\text{max}} = 0.564$ . **c)**  $E = E_{\text{res}} = 29.787 \text{ mV/cm}$  (corresponding to the resonant electric field) with  $F_{\text{max}} = 0.016$ . **d)**  $E = 50 \text{ mV/cm}$  with  $F_{\text{max}} = 0.978$ .

## 4.2 Dependence of the Rydberg blockade on the electric field

First, we show how the blockade radius changes under external homogenous electric fields in arrays of Rydberg atoms. We consider an experimentally realistic 2D tweezer network with a fundamental pitch of  $r_x = 5 \mu\text{m}$  (see Fig. 4.1) in which  $N = 3$  rubidium atoms are placed at a distance  $r = 15 \mu\text{m}$  and subjected to a uniform electric field. The state dynamics in the Fock basis, represented by  $|n_1, \dots, n_N\rangle$  with  $n_i \in \{0, 1\}$ , is shown in Fig. 4.4 by plotting the fidelity  $F = |\langle n_1, \dots, n_N | \Psi(t) \rangle|^2$  between  $|\Psi(t)\rangle$  and  $|n_1, \dots, n_N\rangle$ . For electric fields far away from the Förster resonance ( $E = 0 \text{ mV/cm}$  and  $E = 50 \text{ mV/cm}$  as shown in Fig. 4.4(a) and Fig. 4.4(d) respectively), the system's population oscillates between the ground and fully excited state  $|1_1, \dots, 1_N\rangle$ , as the resulting blockade radius is smaller than the atom separation. However, for electric fields (e.g.,  $E = 25 \text{ mV/cm}$  as seen in Fig. 4.4(b)) approaching the Förster resonance, the population of  $|1_1, \dots, 1_N\rangle$  decreases because the energy defect becomes smaller than the coupling strength. Consequently, the blockade radius increases and becomes comparable to the atom separation. At the Förster resonance ( $E = E_{\text{res}} = 29.787 \text{ mV/cm}$  with  $B_z = 0 \text{ G}$  depicted in Fig. 4.4(c)), the blockade radius reaches its maximum value and surpasses the atom separation. As a result, the probability of the system being fully excited drops to nearly zero.

### 4.2.1 Maximum Fidelity for $N = 3$ atoms

To quantitatively describe the reduction in the probability of the fully excited state around the Förster resonance, we compute the maximum value of the fidelity between  $|\Psi(t)\rangle$  and  $|1_1, \dots, 1_N\rangle$  over a Rabi period  $t \in (0, \tau = 2\pi/\Omega)$  defined as

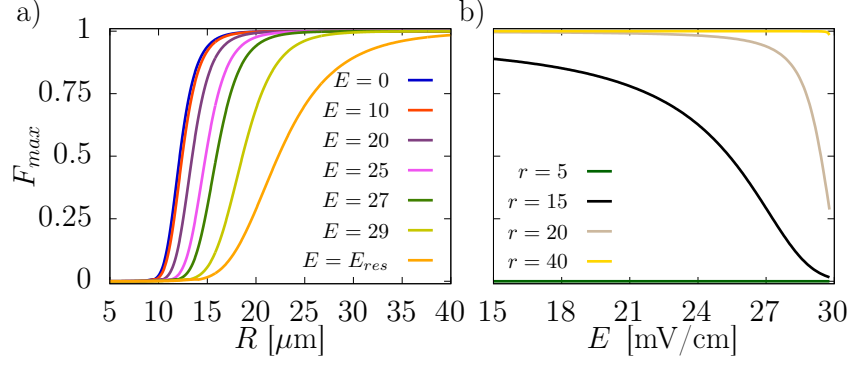


Figure 4.5: **a)** The maximum fidelity for populating the fully excited state,  $F_{max}$  (Eq. (4.13)) for  $N = 3$  over the time period  $t \in (0, 2\pi/\Omega)$ . The atoms have a fixed separation which incrementally increases from  $r = 5 \mu\text{m}$  to  $r = 40 \mu\text{m}$  for the different electric fields  $E = (0, 10, 20, 25, 27, 29, E_{res})$  mV/cm. **b)**  $F_{max}$  as a function of uniform electric field across all  $N = 3$  atoms for fixed separations  $r = (5, 15, 20, 40) \mu\text{m}$ .

$$F_{max} = \max_{t \in (0, \tau)} (|\langle 1_1, \dots, 1_N | \Psi(t) \rangle|^2). \quad (4.13)$$

In Fig. 4.5(a), we showcase  $F_{max}$  for a uniform electric field across the atoms. At small atom spacings, the value of  $F_{max}$  is small as the blockade radius exceeds the separation. However, as the atom distance increases beyond the blockade radius,  $F_{max}$  also rises. This increase happens at different atom separations as the blockade is larger for electric fields closer to the Förster resonance. Furthermore, the gradient of  $F_{max}$  changes due to the electric field. This is a result of the change in nature of the interactions from  $r^{-3}$  to  $r^{-6}$ , which occurs at short atom-atom separation and more abruptly for  $E = 0$  mV/cm compared to  $E = E_{res}$  mV/cm.

Alternatively, we can look at  $F_{max}$  at fixed atom separations in homogeneous electric fields (Fig. 4.5(b)). For  $r = 5 \mu\text{m}$ ,  $F_{max}$  remains low for all electric field values as this atom spacing is much smaller than the blockade radius. Conversely, for  $r = 40 \mu\text{m}$ , the separation is much larger than the blockade radius at all electric fields; therefore,  $F_{max}$  remains high. At the intermediate values  $r = 15 \mu\text{m}$  and  $r = 20 \mu\text{m}$   $F_{max}$  decreases as the electric field approaches the Förster resonance, since the blockade exceeds the atom distance. The non-linear behaviour of these curves stems from the way  $F_{max}$  is shifted in Fig. 4.5(a), which result in a steeper gradient at the larger atom spacings  $r = 20 \mu\text{m}$ .

#### 4.2.2 How System Size Affects Maximum Fidelity

While  $N = 3$  atoms capture the main features of the Rydberg blockade dependence on electric field, adding more atoms enhances Rydberg interactions, which is reflected in on the blockade radii.

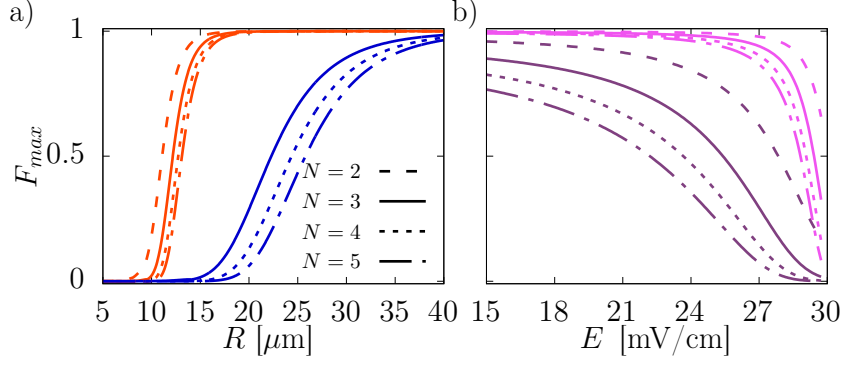


Figure 4.6: The maximum projection  $F_{max}$  of  $|\Psi\rangle$  to the Fock state  $|1_i, \dots, 1_N\rangle$  over the period  $t \in (0, \tau = 2\pi/\Omega)$  for  $N$  atoms, where  $\Omega$  is the Rabi frequency. **a)** All atoms are subject to the same electric field (either  $E = 0$  mV/cm or  $E = E_{res}$  mV/cm) and have atom separation  $r$ . **b)** All atoms have equal spacing (either  $r = 15 \mu\text{m}$  or  $r = 20 \mu\text{m}$ ) with a uniform applied electric field.

The collective effect of the Rydberg blockade is examined by computing  $F_{max}$  for systems with an increasing number of atoms. This serves as an indicator of how the blockade radius evolves with system size. Two electric field values are considered:  $E = 0$  and  $E = E_{res}$ , with atoms arranged at a fixed separation  $r$ , as illustrated in Fig. 4.6(a). As more atoms are introduced,  $F_{max}$  shifts due to the additional interactions in the system. These collective contributions effectively enhance the interaction strength, resulting in an increased blockade radius. The extent of the shift varies with the electric field, as it determines the interaction scaling. At  $E = 0$  mV/cm, interactions follow a van der Waals scaling ( $V \propto r^{-6}$ ), whereas around the Förster resonance ( $E = E_{res}$  mV/cm), they follow a resonant dipole-dipole scaling ( $V \propto r^{-3}$ ). As a result, the stronger interactions at the resonance lead to a more pronounced shift in  $F_{max}$  when atoms are added. However, this effect saturates gradually, as atoms farther away contribute less to the total interaction due to the distance dependence.

Furthermore, for fixed atom separations of  $r = 15 \mu\text{m}$  and  $r = 20 \mu\text{m}$ , the increase in the blockade radius with the number of contributing atoms is illustrated in Fig. 4.6(b). At a given electric field,  $F_{max}$  decreases as the number of atoms grows. Examining the behaviour of the interaction  $V$  at these separations, we observe that for small electric fields, the interaction scales as  $r^{-6}$ ; however, as the electric field increases, it changes to a  $r^{-3}$  scaling. This crossover occurs at a lower electric field for  $r = 15 \mu\text{m}$  compared to  $r = 20 \mu\text{m}$ , leading to a stronger effect on the blockade radius and thus a more pronounced shift in  $F_{max}$  at the smaller separation.

### 4.3 Density-Density Correlator

The main features of the interaction in Rydberg systems are mediated through a two-body process; therefore, employing the two-body density-density correlator  $\langle n_i n_j \rangle$  provides deeper insight into the particles' interaction. This quantity serves as a direct and

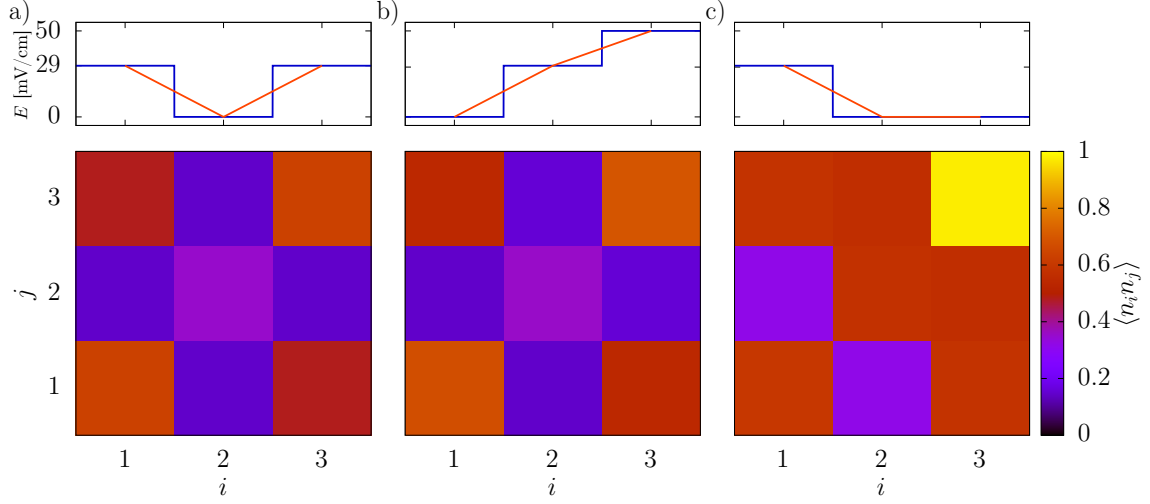


Figure 4.7: **Top:** The applied electric field configuration  $E/E_{res}$  across  $N = 3$  atoms, which are separated by a distance  $R = 15 \mu\text{m}$ . **Bottom:** The corresponding density-density correlator  $\langle n_i n_j \rangle$  for the above electric field configurations recorded at maximum population of the fully excited state. **a)**  $E = E_{res}, 0, E_{res}$  mV/cm. **b)**  $E = 0, E_{res}, 50$  mV/cm. **c)**  $E = E_{res}, 0, 0$  mV/cm.

experimentally accessible measure of spatial correlations and offers a clear signature of the Rydberg blockade phenomenon. Our setup relies on the changes of the blockade radius, therefore this measure offers a direct connection to the applied electric fields.

#### 4.3.1 Density-Density Correlator for $N = 3$ atoms

The density-density correlator  $\langle n_i n_j \rangle$  is calculated for a system of  $N = 3$  atoms separated by  $r = 15 \mu\text{m}$  and subjected to a spatially varying electric field. Results for different electric field configurations are shown in Fig. 4.7. The diagonal elements represent the excitation probability at each site, while the super- and sub-diagonal elements reflect correlations between nearest neighbours. In configurations where one atom is near the Förster resonance, the correlator with its neighbour is suppressed due to the Rydberg blockade—i.e., the blockade radius exceeds the interatomic separation (as observed in Fig. 4.7(a, b)). Conversely, when neighbouring atoms are far from resonance, as in Fig. 4.7(c), the correlators  $\langle n_2 n_3 \rangle$  and  $\langle n_3 n_2 \rangle$  are enhanced, indicating that the blockade is weaker than the separation and simultaneous Rydberg excitation is allowed.

#### 4.3.2 Density-Density Correlator for $N = 19$ atoms

To showcase this dependence, we consider a system of  $N = 19$  atoms with an interatomic separation  $r = 15 \mu\text{m}$ , and calculate the correlator for different electric field configurations at the time where the fidelity of the fully excited state ( $|1_1, \dots, 1_N\rangle$ ) is maximum - Fig. 4.8. We note that the diagonal terms represent the expectation value of the density at each site, which for atoms subject to electric fields close to resonance, takes smaller values

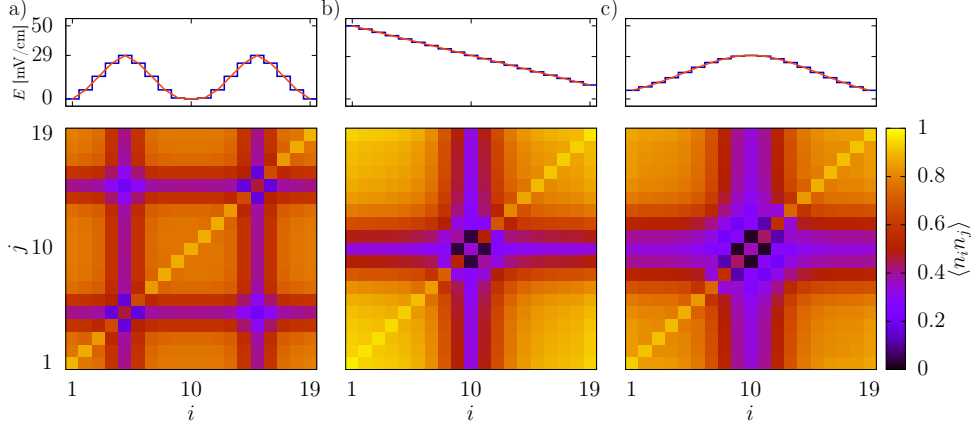


Figure 4.8: **Top:** The applied electric field configuration  $E$  across  $N = 19$  atoms, which are separated by a distance  $r = 15 \mu\text{m}$ . **Bottom:** The corresponding density-density correlator  $\langle n_i n_j \rangle$  for the above electric field configurations recorded at maximum population of the fully excited state. **a)** Sinusoidal function with two resonant peaks, located at  $i, j = 5$  and  $i, j = 15$ . **b)** Gradient field with  $E = E_{res}$  mV/cm for atom  $i, j = 10$ . **c)** Gaussian function mimicking the AC Stark shift of a laser beam.

compared to those with an electric field away from the resonance. Thus, the local density expectation value already provides a signature of the overall shape of the electric field.

The super- and sub-diagonal correlator terms (symmetric under  $i \leftrightarrow j$ ) indicate whether neighbouring atoms can be simultaneously excited. For  $r = 15 \mu\text{m}$ , small  $\langle n_i n_j \rangle$  values indicate fields near the Förster resonance, where the blockade radius exceeds the separation and suppresses excitations, while large values correspond to fields far from resonance, where multiple excitations are allowed. To illustrate this dependence, in Fig. 4.8 we consider several electric-field configurations and calculate the resulting correlations. In Fig. 4.8(a), a sinusoidal electric field produces correlator minima at resonant positions. A constant negative gradient, as depicted in Fig. 4.8(b), yields nearly equal correlators about the resonance, though slight differences arise because  $|\delta|$  and  $C_3$  are not fully symmetric with respect to  $\delta = 0$ . Figure 4.8(c) shows the response to a Gaussian-shaped field, emulating the AC Stark shift from a focused laser beam [273]. All these cases show that  $\langle n_i n_j \rangle$  can capture the overall shape of spatially varying electric fields as this measurement directly reflects interaction-induced spatial correlations.

## 4.4 Application: Sensing of Electric Fields

The effects discussed above provide the ingredients for creating a quantum sensor using arrays of Rydberg atoms. Based on the geometry outlined in Fig. 4.1, we consider a two-dimensional tweezer array with atoms regularly spaced along each row, while the interval between the rows is much larger than the atom-atom separation. Different atom spacings serve as a probe of the distinct blockade radii produced by the specific uniform

electric fields. This feature, quantified by the maximum fidelity  $F_{max}$ , can be effectively exploited to get information about the electric field which the atoms experience. In an experimental setting, the fidelity of state  $|1_1, \dots, 1_N\rangle$  is directly accessible by measuring the Rydberg excitation state of each atom, providing a direct link between theory and observable quantities. The flexibility in controlling the geometry can be used to perform multiple measurements in a single shot.

Indeed in an experimental setting, a single shot cannot provide information such the Fidelity of the states, therefore, in the Appendix, we provide statistical analysis to compare multiple shots for estimating electric field values.

In our scheme, we use different interatomic distances per row. While rows with small and large separations ( $r \ll r_b$  and  $r \gg r_b$  at all electric fields such that the dependence is negligible) provide reference baselines; intermediate separations —comparable to the number of Rydberg blockade radii over the electric field range— serve as the primary probes for electric-field sensing. The sensitivity of these sensing channels can range from broad dynamic range to high precision depending on their pitch separation and the applied field as depicted in Fig. 4.5(b). In particular,  $r = 15 \mu\text{m}$  provides a broad dynamic range for detecting the field as depicted in the black line of Fig. 4.5(b) from  $E \in (15, 30)$ , while  $r = 20 \mu\text{m}$  enables higher sensitivity due to the larger slope of beige line of Fig. 4.5(b), but only near the Förster resonance  $E \in (27, 30)$  mV/cm. The smallest distance between atoms in our array,  $r = 5 \mu\text{m}$ , and the largest distance, which exceeds the maximum blockade radius obtained at the Förster resonance, e.g.,  $r = 40 \mu\text{m}$ , serve as reference values for normalisation and reduction of the signal-to-noise ratio. Altogether, this configuration enables precise and tunable electric field sensing across a range of field strengths.

For spatially varying electric fields on the micrometre scale, Fig. 4.8 illustrates how the Rydberg array can reconstruct the overall field profile. In regions where the field is close to the Förster resonance, the correlator  $\langle n_i n_j \rangle$  takes low values, consistent with a blockade radius exceeding the interatomic separation and suppressing simultaneous excitations of neighbouring atoms. In contrast, far from resonance,  $\langle n_i n_j \rangle$  is large, indicating a reduced blockade radius that permits multiple excitations. By mapping these spatial variations in the correlator, the proposed setup can also resolve and characterise local electric-field distributions.

## 4.5 Conclusion

In this chapter, we investigated the Rydberg blockade under both uniform and spatially varying electric fields. The application of an electric field modifies the blockade radius, which reaches its maximum at the Förster resonance owing to the minimisation of the energy defect between relevant pair states. By employing arrays with tailored interatomic separations, this effect can be exploited to infer the local electric field.

Leveraging this phenomenon, we demonstrate the operating principles of an electric-field sensor based on a two-dimensional Rydberg network, as illustrated in Fig. 4.1. The sensing mechanism relies on monitoring the maximum fidelity  $F_{\max}$  from Eq. (4.13), which corresponds to the probability that all atoms in a given row are excited to a Rydberg state. For a fixed intra-row distances, the suppression (or lack of thereof)  $F_{\max}$  provides a direct signature of the local electric field, owing to the strong dependence of the Rydberg blockade radius on the applied field. The network is arranged such that atoms are uniformly spaced within each row, while the inter-row separation is significantly larger than the intra-row spacing. By engineering distinct intra-row spacings for different rows, the array enables multiple, simultaneous measurements in a single experimental shot. Rows with separations close to the blockade radius exhibit maximal sensitivity to variations in the electric field, whereas rows with off-resonant separations serve as internal reference signals.

Complementarily, the density–density correlator  $\langle n_i n_j \rangle$  can provide information about the electric field spatial profile. In particular, low values of  $\langle n_i n_j \rangle$  indicate strong suppression of neighbouring excitations, pointing to an effective interaction enhanced by the presence of a near-resonant electric field. By examining the spatial distribution of the correlators across the array, the shape and structure of the electric field can be inferred.

Together,  $F_{\max}$  and  $\langle n_i n_j \rangle$  serve as indicators of electric fields: the former captures global suppression patterns indicative of field strength, while the latter reveals local blockade features tied to the spatial profile of the field. While the present implementation is capable of detecting electric fields, its operational range is inherently constrained by the choice of atomic species and the specific Rydberg levels employed. These restrictions arise from the dependence of the blockade radius and level shifts on the principal quantum number and atomic properties. Expanding the dynamic range and enhancing sensitivity could be achieved by incorporating multiple atomic species or by exploiting different Rydberg states within the same array, thereby providing a broader and more tunable response to external electric fields.

Further work could focus on electric fields manipulating Rydberg interactions and the Rydberg blockade. This can be utilised in quantum simulation of models where certain atoms have stronger or weaker interactions, and can be achieved through local addressing of each atom with a designated laser beam.



Rydberg atoms have emerged as a vital platform in quantum technologies in recent years, mainly due to advances in atomic cooling and trapping techniques. Their highly excited energy states exhibit strong dipolar interactions, leading to unique phenomena such as the Rydberg blockade and facilitation. These effects have played a crucial role in advancing various quantum applications, including computation [28–32] and simulation [38, 39]. Additionally, their large electronic wavefunction increases polarisability, making them suitable for quantum sensing of electric fields [37].

In this thesis, we considered two relevant aspects within the most recent evolution of the field of atomtronics: Rydberg atomtronics [136, 189].

In *Chapter 3*, we examined excitation dynamics in various networks of Rydberg atoms. By precisely tuning the laser detuning and designing the specific geometry of the tweezer arrays, we conceived atom arrays that function as counterparts to electronic devices by employing Rydberg excitations. Specifically: we demonstrated a **controlled flow** over a linear network of atoms and use this as a basis for more complex devices. The first proposed device is a **switch** that utilises a specific detuning of a single Rydberg atom to control excitation flow, achieved by alternating between the blockade and facilitation regimes [84–87, 90–93]. Second, we demonstrated how a **non-reciprocal flow** can be engineered via local addressing of an atom’s detuning, positioning it so that excitation propagates in one direction but is restricted in the reverse. Lastly, we propose a scheme to produce **classical logical gates**. The two gates demonstrated are the AND and NOT gates, where the first relies on increasing an output atom’s detuning to reach the facilitation regime while two atoms remain excited. The NOT gate is realised by a  $\pi$  pulse by altering an atom’s detuning from facilitation to blockade, thereby inverting the initial decision. Through their combination we show the principles of a universal gate - the NAND gate.

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The study presented in *Chapter 4* introduces a **protocol for sensing electric fields** using a two-dimensional array of atoms driven into a Rydberg state. This protocol relies on the Stark shift and the subtle phenomenon of Förster resonance. As a result of the latter, dipole-dipole interactions are greatly enhanced, maximising the Rydberg blockade effect. By monitoring, then, the size of the Rydberg blockade we establish a method, employing a suitable collection of linear networks, to measure the applied electric field. Each row is chosen with varied atom separation for distinct roles. Additionally, for schemes investigating **spatially varying fields**, we employ the density-density correlator to analyse the relationship between atom pairs as the interaction propagates via two-body effects. This provides a general overview of the field’s shape and variations across the atoms.

Future work could focus on developing more complex devices and their experimental implementation. Enhancements can also be made as the platform can display dynamics suitable for quantum simulation of models such as the quantum Ising model. Possible future directions for the quantum sensor described in *Chapter 4* include integrating different species into the array—either within or between rows—potentially expanding its detectable electric field range. Finally, as demonstrated in the present work, the interaction strength can be controlled via the electric field; this can be beneficial for quantum simulation where certain interactions are enhanced or suppressed.

Although Rydberg atoms have only recently become accessible in quantum technologies, they offer a promising platform for future developments. Over the past century, quantum theory has achieved remarkable milestones, leading to widely used technologies. Looking ahead, who can foresee the breakthroughs the next century might reveal?

# Appendices



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## Supplementary Material for Chapter 3

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### A.1 Excitation Control in a Magneto-Optical Trap

In our description so far, we only consider Rydberg atoms that are held in place by optical tweezers. However, in the case of transport and the device to control the propagation of excitations, we can consider atoms confined in a MOT and observe the propagation of excitations between a source and drain. Since the atoms are contained in a MOT, they are able to move around the gas cloud, and therefore, our simulation must account for the trajectories of the atoms. For this reason, we employ a Monte Carlo scheme to randomly sample these trajectories and use it to define a switch in a three-dimensional gas.

#### A.1.1 Monte Carlo Method

The Monte Carlo method is a numerical technique that uses randomness to approximate solutions to physical and mathematical problems which are challenging or difficult to analytically solve. The birth of the Monte Carlo method links to the work conducted Los Alamos National Laboratory for the Manhattan project; where the initial idea from Ulam has morally right origins in a card game of solitaire. While wondering the about how likely a game was to win, he developed a concept which used a many random simulations of games and took the average of either winning or not. When discussing this idea with Von Neumann, the technique was adapted for the random trajectories of neutrons in atomic bombs - a vital concept to understand the likelihood of an explosion. This adaptation is an example of probabilistic modelling for the trajectories of the neutrons, however, since the method can be used for problems of optimisation and numerical integration.

The main principle of the technique is that after a large number of simulations of a model, an average can be considered a suitable outcome. This idea takes advantage of key mathematical concepts such as the law of large numbers - which states that the average of a

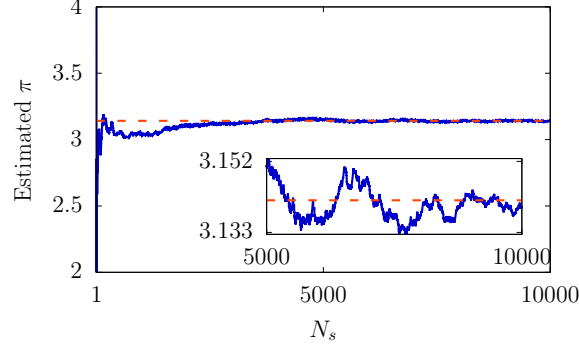


Figure A.1: An estimation of  $\pi$  using a Monte Carlo method.  $N_s$  is the number of samples used in the approximation described in the text. The red dashed line represents the true value of  $\pi$  to five decimal places.

result converges to an expected value as the number of simulations increases. Also, with the central limit theorem, under certain conditions, the average of a large set of independent random values tends to be normally distributed.

To demonstrate the effectiveness of this method, we use a numerical integration example to approximate the value of  $\pi$  using random variables. The premise of this exercise is to utilise a unit square as the domain and divide it into two regions, with a quarter-circle of radius one inscribed within the square. If the random sampling involves placing a point inside the square, which may either fall within the quadrant or outside it. By recording the number of points placed and the number within the quadrant, the ratio is given by  $N_q/N_s$ . Using this and the ratio between the quadrant and square, we derive:

$$\frac{A_q}{A_s} = \frac{\left(\frac{\pi r^2}{4}\right)}{r^2} = \frac{\pi}{4}. \quad (\text{A.1})$$

Therefore, rewriting  $A_q/A_s = N_q/N_s$  gives an expression for  $\pi$  as

$$\pi = \frac{4N_q}{N_s}. \quad (\text{A.2})$$

Fig. A.1, shows this approximation for  $N_s = 10000$ , where the value converges towards  $\pi$ . By using the Monte Carlo method with a sufficiently large random sample size, a stable solution can be achieved to accurately estimate the value of  $\pi$ .

### A.1.2 Rydberg Excitations in a Three-dimensional Gas

In our description, we use the Monte Carlo method to simulate a gas of  $N$  atoms in a three-dimensional potential without controlling their individual positions, where the minimal distance between atoms is  $d_{\min} = 0.1\mu\text{m}$ . This scheme is only suitable for the switch because of the positional dependence in other protocols for producing non-reciprocal flow

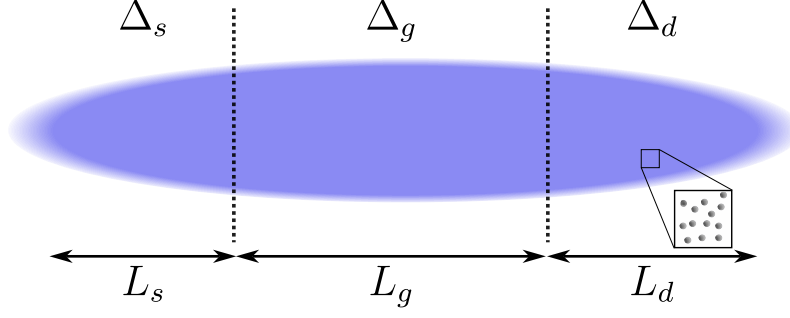


Figure A.2: Schematic of a switch using an extensive Rydberg gas in the limit of strong dephasing Eq. (3.2). The gas is spilt up into three regions: the input with detuning,  $\Delta_s = 0$ , the gate with detuning either  $\Delta_g = \tilde{\Delta}_f/(2\pi)$  (switch on) or  $\Delta_g = -\tilde{\Delta}_f/(2\pi)$  (switch off) and the output with detuning  $\Delta_d = \tilde{\Delta}_f/(2\pi)$ .

of excitations and logical decisions. Figure. A.2 illustrates the protocol, where the gas cloud is divided into three regions, each with a different detuning  $\Delta_s$ ,  $\Delta_g$  and  $\Delta_d$  (which are defined below) each with a length  $L_s = 5\mu\text{m}$ ,  $L_g = 10\mu\text{m}$ , and  $L_d = 15\mu\text{m}$ . The only restriction applied is that  $L_g$  exceeds the facilitation radius from the source, as without this, excitations could directly excite the drain atoms without passing through the gate atoms. In the model, all atoms are subjected to the same driving strength  $\tilde{\Omega}$  and are initialised in the ground state. Each region has a different detuning frequency  $\Delta(x)$ : in the input, Rydberg atoms are excited on resonance with  $\Delta_s = 0$ . In the gate, we have either  $\Delta_g = \tilde{\Delta}_f/(2\pi) = -69.5$  MHz when the switch is on; otherwise, we set  $\Delta_g = -\tilde{\Delta}_f/(2\pi) = 69.5$  MHz to block any transport of excitations. In the output, the detuning is set to the facilitation regime  $\Delta_d = \tilde{\Delta}_f/(2\pi) = -69.5$  MHz.

Operating in a regime of strong dephasing, where  $\tilde{\gamma} \gg \tilde{\Omega}$  (with  $\tilde{\gamma}/(2\pi) = 700$  kHz and  $\tilde{\Omega}/(2\pi) = 50$  kHz), and therefore, we use the classical approximation (Eq. (3.2)) to simulate the dynamics across the gas cloud. In this case, atoms are randomly distributed throughout the cloud, and their positions are randomly chosen to model the excitations' dynamics. This process is repeated for 30 trajectories, recording the average population in the drain. Afterwards, atom positions are randomly reselected, and the process is repeated for 10 different instances. These 10 repetitions are then averaged, as shown in Fig. A.3, where our simulation parameters are chosen closely to the ones from the Rubidium atom experiment in [253]. Our work compared two different decay rates, in both cases, when the gate atoms are subjected to off-resonance detuning ( $\Delta_g = -\tilde{\Delta}_f/(2\pi)$ ), the population in the drain decreases compared to when the atoms experience resonant detuning ( $\Delta_g = \tilde{\Delta}_f/(2\pi)$ ). This demonstrates the switching mechanism, where certain gate atom detuning values can inhibit excitation propagation to the drain. Additionally, an increased decay rate,  $\tilde{\kappa}$ , reduces the drain's population in both detuning scenarios.

To further see the effect of blocking the excitation to flow from the source and drain, the gate atoms detuning could be pushed further away from the resonance. As we see in Sec. 3.3, a larger gate atom's detuning results in a decrease in the drains population,

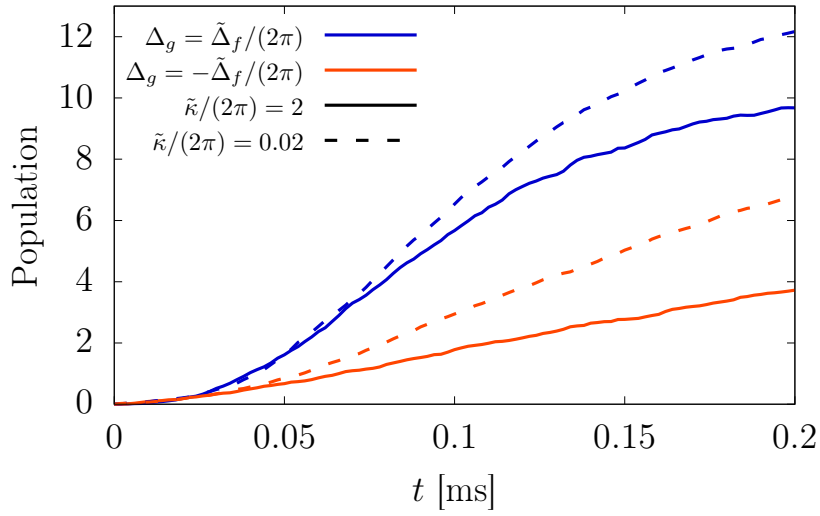


Figure A.3: Switch using  $N = 3000$  atoms trapped in a potential shaped as a cylinder of length  $L_x = 30\mu\text{m}$  and a radius of  $R = 7\mu\text{m}$ . We show the number of output excitations  $N_o$  controlled by gate detuning  $\Delta_g$  over the time  $t$ . For this setup, we use explicit dimensionfull parameters, which are denoted by a tilde, we have  $\tilde{C}_6/(2\pi) = 869\text{GHz}\mu\text{m}^6$ ,  $L_s = 5\mu\text{m}$ ,  $L_g = 10\mu\text{m}$ ,  $L_d = 15\mu\text{m}$ ,  $\tilde{\gamma}/(2\pi) = 700\text{kHz}$ ,  $\tilde{\kappa}/(2\pi) = 2\text{kHz}$ ,  $\tilde{\Omega}/(2\pi) = 50\text{kHz}$ ,  $\Delta_f = \tilde{\Delta}_f/(2\pi) = -69.5\text{MHz}$ . We have  $\tilde{r}_f = 4.8\mu\text{m}$ ,  $\tilde{r}_b = 10.4\mu\text{m}$  and a gas density of  $2.3 \cdot 10^{12}\text{cm}^{-3}$ . The numerical simulation is averaged over 10 random instances of atom positions with 30 simulation trajectories each.

which is also applicable in this situation.



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Supplementary Material for Chapter 4

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## B.1 Bayesian Statistics

To complement the analysis in the main text, we offer an alternative approach to estimate a single value of an electric field. Considering that the electric field might not be constant across an array of  $N = 3$  atoms, we utilise Bayesian statistics to determine an electric field given the other two field values. Bayesian statistics is grounded in the principle of updating beliefs or probabilities in light of new evidence [284, 285]. The theory serves as a versatile tool in quantum metrology [286, 287].

### B.1.1 Derivation of Bayes' Theorem

This technique is used to estimate an unknown parameter  $\theta$  of a system which has been measured with the following outcome,  $S = \{x_1(\theta), x_2(\theta), \dots, x_n(\theta)\}$ . Assuming the parameter exists within the space  $\theta = [\theta_{min}, \theta_{max}]$ , the use of Bayes' theorem estimates the Posterior distribution  $P(\theta|S)$  around the target parameter. The conditional probability that event has  $\theta$  occurred is defined as:

$$P(\theta|S) = \frac{P(\theta \cap S)}{P(S)}, \quad (\text{B.1})$$

where  $P(\theta \cap S)$  is the joint probability of both events happening. Similarly, the conditional probability of  $S$  given  $\theta$  is

$$P(S|\theta) = \frac{P(\theta \cap S)}{P(\theta)}. \quad (\text{B.2})$$

Re-writing both Eq. B.1 and Eq. B.2 for the joint probability gives

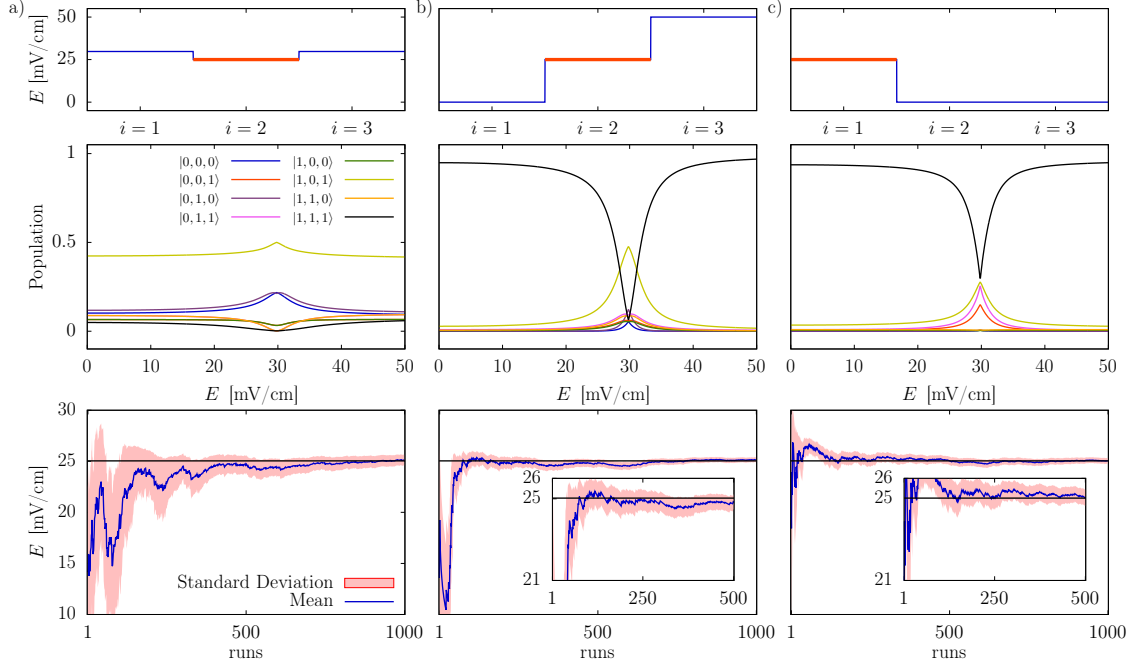


Figure B.1: Bayesian analysis for  $N = 3$  atoms separated by  $r = 15 \mu\text{m}$  to estimate a single value of an electric field. **Top:** The applied electric field configuration across the atoms, with the highlighted field corresponding to the parameter to estimate  $E = 25 \text{ mV/cm}$ . **Middle:** The population of each of the state when the highlighted electric field is varied from  $E = 0 \text{ mV/cm}$  to  $E = 50 \text{ mV/cm}$ , recorded at  $t = \pi/\Omega$ . **Bottom:** The mean value posterior calculated through Eq. (B.4) for runs = 1000. The shaded area is the standard deviation of the posterior.

$$P(\theta \cap S) = P(\theta|S)P(S) \quad \text{and} \quad P(\theta \cap S) = P(S|\theta)P(\theta). \quad (\text{B.3})$$

Setting these two equal and re-arranging gives the expression

$$P(\theta|S) = \frac{P(S|\theta)P(\theta)}{P(S)}, \quad (\text{B.4})$$

where  $P(\theta)$  is the pre-known knowledge (distribution),  $P(S|\theta) = p_i(x_i(\theta))$  is the conditional probability of making the observation  $x_i(\theta)$ . The posterior<sup>1</sup> is an updated distribution, which is normalised via  $P(S)$ , and can be reused as  $P(\theta)$  in another iteration of Eq. (B.4).

### B.1.2 Electric Field Parameter Estimation using Bayes' Theorem

In the context of sensing electric fields, we employ Bayes' theorem to estimate a single value parameter value. We use an array of  $N = 3$  atoms which all experience an independent electric field, considering three variations of configurations which are shown in the

<sup>1</sup>originating from the Latin *posterus* meaning 'coming after'.

top row of Fig. B.1. For ease, we select the value to estimate as  $E_{true} = 25$  mV/cm which in the above description is  $\theta$ . However, as we are considering a system which is primarily unmeasured, therefore we assume no initial knowledge of  $E_{true}$ , the prior distribution is set to a uniform distribution  $P(E_i)$  where  $E_i = [0, 50]$  mV/cm. To obtain the conditional probability, we investigate the state populations (amplitudes) when the electric field on the atom we want to measure varies over  $E_i$  - this can be seen in the middle row of Fig. B.1. In doing this, we denote  $x_i$  as each of the states (which for  $N = 3$  are eight in total) and their population correspond to the probability  $p_i$ .

Applying Bayes' theorem for the three electric field configurations in Fig. B.1, we iterate through the algorithm 1000 runs to show the estimation converges on  $E_{true}$ . If the applied electric field on either of the two auxiliary atoms is close enough to the resonance, so that the resulting blockade radius is greater than the atom separation, the population of the fully excited state remains low and relatively constant for all  $E$ . This situation is shown in Fig. B.1(a), where the difficulty arises that due to the non-varying state populations, Bayes' theorem cannot converge on  $E_{true}$  as the probability of each measurement is similar for all values of  $E$ . However, suppose the auxiliary atoms are subject to an electric field where the blockade radius is smaller than the atom separation. In that case, we observe a change in the population of the fully excited state as  $E$  changes, because this atom now dominates whether a blockade occurs or not. This situation is given in both Fig. B.1(b, c), where, due to the changing population for the applied  $E$ , Bayes' theorem can estimate  $E_{true}$  for a small number of runs.



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