

ATOMIC CHAINS WITH RYDBERG EXCITATIONS: BOSE-HUBBARD PARAMETERS TO CORRELATION DYNAMICS

A DISSERTATION
SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENT OF THE
DEGREE OF DOCTOR OF PHILOSOPHY IN PHYSICS

BY

YASHWANT CHOUGALE

REGISTRATION NUMBER: 20142031

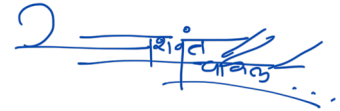


DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH
PUNE 411008, INDIA
2021

Dedicated to Baba, Aai, Pappa & Didi

DECLARATION

I, **Yashwant Chougale**, declare that the written submission entitled “**Atomic Chains with Rydberg Excitations: Bose-Hubbard Parameters to Correlation Dynmaics**” represents my ideas in my own words and where others ideas have been included, I have adequately cited and referred original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that violation of the above will be cause for disciplinary action by the institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed. The work reported in this thesis was done under the guidance of Dr. Rejish Nath.



Yashwant Chougale

CERTIFICATE

I certify that the thesis entitled “**Atomic Chains with Rydberg Excitations: Bose-Hubbard Parameters to Correlation Dynamics**” presented by **Yashwant Chougale** represents his original work which was carried out by him at IISER, Pune under my guidance and supervision during the period from Aug 2016 to July 2021. The work presented here or any part of it has not been included in any other thesis submitted previously for the award of any degree or diploma from any other university or institutions. I further certify that the above statements made by him in regard to his thesis are correct to the best of my knowledge.



Dr. Rejish Nath
(supervisor)

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Acknowledgements

First and foremost I would like to thank my supervisor, Dr. Rejish Nath, for his guidance on various projects. He is been patient throughout the duration of my Ph.D. I would like to thank him for his feedback on the thesis. I am also grateful to him for making me aware of career opportunities outside academia other than Physics.

I thank my RAC members Prof. T S Mahesh and Dr. Sreejith G J for their continuous valuation of my work. I would like to thank my collaborators Dr. Tomas Ramos, Jugal Talukdar, and Sagarika Basak with whom I had an opportunity to work. I would like to thank Dr. Tapan Mishra from IIT Guwahati for giving me an opportunity to visit his group. I thank Suman Mondal for teaching me DMRG.

I thank IISER Pune for the uninterrupted funding provided throughout my Ph.D. tenure. I am grateful for the partial travel support provided by the Infosys Foundation for attending a conference at OIST Japan. I am thankful to ICTP Italy for fully funding the visit to summer school.

A special thanks to Prabhakar and Dhanashree from the Physics office and Tushar and Sayali from the academic office for their help with all the official matters. I would like to specially thanks Tushar for the genuine care he showed while solving our problems. The stay at IISER would not have been smooth without the tremendous efforts of the non-teaching staff at IISER Pune including the IT department, electrical department, housekeeping staff, mess, and canteen staff. I would like to thank the gardening department for beautifully maintaining the campus. I would like to thank gym trainer Mr. Santosh Bhosale for his training.

Over the years of my time at IISER, I had the privilege to share the office with two wonderful colleagues and good friends, Ankita and Chinmayee. I would like to thank them for their unique perspective on various topics ranging from feminism to entertainment. Their presence has helped me immensely during the highs and lows of my Ph.D. life. I would like to thank my former and current group members

Supriti, Ratheejit, Sandra, Gopal, Pranay, Vighnesh, Banibrata, and Vineesha. I would like to thank my roommate Deepak for being a reliable company for misal pav outings to which he never said no. Thank you for helping me with choosing clothes and improving my dressing sense. I would like to thank Mayur for all the snacks he bought every time he came back from home. Also many thanks to friends Sayali, Tejal, Punita, Dipti, Vikhyaat, and Payal, Pankhuri.

Lastly, this all would not have been possible without the rock-solid support from my family. I am sincerely grateful to my parents Kerba Chougale and Ashwini Chougale for the constant support they provided in pursuit of my dream of doing a Ph.D. I would like to thank my sister Chirta (Didi) for all her efforts. And finally, my late grandpa Krisha Patil whose passion for higher education has always been an inspiration.

Abstract

Synthetic quantum systems are simplified versions of real-world, complex, quantum many-body systems. They provide a versatile testbed for understanding the complex phenomenons of condensed matter physics, nuclear physics, high energy physics, and chemistry. In the context of quantum many-body physics, these systems have mainly been used to study various spin models and Hubbard-type models. The major advantage of synthetic quantum systems is the possibility to have control over system parameters such as dimension, scale, the strength of interaction, and range of the interaction. The tremendous experimental progress in the area of laser cooling and trapping has boosted the development of various synthetic quantum systems based on different architectures. The platforms based on ultracold atoms, ions, superconducting circuits, photons have emerged in the past two decades and have succeeded in revealing exotic quantum phenomena. Among all the platforms, Rydberg atom-based quantum systems stand out because of strong controllable interaction, single-site addressability, scalability, and large coherence times. These systems have been used to study both the ground state physics as well as non-equilibrium dynamics of various spin models.

This work is focused on utilizing the properties of Rydberg atoms along with other tools to achieve control over the interactions, population dynamics, correlations, and entanglement in the system. In three independent setups, we show how the specific properties of the system along with the properties of Rydberg atoms can be used to achieve the same. Towards that goal, in Chapter 1, we give a brief overview of the developments in the field of ultra-cold atoms. We then discuss the basic properties of Rydberg atoms such as Rydberg blockade, Rydberg dressed interaction, Bose-Hubbard model, photonic crystal waveguides. These properties will be used in subsequent chapters.

In chapter 2, we calculate the Hubbard parameters for Rydberg-dressed interaction using maximally localized Wannier functions. We show that by varying

the external laser parameters we can vary the shape of Rydberg-dressed potential such that the extended Bose-Hubbard model can be realized. We also identify the dominant density-assisted tunneling processes for Rydberg-dressed interaction.

In chapter 3, we study a chain of Rydberg atoms in which the detuning is periodically varied in time. We identify the correlated Rabi oscillations emerging due to Rydberg interaction and study the effect of periodic driving onto the correlation functions characterizing the correlated Rabi oscillations.

Chapter 4 studies the single excitation dynamics of an atomic excitation coupled to a photonic crystal waveguide. The coupling of atoms to photonic modes of the photonic crystal waveguide gives rise to an effective exchange Hamiltonian with a controllable exchange interaction range. We study the excitation dynamics as a function of exchange interaction range and characterize the change in the dynamics using various parameters.

In the final chapter, we introduce one more excitation to the system and study the effect of that excitation on the dynamics. Firstly, for the non-interacting excitations, we show the anti-bunching dynamics and quasi-localization. Secondly, for the Rydberg excitations, we take into account the van der Waals interaction and study its effect on the excitation dynamics. By varying the strength of vdW interaction we go from anti-bunching dynamics to bound state dynamics. We also investigate the effect of initial separation on the population dynamics and entanglement.

Symbols & Abbreviations

Physical constants

$\hbar \rightarrow$ Planks constant

Abbreviations

BEC $\rightarrow$ Bose Einstein Condensate

BHM $\rightarrow$ Bose Hubbard Model

EBHM $\rightarrow$ Extended Bose Hubbard Model

WF $\rightarrow$ Wannier Functions

MLWF $\rightarrow$ Maximally Localized Wannier Functions

BZ $\rightarrow$ Brillouin Zone

HO $\rightarrow$ Harmonic Oscillator

NN $\rightarrow$ Nearest Neighbor

NNN $\rightarrow$ Next Nearest Neighbor

DAT $\rightarrow$ Density Assisted Tunneling

MWOL $\rightarrow$ Magic Wavelength Optical Lattice

PWC $\rightarrow$ Photonic Crystal Waveguide

LTPD $\rightarrow$ Long Time Probability Distribution

CTQW $\rightarrow$ Continuous Time Quantum Walk

IPR $\rightarrow$ Inverse Participation Ratio

vdW $\rightarrow$ van der Waals

RRI $\rightarrow$ Rydberg-Rydberg Interaction

List of Publications

1. *Ab initio* calculation of Hubbard parameters for Rydberg-dressed atoms in a one-dimensional optical lattice,
Yashwant Chougale and Rejish Nath,
[J. Phys. B: At. Mol. Opt. Phys. 49, 144005 \(2016\)](#)
2. Periodically driven array of single Rydberg atoms
Sagarika Basak, **Yashwant Chougale** and Rejish Nath
[Phys. Rev. Lett. 120 \(12\), 123204 \(2018\)](#)
3. Dynamics of Rydberg excitations and quantum correlations in an atomic array coupled to a photonic crystal waveguide
Yashwant Chougale, Jugal Talukdar, Tomas Ramos and Rejish Nath
[Phys. Rev. A 102 \(2\), 022816 \(2020\)](#)

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Chapter 1

Introduction

1.1 Overview

Bose-Einstein Condensate (BEC), the fifth state of matter, was predicted by Satyendra Nath Bose and Albert Einstein in 1920. The results predicted were so groundbreaking that Einstein in his 1925 paper claimed them to be “as good as impossible”. Seventy years later in 1995, experimentalists at JILA, lead by C. E. Weiman and E. A. Cornell, were successful in observing the “fifth state of matter”. For the first time, they observed the signatures of BEC in a cloud of Rubidium atoms at a temperature of 170 nanokelvin [1]. This remarkable feat was possible due to the tremendous progress in the area of laser cooling and trapping. The development of trapping techniques of Magneto-optical-trap and the cooling techniques such as Zeeman cooling, Doppler and sub-Doppler cooling, evaporative cooling, lead to the achievement of temperatures in the micro kelvin to nano kelvin range. Such a low temperature made it possible to trap atoms using various methods.

In 1978, Ashkin proposed cooling and trapping of atoms using the dipole force arising from the dipole moment of atoms interacting with the electric field [2, 3]. Building upon these proposals, trapping of neutral atoms was achieved for the first time [4] and later using a far off-resonant trap for Rb atoms [5]. After these initial developments, various other methods of trapping atoms have been proposed [6]. Amongst them, the trapping of atoms in the optical lattice has emerged as a versatile method because of its controllability. The potential landscape formed by interference of counter-propagating laser beams gave rise to the possibility of forming a lattice of trapped atoms. The optical lattices provide the tunability of lattice depths and also the dimensionality of lattices [7, 8]. Recently a new way of trapping

atoms using nanophotonic structures has emerged with a motivation of interfacing atomic systems with the nanophotonic system [9, 10].

With all the progress made over the past two decades, the field of ultra-cold atoms has made a major impact on other fields such as condensed matter, quantum information, metrology, material science, chemistry, and even biology. The techniques of laser cooling and trapping has particularly boosted the development of large scale quantum simulator and programmable quantum computer. The biggest advantage of ultracold atomic systems is that they are almost defect-free, highly tunable, and scalable. For the ultracold atomic system, it is relatively easy to trap, manipulate and detect individual quantum elements of the system compared to other platforms. They also provide the possibility of varying the parameters of the system with external fields e.g. method of Feshbach resonance allows one to tune the strength of atom-atom interactions. All these features have resulted in some remarkable experiments such as supersolid formation in dipolar BEC [11], observation of degenerate fermi gas [12, 13], the observation of Kosterlitz-Thouless type transition in two-dimensional atomic gas [14, 15], Mott insulator to the superfluid phase transition of atoms loaded in optical lattice [16] and a very recent one where non-equilibrium dynamics of a quantum system is studied with 256 atom Rydberg quantum simulator [17].

Among all the experiments featuring ultracold atoms, the one having Rydberg atoms has gained a lot of traction over the past two decades. The exaggerated properties of Rydberg atoms make them a perfect candidate for quantum simulations, quantum computing, and metrology. Rydberg atoms are highly sensitive to the external fields due to their large polarizability [1.1]. This property of Rydberg atoms has been exploited to build sensors that can detect very small electric fields in a wide range of frequencies [18, 19]. The most important property of the Rydberg atoms is their huge transition dipole moment which results in the strong, anisotropic, tunable interaction between the two Rydberg atoms. The strength of the interaction can be orders of magnitude more than the ground state atoms, which is crucial for many applications. Particularly, the phenomena of “Rydberg blockade” which arises due to strong interaction has been exploited for quantum computing applications. In 2000, Jaksch *et al* proposed the use of Rydberg blockade for logic gate implementation [20]. In 2009, the Rydberg blockade was experimentally observed for two individually trapped atoms and using which the controlled-NOT gate was implemented [21]. Further experiments have also achieved the preparation of

highly entangled states using Rydberg blockade with high fidelity [22, 23]. This has boosted the progress for quantum information related applications.

On the quantum many-body side, Rydberg atoms based setups are used to implement and study various types of spin models [24, 25]. Many experiments have demonstrated exotic phases of matter as well as interesting non-equilibrium dynamics. To name a few, the dynamical crystallization of Rydberg excitations in a two-dimensional lattice [26, 27], the realization of Ising type quantum spin chain [28], implementation of 2D transverse field Ising model with 196 atoms, the study of exotic phases of quantum spin models with up to 256 atoms, the stabilization of coherent revivals associated with quantum scars by periodic driving [29], etc have proven the versatility of Rydberg based platforms. Taking motivation from these developments we make use of Rydberg atoms along with other system properties to explore interesting physics revealed. In the system consisting of Rydberg atoms, we demonstrate the control over the interactions, correlations, and entanglement in the system. Since the Rydberg atoms are common to all the setups, it's of importance to understand the properties of Rydberg atoms. In the next section, we begin by discussing the useful properties of Rydberg atoms as well as other systems, which will be used in the upcoming chapters.

1.2 Rydberg Physics

Rydberg atoms are atoms in which the valence electron is excited to a very high principal quantum number n . For a typical experiment involving Rydberg atoms, the principal quantum number, n , is generally greater than 30. For such high values of n , the valence electron is far away from the nucleus and the multi-electron system can be effectively treated as a Hydrogen atom Fig[1.1a]. This approximation works well for high angular momentum (l) quantum states, for which the electron is far away from the core. In this thesis, we shall use the properties of low angular momentum states. For such states, the interaction between the valence electron and atomic core can not be neglected due to the higher level of penetration of the electron into the core. The theory of quantum defects takes into account this interaction by modifying the principal quantum number n by an amount $\delta(n, l, j)$, called the quantum defect, for state with principal quantum number n , angular momentum quantum number l , and magnetic quantum number j . Taking into account the quantum defect, the energy of the atom is given by,

Properties	n scaling	Rb(5S)	Rb (43S)
Binding energy	n^{-2}	4.18 eV	8.56 meV
Level spacing	n^{-3}	2.5 eV	413.76 μeV
Polarizability	n^7	$-79.4 \text{ MHz}(\text{V cm}^{-1})^{-2}$	$-17.7 \text{ MHz}(\text{V cm}^{-1})^{-2}$
Lifetime	n^3	26.2 ns	42.3 μs
Transition dipole moment	n^{-2}	4.227 ea_0	1069 ea_0
vdW coefficient C_6	n^{11}	4707 au	-1.697×10^{19} au

Table 1.1: Comparison between properties of Rydberg state (43S) and ground state (5S)

$$E(n, l, j) = -\frac{R'}{(n - \delta(n, l, j))^2} \quad (1.1)$$

where R' is the Rydberg constant, whose value for Rubidium atom is $109736.605 \text{ cm}^{-1}$. In this thesis, we will focus on the properties of the Rubidium atom as it is commonly used in most Rydberg-based experiments. With the help of these energies, the Schrodinger equation for the Hydrogen like atom can be solved analytically and the wavefunctions can be obtained. The wavefunctions in the spherical polar coordinate are given by,

$$\psi(r, \theta, \phi) = N \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]}} e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}(2r/na_0) \times e^{ij\phi} P_l^j(\cos \theta) \quad (1.2)$$

where, $P_l^j(\cos \theta)$ are associated Legendre polynomials and L are a generalized Laguerre polynomial. We make use of these wavefunctions to calculate the dipole matrix elements between various states. The knowledge of which is crucial in calculating the lifetimes and the van der Waals coefficients. The table below compares the properties of Rubidium atoms in two states, one being the ground state 5S and the other being the Rydberg state 43S Table [1.1] [30].

The properties which scale polynomially with n are orders of magnitude large for the Rydberg state compare to the ground state. These exaggerated properties of Rydberg states are advantageous for the controllability and tunability of interactions. We shall be focusing on the strong interaction between two atoms in the Rydberg state which are separated by a distance of R . In the next sections, we

study how the interaction between Rydberg atoms gives rise to the phenomenon of Rydberg blockade and the Rydberg-dressed interaction.

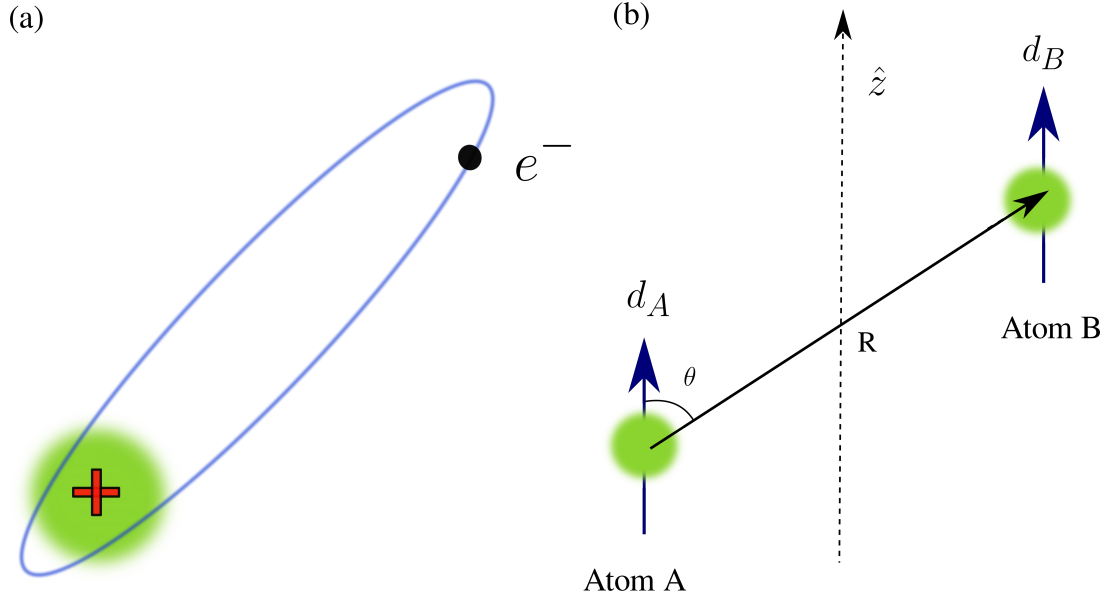


Figure 1.1: (a) A schematic of Rydberg atom (b) A schematic of two Rydberg atoms with dipole moment interacting via vdW interaction

1.2.1 Rydberg Blockade

The Rydberg blockade arises due to strong interaction between two atoms excited to Rydberg states. The large dipole moments of Rydberg atoms make them interact strongly even at large separation. We consider two atoms labeled A and B . We assume that both the atoms are excited to the same state $|nl\rangle$, with n and l being the principal quantum number and orbital angular momentum quantum number respectively. Let R be the separation between two atoms Fig[1.1 b]. The atoms interact mostly via strong dipole-dipole interaction given by,

$$\hat{V} = \frac{1}{4\pi\epsilon_0 R^3} (\hat{d}_A \cdot \hat{d}_B - 3(\hat{d}_A \cdot \hat{r})(\hat{d}_B \cdot \hat{r})) \quad (1.3)$$

where $\hat{d}_A$ and $\hat{d}_B$ are the dipole moments of atoms A and B respectively. This interaction term couples the two-atom state $|nl, nl\rangle$ to nearby states $|n'l', n''l''\rangle$. However it predominantly couples to only one nearby state e.g. the state $|ns, ns\rangle$ is mainly coupled to the state $|np, (n-1)p\rangle$. For the other states, the difference between energy from $|ns, ns\rangle$ is much larger and hence can be neglected. With this

assumption, the system can be considered as an effective two-level system consisting of states $|ns, ns\rangle$ and $|np, (n-1)p\rangle$. The Hamiltonian in this basis is given by,

$$\hat{H} = \begin{pmatrix} 0 & C_3/R^3 \\ C_3/R^3 & \delta \end{pmatrix} \quad (1.4)$$

where the Forster defect $\delta = 2E_{ns} - E_{np} - E_{(n-1)p}$ is the energy difference between the states $|ns, ns\rangle$ and $|np, (n-1)p\rangle$. The effective Hamiltonian can be diagonalized to find the energy of the two eigenstates as

$$\Delta E_{\pm} = \frac{\delta}{2} \pm \frac{1}{2} \sqrt{\delta^2 + \left(\frac{C_3}{R^3}\right)^2} \quad (1.5)$$

We are interested in the case where atoms separated by distance R in such a way that $C_3/R^3 \ll \delta$. In this case the interaction hardly couples the state $|ns, ns\rangle$ to $|np, (n-1)p\rangle$ and the energy level shift due to this interaction is given by

$$\Delta E_{ns, ns} \approx \frac{C_6}{R^6} \quad (1.6)$$

This is the van der Waals interaction between two atoms excited to the $|ns, ns\rangle$ state. The effect of this interaction is to shift the energy level by amount $\Delta E_{ns, ns}$. For this simple case, the scaling of the C_6 can be easily calculated by the fact that dipole matrix element scales as $d \sim n^2$ and the energy difference scales as $\delta \sim n^{-3}$ giving rise to $C_6 \sim (n^2)^4/n^{-3} = n^{11}$. For the case of Rb atoms, the dispersion coefficient has following dependence [31]

$$C_6^{\text{Rb-Rb}} = n^{11}(c_0 + c_1 n + c_2 n^2) \quad (1.7)$$

with $c_0 = 11.97$, $c_1 = -0.8486$ and $c_2 = 0.003385$. However for a more general case, where more than one state gets coupled to the $|ns, ns\rangle$ state, the energy shift of the state $|ns, ns\rangle$ is given by,

$$\Delta E_{ns, ns} = \sum_{n', l', n'', l''} \frac{|\langle ns, ns | \hat{V} | n' l', n'' l'' \rangle|^2}{2E_{ns} - E_{n' l'} - E_{n'' l''}} \quad (1.8)$$

For the computation in upcoming chapters, we take into account ten nearest states so that convergence is achieved.

With the knowledge that two atoms in the Rydberg state interact via strong vdW interaction which diverges at small atomic separation, R , we now look at how this interaction leads to the phenomenon of Rydberg blockade. For this, we consider

two two-level atoms with two states being the ground state $|g\rangle$ and the excited state, which is a Rydberg state $|r\rangle$. The ground state is coupled with the excited state by a laser with Rabi frequency Ω and the detuning from the excited state is Δ . For this system the basis states can be formed by states $|gg\rangle$, $|gr\rangle$, $|rg\rangle$ and $|rr\rangle$. In this basis, the two atom Hamiltonian is given by,

$$\hat{H}^{(2)} = \begin{pmatrix} 0 & \Omega/2 & \Omega/2 & 0 \\ \Omega/2 & \Delta & 0 & \Omega/2 \\ \Omega/2 & 0 & \Delta & \Omega/2 \\ 0 & \Omega/2 & \Omega/2 & 2\Delta + V_0 \end{pmatrix} \quad (1.9)$$

where, $V_0 = C_6/R^6$ takes into account the vdW interaction for the doubly Rydberg excited state $|rr\rangle$.

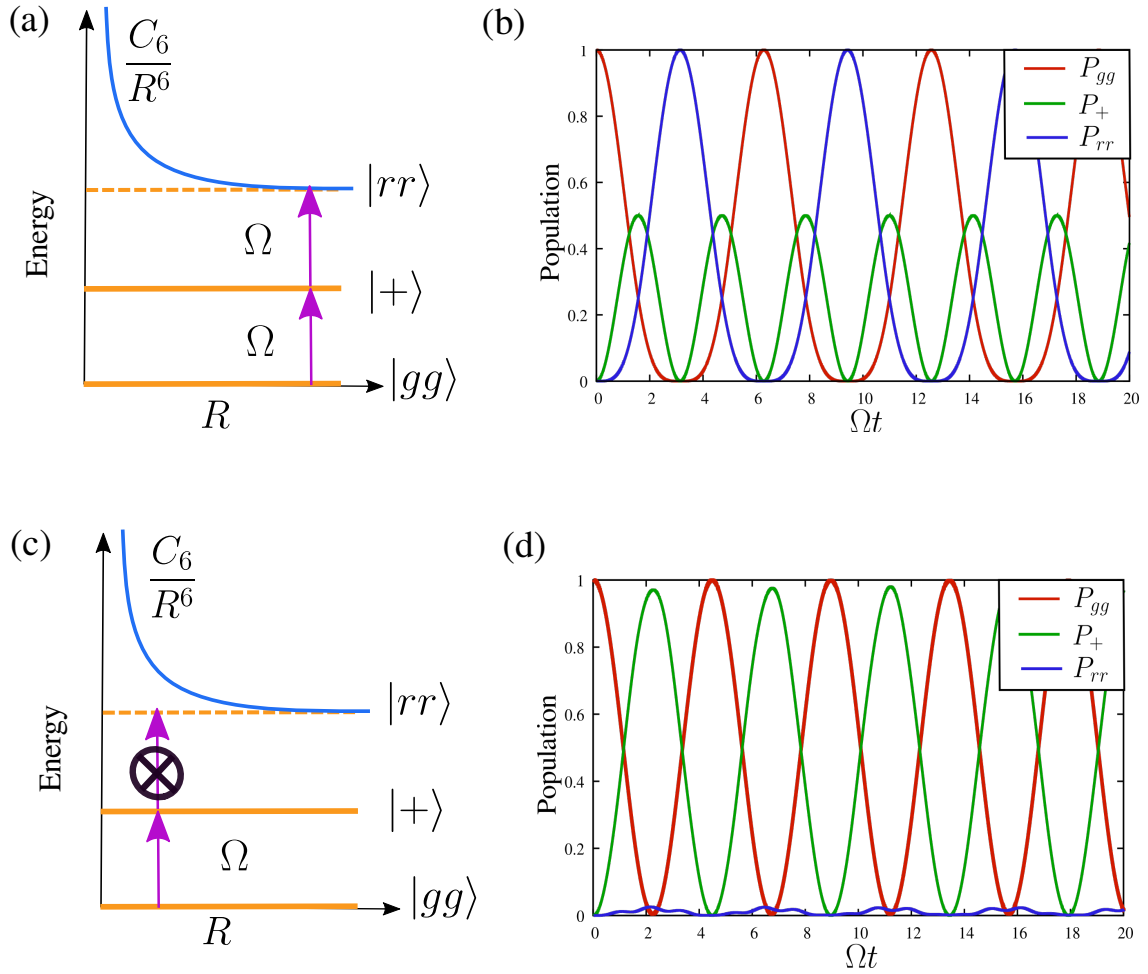


Figure 1.2: (a) Schematic representing two atoms at large separation in the ground state atoms coupled to Rydberg state, (b) Population dynamics for case (a), (c) Rydberg blockade at small separation (d) The population dynamics for (c)

After diagonalizing the Hamiltonian the energies of different states can be plotted as a function of separation between the atoms R . Fig [1.2] schematically shows the energies of different states as a function of R . The energy levels $|gg\rangle$ and $|+\rangle = (|gr\rangle + |rg\rangle)/\sqrt{2}$ are unaffected by the separation between the atoms. The state $|-\rangle = (|gr\rangle - |rg\rangle)/\sqrt{2}$ is decoupled from the dynamics due to vanishing dipole moment. The doubly excited state $|rr\rangle$ is maximally affected by vdW interaction. For large separation, this effect is small and the atoms can be driven to all the states including $|rr\rangle$. For this case, the population is transferred to all the states as shown in Fig [1.2 b] which shows the population dynamics starting from the state $|gg\rangle$. However, for a small separation, as shown in Fig [1.2 c], the energy level of $|rr\rangle$ gets shifted due to strong vdW interaction. This shift in the energy drives the lasers off-resonant from the previous energy level which prohibits the transition to the $|rr\rangle$. The effect of which can be observed in the population dynamics in which the population of $|rr\rangle$, denoted by P_{rr} is suppressed Fig [1.2 d]. This suppression of a doubly excited state due to strong vdW interaction is called Rydberg blockade. The condition for the blockade can be written as,

$$\hbar\Omega < \frac{C_6}{R^6} \quad (1.10)$$

which implies that the level shift due to vdW interaction should be greater than the line width of the laser used for excitation in case of resonant excitation. In the case of off-resonant excitation, detuning Δ is taken into consideration. The separation at which the level shift due to vdW to interaction is equal to the linewidth of the laser is called blockade radius, R_b given by,

$$R_b = \left(\frac{C_6}{\hbar\Omega} \right)^{1/6} \quad (1.11)$$

In chapter 3, when we study a periodically driven array of Rydberg atoms where we give an alternative explanation for Rydberg blockade in terms of correlated Rabi oscillations. In the next section, we look at the case where the ground state $|g\rangle$ is off-resonantly coupled to the Rydberg state $|r\rangle$. In this case atoms in the dressed ground state interacts via Rydberg-dressed interaction. The following section derives the Rydberg-dressed interaction between the ground state atoms

1.2.2 Rydberg dressed interaction

Rydberg dressed interaction arises as an effective interaction between two ground-state atoms which are weakly admixed with Rydberg state. We consider the case of N two-level atoms with ground state $|g\rangle$ and the excited state $|r\rangle$. The levels are coupled off-resonantly by a laser with Rabi frequency Ω and detuning Δ . The two atoms in the Rydberg state interact via vdW, $V_{ij} = C_6/(r_i - r_j)^6$, mentioned in the previous subsection. The Hamiltonian for the system is given by

$$\hat{H} = -\Delta \sum_1^N \hat{\sigma}_{rr}^i + \frac{\hbar\Omega}{2} \sum_i^N \hat{\sigma}_x^i + \sum_{i<j}^N V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \quad (1.12)$$

where the first term is detuning from the excited state. The second term represents the single atom Rabi coupling of the ground state and the excited state. The third term is the vdW interaction between two atoms when they are in the Rydberg state. We consider the case of off-resonant coupling with the condition $C_6/\Delta < 0$ with $C_6 > 0, \Delta < 0$ and the large detuning $\Omega/\Delta \ll 1$. With these conditions, we can treat the single-particle Rabi oscillation term perturbatively with $\Omega/2\Delta$ being the perturbation parameter. We rewrite the Hamiltonian as

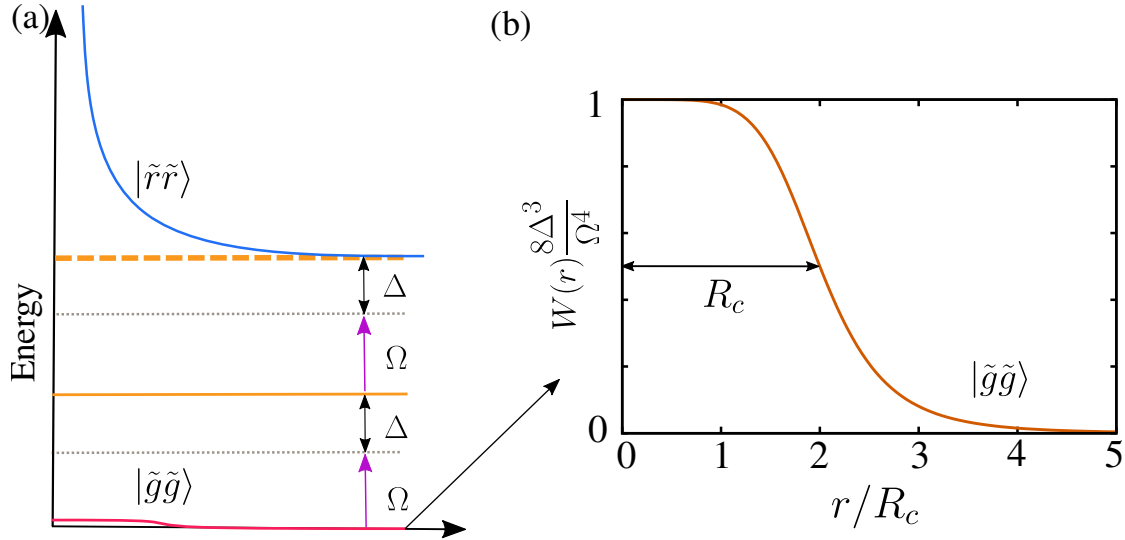


Figure 1.3: (a) Energy level scheme for dressed ground state atoms $|g\rangle$. Bare ground state atoms $|g\rangle$ are coupled to the Rydberg state $|r\rangle$ by laser with Rabi frequency Ω and detuning Δ (b) The Rydberg-dressed interaction potential as a function of separation between two atoms.

$$\hat{h} = \frac{\hat{H}}{\Delta} = \hat{h}_0 + \hat{X} \quad (1.13)$$

with $\hat{h}_0 = \sum_1^N \hat{\sigma}_{rr}^i + \frac{1}{\Delta} \sum_{i<j}^N V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j$ being the unperturbed Hamiltonian and $\hat{X} = (\Omega/2\Delta) \sum_i^N \hat{\sigma}_x^i$ being the perturbation.

We need to solve for the eigenenergies of the equation using the perturbation theory

$$\hat{h} |\Psi(r_1 \dots r_N)\rangle = w(r_1 \dots r_N) |\Psi(r_1 \dots r_N)\rangle \quad (1.14)$$

where, $|\Psi(r_1 \dots r_N)\rangle$ is the wavefunction of N atoms located at positions $r_1, r_2 \dots r_N$. Using the methods of perturbation theory, we expand the $w(r_1 \dots r_N)$ in perturbative series as

$$w(r_1 \dots r_N) = \sum_l^\infty \left(\frac{\Omega}{2\Delta} \right)^l w^{(l)}(r_1 \dots r_N) \quad (1.15)$$

We truncate the series up to the fourth order and calculate the first four terms of the series. Since we are looking at the perturbation over the state with all the atoms in their electronic the ground state $|g\rangle$ and perturbation operator $\hat{X}$ either excites or de-excites an atom locally, the odd order perturbation terms vanish i.e. $w^{(1)} = w^{(3)} = 0$. For even-order terms we get

$$w^{(2)} = N \quad (1.16)$$

$$w^{(4)} = \Delta \sum_{i<j}^N \frac{4}{2\Delta - V_{ij}} - N^2 \quad (1.17)$$

Rewriting in terms of the original parameters we get the fourth order correction as

$$W(r_1 \dots r_N) = \left(\frac{\Omega}{2\Delta} \right)^4 \Delta w^{(4)} = \frac{\Omega^4}{4\Delta^2} \sum_{i<j}^N \frac{1}{2\Delta - W_{ij}} - \left(\frac{\Omega}{2\Delta} \right)^4 \Delta N^2$$

Notice that the last term in the equation above is independent of the position of atoms and hence the energy can be rescaled by subtracting the constant offset, which leads to only a position-dependent fourth-order term. We also re-substitute for the $V_{ij} = C_6/r_{ij}^6$, with $r_{ij} = r_i - r_j$ to obtain,

$$W(r_1 \dots r_N) = \left(\frac{\Omega}{2\Delta} \right)^4 \sum_{i<j}^N \frac{C_6}{R_c^6 + r_{ij}^6} \quad (1.18)$$

The expression above is a sum of two-body interactions, which for the case of two atoms becomes,

$$W(r_i, r_j) = \left(\frac{\Omega}{2\Delta} \right)^4 \frac{C_6}{R_c^6 + r_{ij}^6} \quad (1.19)$$

where, $R_c = [C_6/(2\Delta)]^{1/6}$. We now look at the two limits, one for the large inter particle separation, $r_{ij} \gg R_c$ and the other of small separation $r_{ij} \ll R_c$. In the first case, the potential reduces to the vdW interaction with a prefactor of $(\Omega/2\Delta)^4$. Interestingly for later case, the potential saturates to a constant value of $\Omega^4/8\Delta^3$. The eigenstates of the Hamiltonian are the new dressed ground states, $|\tilde{g}\rangle = |g\rangle - (\Omega/2\Delta)|r\rangle$. The Fig. [1.3 b] shows the shape of the potential.

1.3 Bose-Hubbard Model

The Hubbard model was first introduced in 1963, in the context of solid-state physics, to study the properties of electrons in transition metal [32]. The model could capture the interaction between the electrons in the lowest band and also explained the transition from an insulating state to a conducting state. A similar model was used by Fisher *et al* [33] to investigate the phases of bosons loaded in an optical lattice. The transition from the Mott insulator phase to a superfluid phase was studied for the first time in the case of bosons. In this section, we briefly give an overview of the standard Bose-Hubbard model, Hubbard parameters, and its phases.

The hamiltonian for the standard Bose-Hubbard model is given by

$$\hat{H}_{BH} = -J \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + \text{H.c.}) + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i \quad (1.20)$$

where $\hat{a}_i^\dagger$ ($\hat{a}_i$) is a boson creation (annihilation) operator at site i . $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is a number operator at site i . The first term is the kinetic energy or the hopping term which represents bosons tunneling from a site i to site j . The standard BHM takes into account only the nearest neighbor hopping represented by $\langle \dots \rangle$. The second term is the interaction between two bosons when they are at the same lattice site. We assume that in the standard BHM, bosons interact only by a short-range contact interaction. The final term is the chemical potential which determines the energy required to add or remove a particle from the system. The coefficients J and U are called Hubbard parameters and are given by,

$$J = - \int dx w_i^*(x) \left[\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V_0 \sin^2(kx) \right] w_{i+1}(x) \quad (1.21)$$

$$U = g \int dx |w_i(x)|^4 \quad (1.22)$$

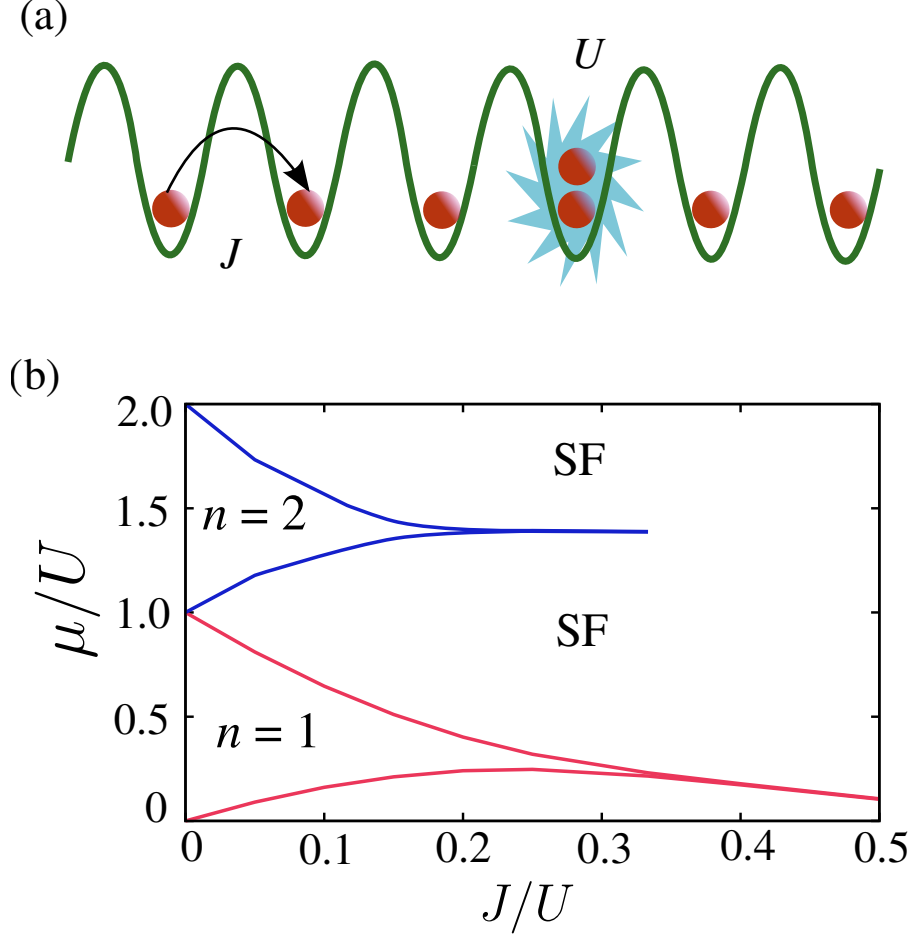


Figure 1.4: (a) A schematic representation of bosons loaded in optical lattice. Two processes denoted by J and U represent nearest neighbor hopping and onsite interaction respectively (b) A phase diagram of BHM calculated using Density Matrix Renormalization Group calculations.

The exact knowledge of these parameters is crucial in understanding the phases of the system. The relative strengths of these parameters determine the ground state of the system. For a large value of J/U we have a superfluid phase whereas for a small J/U we have a Mott insulator phase with integer number density at each site [1.4 b].

The experimental observation of MI-SF phase transition was possible due to experimental progress in atom cooling, trapping, and detecting techniques [16]. This paved way for more complex models with long-range interactions, higher bands, and mixtures of boson and fermions, also called Extended Bose Hubbard models (EBHM). These models have given rise to a plethora of exciting phases such as density waves, supersolid, Haldane Insulator etc. [34–36]. The EBHM was implemented with magnetic atoms [37]. In the second chapter, we calculate the Hubbard

parameters for Rydberg dressed atoms in a 1D lattice and study their behavior as a function of a Rydberg-dressed potential parameter, studied in the previous section.

1.4 Photonic Crystal Waveguides

So far, the strong interaction between atoms was achieved by varying the atomic properties i.e. by exciting them to a Rydberg state. A strong interaction can also be achieved with the help of magnetic atoms, polar molecules, and ions. However, a new way of engineering strong atom-atom interaction has been demonstrated by using so-called Photonic Crystal Waveguides (PCW). They are periodic dielectric structures that can modify the flow of light. Similar to the electrons in a solid, which feel periodic Coulomb potential, photons feel the periodic dielectric structure of PCW. This gives rise to band structure for a light similar to that of electronic band structure, implying that for certain frequencies the propagation of light through the PCW is prohibited. Also, the guided photonic modes of PCW can be used to trap the atoms near the surface of PCW [10]. This trapping is possible due to the Casimir-Polder forces and light shifts arising from the far-off-resonant traps (FORT) [9, 10]. As shown in Fig [1.5] the atoms are trapped above the surface of the dielectric structure where the electric field minima/maxima are located.

When atoms with a two-level structure are trapped near PCW such that the atomic frequency lies in the bandgap of the PCW, see Fig [1.6 a], we get a bound state of photon and atom. The excited state which lies in the bandgap gets dressed by exponentially decaying photonic profile. The exponential profile of the photonic mode associated with the atom can be tuned by varying the length parameter L dependent on PCW structure and external laser. In chapter 4, we study in detail the system of atoms coupled to PCW and show how the L can be varied. By making use of this property we study the dynamics of atomic excitation coupled to a PCW as a function of L and characterize the change in the dynamics.

1.5 Entanglement and Correlations

Entanglement is an elite feature of quantum mechanics which distinguishes it from classical mechanics. The entanglement forms a basis for many applications in quantum computing and quantum information processing. It has been useful for quantum cryptography [38, 39], quantum teleportation [40] and quantum dense coding

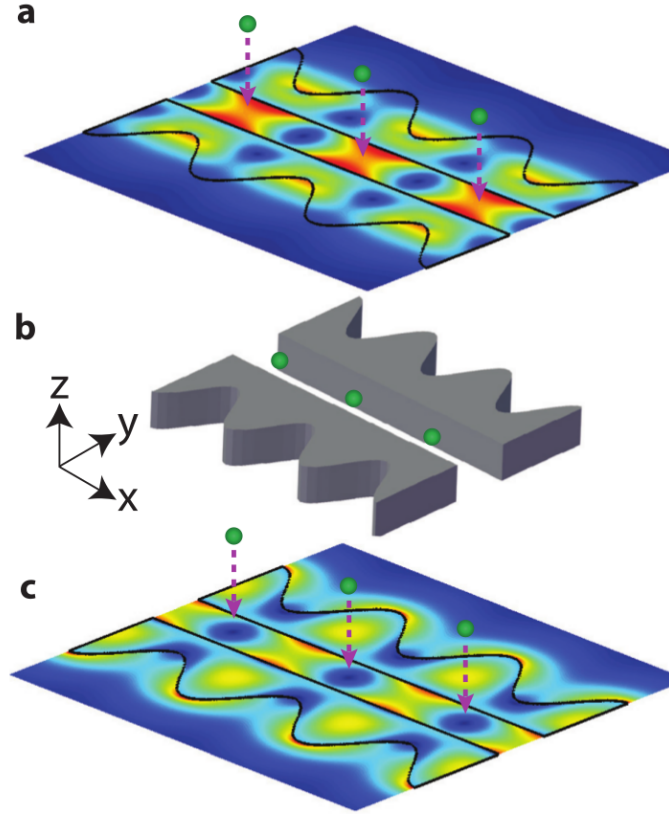


Figure 1.5: (a), (c) Electric field profile for various guided modes (b) The structure of PCW and the green dots represent the position of atoms. Figure taken from [9].

related applications. On the more fundamental side, entanglement has been found to be relevant in the areas such as condensed matter and high energy physics. In condensed matter, the behavior of entanglement entropy is crucial in understanding the phase transitions for the systems with topological order [41, 42]. In the many-body systems, the behavior of entanglement is crucial for understanding universal scalings at quantum phase transitions [43–47]. Because of such wide applications of entanglement, it becomes crucial to quantify it with a proper parameter. Various parameters such as purity, Renyi entropy, von-Neumann entropy are used to quantify the entanglement entropy of the system. The von Neumann entropy of a bipartite system is widely used in the case of quantum many-body systems. For a one dimensional system, which can be partitioned into two subsystems namely A and B, the von-Neumann entropy is defined as

$$S_A = -\text{Tr}(\rho_A \log \rho_A) \quad (1.23)$$

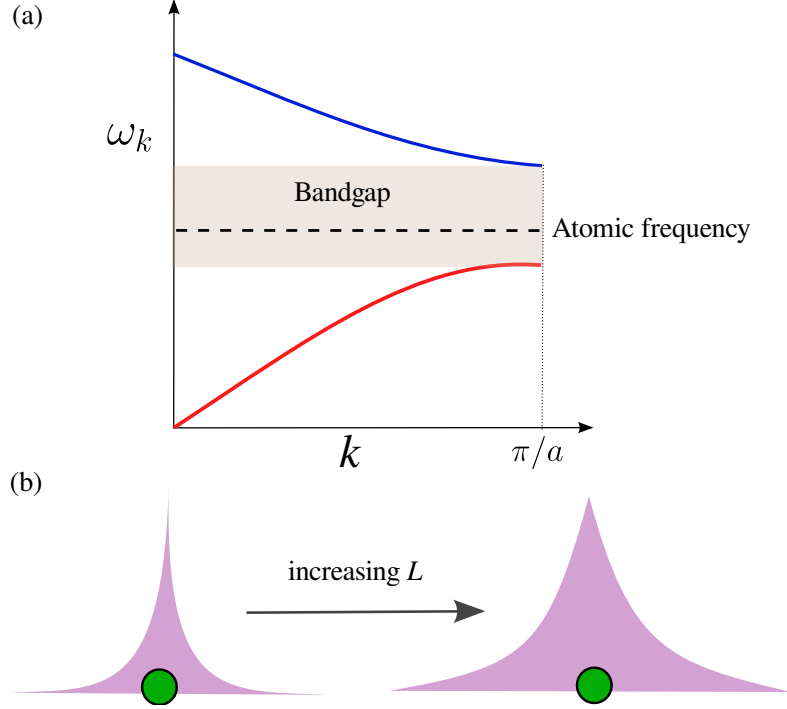


Figure 1.6: (a) The bandstructure of a photonic crystal waveguide. The shaded region is bandgap region and the atomic frequency of two level atom lies in the bandgap (b) The exponentially decaying profile of a photonic mode associated with an atom which can be tuned by varying L

where, ρ_A is a density matrix of the sub-system A, obtained by partially tracing the subsystem B. Also, the correlations building up during the non-equilibrium state of a system are studied in recent experiments with ultracold atoms [48, 49]. The study of these correlations is important in understanding how the different parts of the systems get correlated over time [50] and also how the information propagates during the time evolution. The dynamics of correlations also provide an understanding of how the system relaxes far from equilibrium. To characterize these correlations in the system, two-point correlation functions are widely used in the literature. For a pair of spins, separated by distance d , the correlation function in terms of spin operators $\hat{S}$ is given by,

$$C(d, t) = \sum_i \langle \hat{S}_i(t) \hat{S}_{i+d} \rangle - \langle \hat{S}_i(t) \rangle \langle \hat{S}_{i+d} \rangle \quad (1.24)$$

where $\langle \dots \rangle$ is an expectation with respect to the state of the system at time t . The behavior of these two-point correlation functions as a function of distance (d) and time (t) reveals the nature of the propagation of correlations in the system. These are widely used to verify the applicability of Lieb-Robinson bounds for the short-

range interacting systems. We use both the von Neumann entropy and two-point correlation function to study the entanglement and correlation dynamics of atomic excitation coupled to a PCW in chapter 4 and chapter 5.

1.6 Periodic Driving

The unprecedented control over atomic systems, provided by experimental developments, has allowed for complex ways to manipulate the state of a quantum system. Periodic driving of a parameter in the hamiltonian is one such way of controlling the state of a quantum system. This is similar to a classical example of the Kapitza pendulum [51]. A simple pendulum has an unstable equilibrium point in the inverted position. However, Kapitza in his paper showed that a pendulum, whose pivot point is driven periodically with a high frequency, has a stable equilibrium point in the inverted position Fig [1.7]. The usual equilibrium point of a simple pendulum becomes unstable for the Kapitza pendulum.

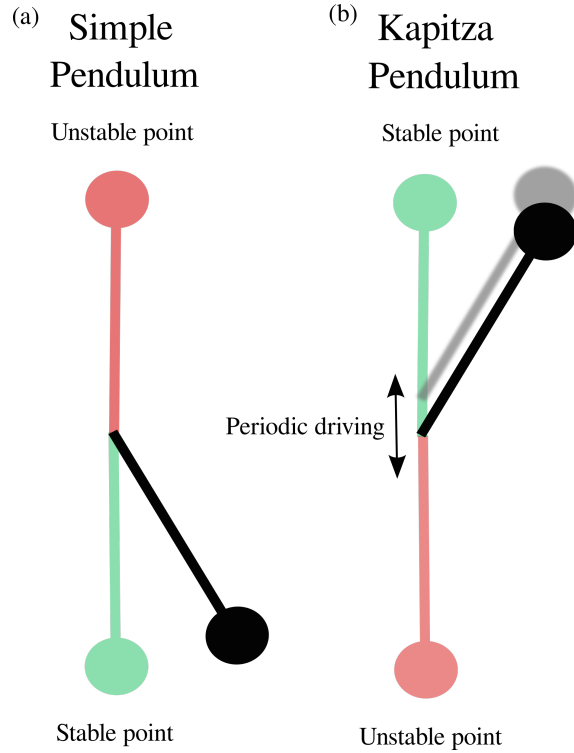


Figure 1.7: (a) A simple pendulum without periodic driving has a stable point at the bottom and unstable point in the inverted position (b) Kapitza pendulum with periodic driving of a pivot has stable point in the inverted position where as the bottom point is unstable

Similarly, for a quantum system, periodic driving of a parameter in the system

leads to interesting dynamics which is unexpected from a non-driven system. One such example is coherent destruction of tunneling for the driven double-well system [52]. The particles trapped in a double-well potential tend to move from one well to another due to the tunneling effect. However, if the double-well potential is perturbed by a high frequency periodic driving, the tunneling of particles from one well to another can be suppressed. Hence if the particles are located in one of the wells at the beginning, they remain in the same well over a long time for the driven case. Recently, the method of periodic driving was utilized in the case of the Rydberg atom-based quantum simulator. A two-dimensional array of Rydberg atoms was driven periodically in time. The periodic driving of the system helped in stabilizing the coherent revivals of the system [29]. In our case, we use periodic driving to control the correlation dynamics in the system, details of which are outlined in chapter 3.

1.7 Thesis overview

In the upcoming chapters, we use the properties mentioned above along with other system-specific properties to observe interesting physics. We demonstrate the control over various parameters such as interaction, correlations, populations, and entanglement. In the second chapter, we extend the standard Bose Hubbard model to incorporate the Rydberg-dressed interaction. We calculate the Hubbard parameters for Rydberg-dressed interaction using maximally localized Wannier functions. We show that the behavior of Hubbard parameters can be controlled by tuning the Rydberg dressed interaction and it has an advantage over standard BHM or other extended BHM. We also identify the most dominant density assisted tunneling processes arising from the Rydberg-dressed interaction. We show that their strength can be manipulated by varying the shape of Rydberg-dressed interaction.

In the third chapter, we study the periodically driven chain of Rydberg atoms. We show how the periodic driving of a parameter in hamiltonian can be used as a tool to control the dynamics of correlated Rabi oscillations. The behavior of correlated Rabi oscillations quantified by computing various correlation functions and role of it in the excitation dynamics is explained by calculating the effective hamiltonian in various limits.

In chapter 4, we study the dynamics of a single excitation, coupled to a photonic crystal waveguide. The coupling of atoms to PCW gives rise to an effective

exchange Hamiltonian in which the range of the exchange can be varied. We study the population dynamics of excitation as a function of a range of interactions. The characteristic change observed in the excitation dynamics is quantified using various parameters such as kurtosis, Shannon entropy, edge-center population imbalance, and inverse participation ratio. We also study the entanglement dynamics.

In the final chapter, we introduce one more excitation and study the effect of the presence of one excitation on the other excitation. When the excitations are Rydberg nature they interact strongly via van der Waals (vdW) interaction. This creates a competition between exchange interaction arising from PCW and vdW interaction from Rydberg excitation. We show how by varying the system parameters correlation and population dynamics can be controlled. We also study how the relative separation between two excitation affects the dynamics.

Chapter 2

Rydberg Dressed Extended Bose-Hubbard Model

Rydberg-dressed atoms have emerged as a promising candidate in the field of many-body physics from both theoretical and experimental standpoints. Rydberg atoms are excited-state atoms with high principal quantum numbers whereas Rydberg-dressed atoms are the ground state atoms with a very small fraction of the Rydberg state. Because of the small Rydberg state fraction, the new dressed ground state has characteristics of the Rydberg state. Firstly, the Rydberg blockade effect leads to the soft-core potential having a plateau at small atomic separations and $1/r^6$ type of tail at large separations. The length of the plateau, which determines the range over which potential remains constant, can be controlled by varying the external laser parameters. This gives us controllability over the range and the strength of the interaction. This unusual shape of the potential and its controllability stands out compared to conventional potentials such as Coulomb, dipolar, and van der Waals. Rydberg-dressed interaction and its effect were studied in two recent experiments. In one of them, the effective interactions in the strong dressing limit were demonstrated with two individual atoms trapped in optical tweezers [53] whereas the second experiment involves a two-dimensional (2D) lattice setup [54]. Realization of Rydberg dressed interaction has led to exciting studies in the area of quantum many-body physics [55–61] where roton excitation, supersolid formation, crystallization, and soliton formation is observed in Rydberg-dressed Bose-Einstein condensates. Topological density waves for fermionic systems [62] and topological mott insulators for bosonic systems have been studied in the context of Rydberg dressed interaction [61]. Also, the quantum spin models which are used to study

frustrated quantum magnets, lattice gauge theories make use of the versatility of Rydberg-dressed interaction in terms of angular and spatial dependence [63, 64]. On the application side, the Rydberg-dressed scheme is used for adiabatic quantum computation to perform gate operations and entanglement generation [65, 66].

The Bose-Hubbard model (BHM) is widely used to study the quantum phase transition for ultracold atoms trapped in an optical lattice. From the very first prediction of Mott insulator to superfluid phase transition prediction by Fisher *et al* [33] and its experimental observation in cold atom setup [16] the field has made tremendous progress both on theoretical and experimental fronts. On the theoretical side, the BHM has been extended to include different types of interactions such as long-range, anisotropic dipolar interaction, vdW interaction, cavity mediated infinite range interactions with the help of magnetic atoms, polar molecules, or cavities. BHM has also been extended to include higher orbitals and excited states. These extensions have given rise to the so-called extended Bose-Hubbard models (EBHM), which host a variety of quantum phases such as stripes, checkerboard phases, supersolids, Haldane insulators, etc [34].

In this chapter, we extend the BHM by taking into consideration the Rydberg-dressed interaction and the two lowest bands. We calculate the Hubbard parameters using maximally localized Wannier functions (MLWF) for the Rydberg-dressed interaction. We show that the EBHM with Rydberg dressed interaction has an advantage over the standard BHM or other EBHM. Among them, the most striking property is the possibility of engineering the strengths of offsite couplings to the same magnitude as that of onsite ones by varying the range of the Rydberg dressed interaction. This may have far-reaching consequences in the context of quantum many-body physics [67] especially in frustrated magnetism [63, 64] to impose local constraints or conservation laws. Also, we identify the density-assisted tunnelings which are most relevant to Rydberg dressed interaction and study their behavior as a function of lattice parameters and interaction parameters.

This chapter is structured as follows. In section 2.1 we discuss the Rydberg-lattice setup, the governing many-body Hamiltonian, and derive ab initio the extended Hubbard model using the maximally-localized Wannier functions. In section 2.2 we discuss how MLWFs are calculated using a unitary diagonal phase transformation in the isolated Bloch bands for a sinusoidal 1D optical lattice potential. We compare the results with the tight-binding approximation where harmonic oscillator wavefunctions are used as an approximation for MLWF. The results for

the Hubbard parameters are discussed in section 2.3. In section 2.4 we discuss the validity of our model and we also provide realistic numbers for the state-of-the-art experimental Rubidium lattice setup in 2.5. Finally, we summarize all the results in 2.6.

2.1 Rydberg dressed atoms in an one-dimensional optical lattice

2.1.1 The atom-lattice setup and Rydberg-Rydberg interactions

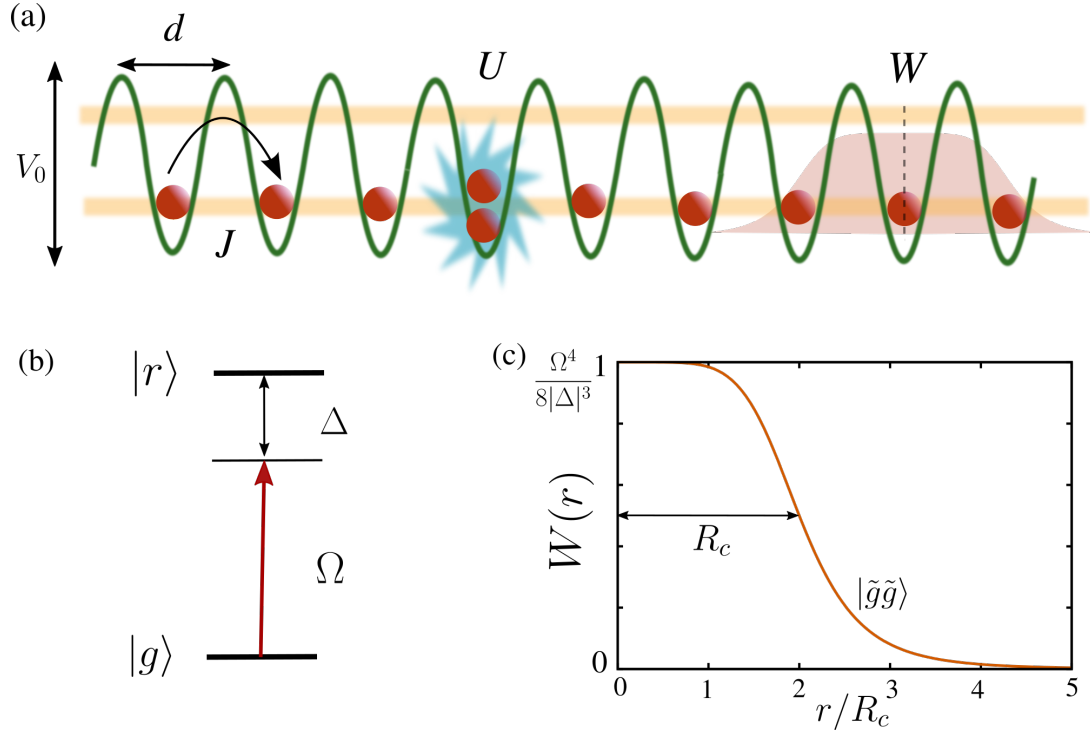


Figure 2.1: (a) Atoms loaded in one dimensional optical lattice with lattice depth V_0 and lattice spacing d . J, U and W represent the hopping, on-site interaction and Rydberg-dressed interaction respectively. The yellow bands are the two lowest vibrational bands (b) The two-levels, ground state $|g\rangle$ and the excited state $|r\rangle$ coupled off-resonantly by a laser with detuning Δ and Rabi frequency Ω . (c) The effective Rydberg-dressed interaction between two dressed ground state atoms.

Our setup consists of bosonic atoms trapped in a one-dimensional optical lattice. The optical lattice potential of the form $V_{OL}(x) = V_0 \sin^2(k_0 x)$ is formed by two

counter-propagating lasers with wavenumber given by $k_0 = \pi/d$ where, d is the lattice spacing of the resulting optical lattice. The atoms in the ground state $|g\rangle$ are coupled to the Rydberg state $|r\rangle$ with frequency Ω and detuning Δ . We assume large detuning condition $|\Delta| \gg \Omega$, which leads to the weak admixing of Rydberg state $|r\rangle$ to the ground state $|g\rangle$. The weak admixing of Rydberg state with the ground state results in a dressed ground state $|\tilde{g}\rangle = |g\rangle - (\Omega/2|\Delta|)|r\rangle$. Although the two atoms in the Rydberg state $|r\rangle$ separated by distance r , interact via vdW interaction of the form C_6/r^6 , the atoms in the dressed ground state $|\tilde{g}\rangle$ interact via tunable soft-core potential given by, (see section 1.2.2)

$$W(r_{ij}) = \left(\frac{\Omega}{2|\Delta|} \right)^4 \frac{C_6}{(r_{ij}^6 + R_c^6)}. \quad (2.1)$$

where r_{ij} is the separation between two atoms at lattice sites i and j . For small values of $r_{ij} \ll R_c$, when the vdW interaction is strong enough to induce the blockade, the dressed interaction $W(r_{ij})$ saturates to the value $W(r_{ij}) \approx (1/8)(\Omega^4/|\Delta|^3)$. At large separations, the potential decreases as a vdW potential but with a pre-factor proportional to laser parameters given by $W(r_{ij}) \approx (\Omega/2|\Delta|)^4 C_6/r_{ij}^6$. Hence the Rydberg-dressed interaction gives us a unique feature that allows us to control the range of the potential $R_c = (C_6/2\hbar|\Delta|)^{1/6}$. By either varying the detuning Δ or C_6 (varying the Rydberg state) we can control the range of the interaction. Rydberg dressing also modifies the decay rate of the dressed state. The spontaneous decay rate of $|\tilde{g}\rangle$ is approximately given by $(\Omega/2|\Delta|)^2 \gamma_r$, where γ_r is the decay rate of Rydberg state. The smaller decay rate of atoms in the dressed state is crucial when long coherence times are desired.

2.1.2 Many body Hamiltonian and the extended Hubbard model

To describe the system of atoms interacting via contact interaction and Rydberg-dressed interaction, we start with the many-body atomic Hamiltonian containing the single-particle term and two-body interactions.

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \hat{h}_0 \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') U_I(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}'), \quad (2.2)$$

where the field operator $\hat{\Psi}(\mathbf{r})$ [$\hat{\Psi}^\dagger(\mathbf{r})$] annihilates [creates] a boson at the position $\mathbf{r}$. The term $\hat{h}_0 = -\hbar^2 \Delta^2/2m + V_{OL}(\mathbf{r})$ contains the single particle kinetic energy and optical lattice potential term. The two-particle interactions are given by, $U_I(\mathbf{r} - \mathbf{r}') =$

$U(\mathbf{r} - \mathbf{r}') + W(\mathbf{r} - \mathbf{r}')$ with the first term being the typical contact interactions: $U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$ arising due to the scattering of bosons at low temperatures. The strength of the interaction is characterized by the parameter, $g = 4\pi\hbar^2 a/m$ where a is the s -wave scattering length. The second term represents the Rydberg-dressed interaction. To obtain the Hamiltonian in form of EBHM, we expand the field operators in the basis of maximally localized single particle Wannier functions $w_n(\mathbf{r} - \mathbf{R}_j)$ (see section 2.2). The Wannier function $w_n(\mathbf{r} - \mathbf{R}_j)$ represents a bosonic particle in n^{th} band, centered at the lattice site $\mathbf{R}_j = j\mathbf{R}$. Where $\mathbf{R}$ is a lattice vector such that $V_{OL}(\mathbf{r} + \mathbf{R}) = V_{OL}(\mathbf{r})$. Hence, the field operator can be expanded in the Wannier function basis as

$$\hat{\Psi}(\mathbf{r}) = \sum_j \sum_n w_n(\mathbf{r} - \mathbf{R}_j) \hat{a}_{jn}, \quad (2.3)$$

where $\hat{a}_{jn}$ ($\hat{a}_{jn}^\dagger$) annihilates (creates) a boson in the mode represented by the Wannier function $w_n(\mathbf{r} - \mathbf{R}_j)$ at j^{th} lattice site and n^{th} band. They satisfy the commutation relation $[\hat{a}_{in}, \hat{a}_{jm}^\dagger] = \delta_{ij}\delta_{nm}$. Inserting the above expression for field operator in Equation 2.2, we arrive at a general extended Hubbard model:

$$\hat{H} = - \sum_{i,j} \sum_{n,m} J_{ij}^{nm} \hat{a}_{in}^\dagger \hat{a}_{jm} + \frac{1}{2} \sum_{i,j,i',j'} \sum_{n,m,n',m'} (U_I)_{ij i' j'}^{nm n' m'} \hat{a}_{in}^\dagger \hat{a}_{jm}^\dagger \hat{a}_{j'm'} \hat{a}_{i'n'} \quad (2.4)$$

where the hopping and the interaction matrix elements are respectively

$$J_{ij}^{nm} = - \int d\mathbf{r} w_n^*(\mathbf{r} - \mathbf{R}_i) [-\hbar^2 \Delta^2 / 2m + V_{OL}(\mathbf{r})] w_m(\mathbf{r} - \mathbf{R}_j) \quad (2.5)$$

$$(U_I)_{ij i' j'}^{nm n' m'} = \iint d\mathbf{r} d\mathbf{r}' w_n^*(\mathbf{r} - \mathbf{R}_i) w_m^*(\mathbf{r}' - \mathbf{R}_j) U_I(\mathbf{r} - \mathbf{r}') w_{m'}(\mathbf{r}' - \mathbf{R}_{j'}) w_{n'}(\mathbf{r} - \mathbf{R}_{i'}). \quad (2.6)$$

where, J_{ij}^{nm} is the Hubbard parameter for particle hopping from site j and band m to site i and band n . $(U_I)_{ij i' j'}^{nm n' m'}$ is the generalized interaction Hubbard parameter which includes both density-density interaction and density induced intersite and inter-band hoppings. Here we assume that the depth of the lattice V_0 is such that the summation over the band index can be restricted to the two lowest Bloch bands. As seen from the expressions of Hubbard parameters, the knowledge of Wannier functions is essential for their computation. In the next section, we show how the Wannier functions for the two lowest bands can be computed from the Bloch functions.

2.2 Maximally localized Wannier functions

The generalized Wannier functions are calculated by the unitary mixing of N degenerate or closely spaced Bloch eigenstates and in 1D it is written as,

$$w_n(x - X_j) = \frac{d}{2\pi} \int_{BZ} dq e^{-iqX_j} \sum_{m=1}^N U_{nm}(q) \psi_q^m(x), \quad (2.7)$$

where $\psi_q^m(x)$ is the Bloch function for the m^{th} Bloch band for a quasi-momentum q and $U_{nm}(q) \in U(N)$ is a unitary matrix satisfying the periodic boundary condition in the momentum space: $U_{nm}(q + 2q_B) = U_{nm}(q)$ with $q_B = \pi/d$ and N corresponds to the number of lattice sites in the unit cell. BZ indicates that the integration is carried over the first Brillouin zone.

Here we make use of the conjecture that MLWFs are real functions up to a global phase factor. In our case ($N = 1$) the generalized Wannier functions are

$$w_n(x - X_j) = \frac{d}{2\pi} \int_{BZ} dq e^{-iqX_j} e^{i\phi_q^n} \psi_q^n(x). \quad (2.8)$$

The periodic Bloch functions $\psi_q^n(x)$ are calculated as prescribed in 2.7.1. The phases ϕ_q^n for the unitary transformation is obtained by minimizing the absolute value of the imaginary part of the Wannier function in equation 2.8 and it leads to

$$\phi_q^n = \arctan \left(\frac{\Re[u_q^n(x_0)]}{\Im[u_q^n(x_0)]} \right) - qx_0. \quad (2.9)$$

In our numerics, for symmetric $u_q^n(x)$ we took $x_0 = 0$ and for anti-symmetric $u_q^n(x)$ we took the point at which the imaginary part of $u_q^n(x)$ is maximum. The resulting Wannier functions match perfectly with those obtained via the spread minimization procedure. Fig [2.2] shows the MLWF for two different lattice depths $V_0 = E_R$ and $10E_R$ where $E_R = \hbar^2 k^2 / 2m$ is the recoil energy. For a given V_0 , the Wannier functions for both the first band (solid green) and the second band (dashed red) band decay exponentially as we move away from the center of the unit cell Fig [2.2a,b]. The Wannier functions for the second band are more delocalized pertaining to its higher energy. For the higher value of lattice depth, Wannier functions in both the band get more localized Fig [2.2c]. The exponentially fast decay of WF is apparent on the log scale plot shown in Fig [2.2d]. The localization of WF with the increase in the lattice depth V_0 , is crucial in understanding the behavior of Hubbard parameters as a function of lattice depth V_0 .

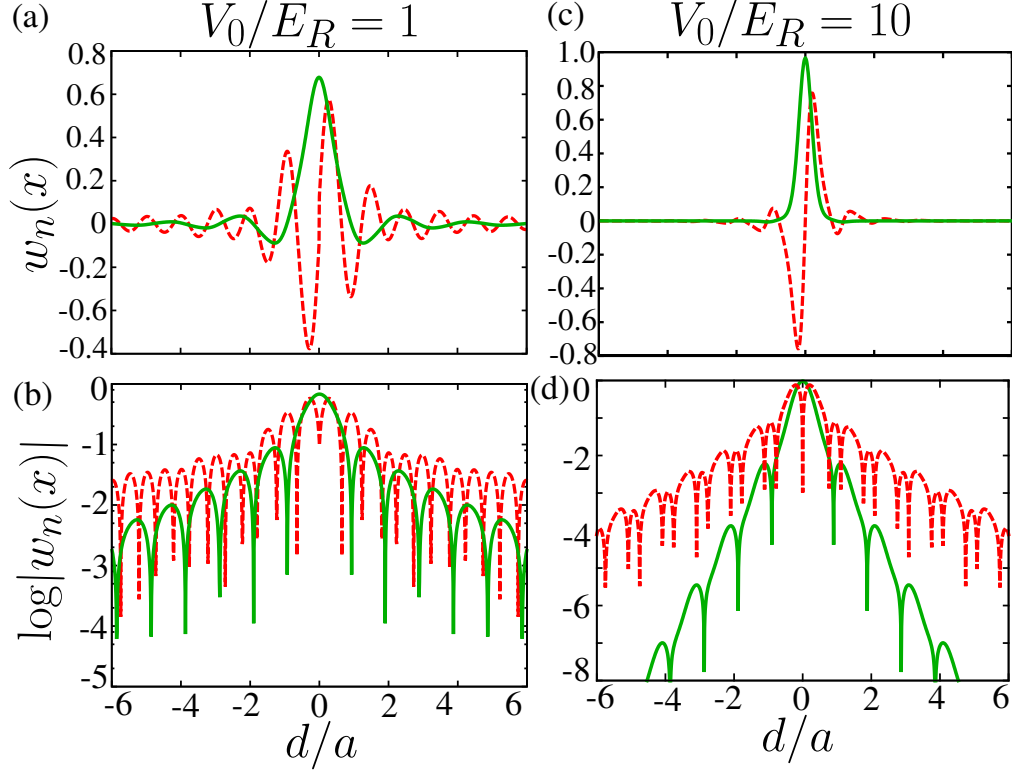


Figure 2.2: The maximally localized Wannier functions $w_n(x)$ for the two lowest Bloch bands, band 1 (solid green) and band 2 (dashed red) with (a) $V_0 = 1E_R$ and (c) $V_0 = 10E_R$. (b),(d) Wannier function of the top panel on a logarithmic scale.

For large values of V_0 , WF can be approximated by Harmonic Oscillator (HO) wavefunctions obtained by approximating the sinusoidal potential with the parabolic potential given by,

$$V_{OL}(x) = V_0 \sin^2(k_0 x) \approx V_0 k_0^2 x^2 \quad (2.10)$$

comparing this with the parabolic potential of the form $\frac{1}{2}m\omega_{ho}^2 x^2$, we get the expression for the HO frequency ω_{ho} as,

$$\omega_{ho} = 2\sqrt{V_0 E_R} \quad (2.11)$$

The Gaussian wavefunctions for the first two bands are given by

$$\phi^1(x) = \left(\frac{1}{\pi\sigma_{ho}^2}\right)^{1/4} e^{-x^2/2\sigma_{ho}^2} \quad (2.12)$$

$$\phi^2(x) = \sqrt{2\pi} \left(\frac{1}{\pi\sigma_{ho}^2}\right)^{3/4} x e^{-x^2/2\sigma_{ho}^2} \quad (2.13)$$

where, $a_{ho}^2 = \frac{1}{m\omega_{ho}^2}$ is the corresponding Harmonic oscillator length scale.

The plots below compare the Wannier functions with their Gaussian counterparts for different values of V_0 and for different bands. For small values of V_0 , HO wavefunctions are poor approximations to WF because of the lack of oscillations in HO wavefunctions. For a given V_0 , the discrepancy between WF and HO wavefunctions increases with increasing band index. For a fixed band, at large values of V_0 , HO wavefunctions match the Wannier functions because for large lattice depths the potential is closer to the parabolic approximation. The strong localization of HO wavefunctions makes them inadequate for calculating the offsite interaction Hubbard parameters.

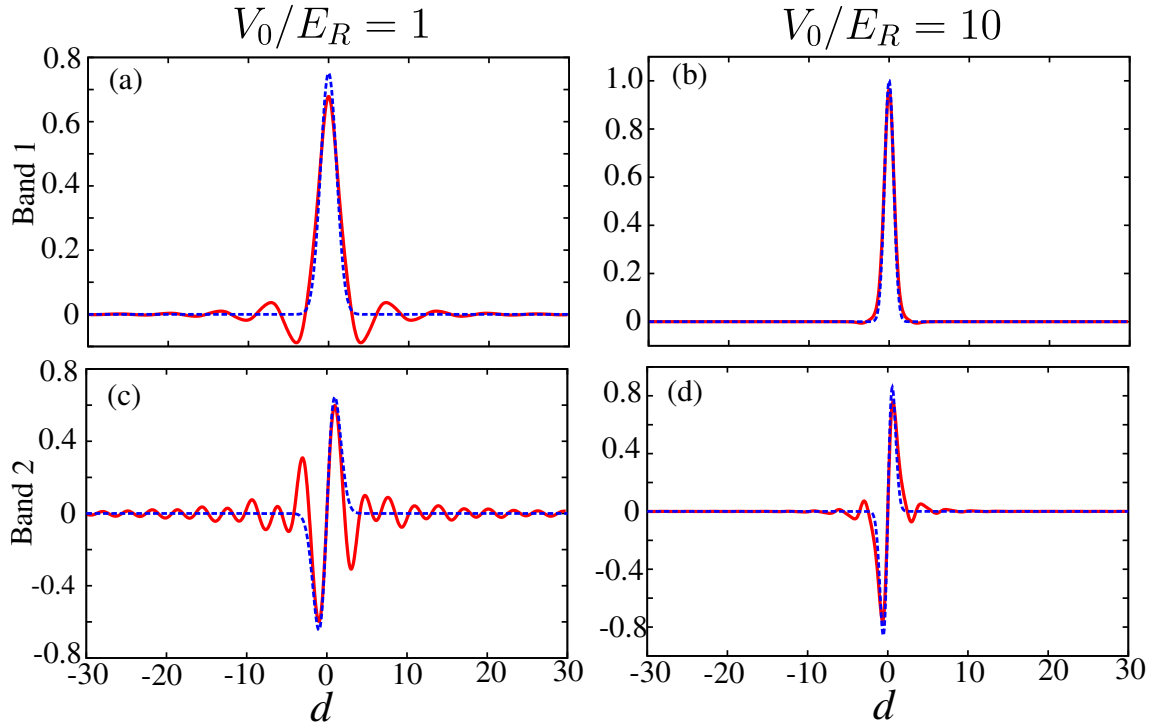


Figure 2.3: Comparison of Wannier functions (solid red line) with corresponding harmonic oscillator wavefunctions (dashed blue) for (a-b) band 1 ($V_0/E_R = 1, 10$) and (c-d) band 2 ($V_0/E_R = 1, 10$)

2.3 Hubbard Parameters

2.3.1 Hopping and short-range interaction parameters

In this section, we calculate the Hubbard parameters for contact interaction U and study their behavior as a function of depth of the lattice V_0 . Firstly, for the interaction parameter, we have onsite and nearest-neighbor interactions for particles being

in the same or two different bands. The onsite interaction between the particles in band n is given by

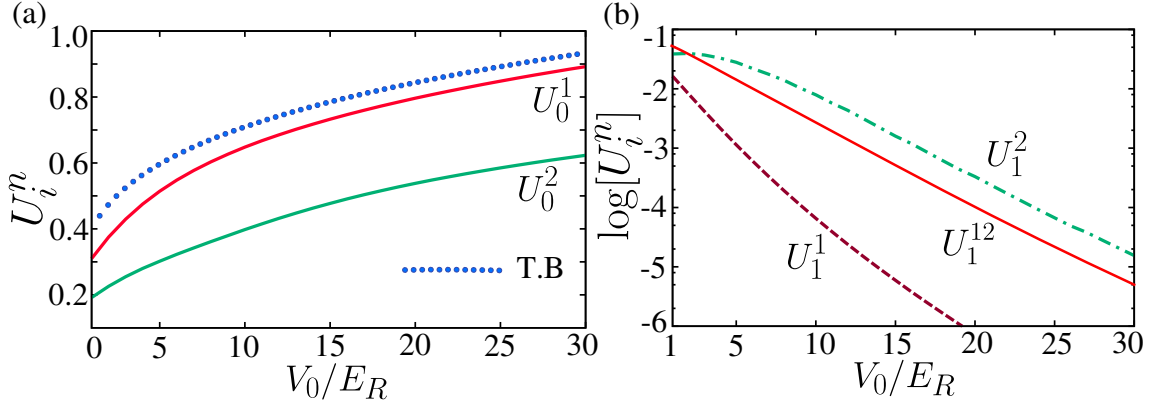


Figure 2.4: (a) Onsite interaction energy for contact interaction as a function of lattice depth for band 1 (green) and band 2 (red). Tight binding approximation for band 1 (dotted line) (b) Nearest neighbour interaction for two particles in band 1 (dashed brown line), band 2 (solid red line) and one particle in band 1 and other in band 2 (dot dashed green line)

$$U_0^n = U_{0000}^{nnnn} = g \int |w_n(r)|^4 dr \quad (2.14)$$

As shown in Fig [2.4a], U_0^n increases with increase in V_0 for both $n = 1$ and $n = 2$ bands. This can be attributed to the localization of WF with the increase in V_0 . The onsite interaction is more for a lower band due to larger localization than higher bands which are more delocalized due to higher energy. The tight-binding approximation with Gaussian wavefunction approaches the one with WF in a large V_0 limit. The onsite interaction between two particles in different bands vanishes owing to the orthogonality of the WF of the two bands. In the case of nearest neighbor (NN) interactions, the matrix element is given by,

$$U_1^{nm} = U_{0101}^{nmnm} = g \int |w_n(r)|^2 |w_m(r-R)|^2 dr \quad (2.15)$$

Here, the strength of the matrix element depends on the overlap between the WF of the particles located at two different sites. With the increase in V_0 the overlap between the WF decreases due to localization. Hence the matrix elements for both the bands decrease with an increase in V_0 . The NN interaction for particles in the higher band is more because of the larger overlap between the wavefunctions of the higher bands Fig [2.4 b]. Unlike onsite interaction, the NN interband interaction ($U_1^{12} = U_{0101}^{1212}$) is non-zero and its strength lies in between the interaction elements U_1^1 and U_1^2 Fig [2.4 b].

In the case of hopping, we consider only the nearest neighbor hopping matrix element for two lowest bands given by $J_1 = J_{i,i+1}^{11}$ and $J_2 = J_{i,i+1}^{22}$. The interband hopping is zero due to the orthogonality of the wavefunctions. As shown in Fig [2.5 a] the hopping matrix elements for both the bands decrease exponentially with an increase in V_0 due to localization of WF. The hopping in the second band is more compared to the first band due to its higher energy. The hopping matrix element for the first band can be calculated analytically using WKB approximation in a large V_0 limit, which results in the expression of the form,

$$J_{\text{WKB}} = \frac{16}{\sqrt{\pi}} \left(\frac{V_0}{E_R} \right)^{0.75} e^{-2\sqrt{V_0/E_R} E_R} \quad (2.16)$$

Along with the single-particle hoppings (J) arising from the kinetic energy of particles we also get hoppings resulting from the interaction, called Density Assisted Tunnelings (DAT). In the case of DAT, particle tunnel intersite and/or interband due to the presence of another particle. The standard Bose-Hubbard model gets augmented by the terms of the form $\sim \sum_i \hat{a}_i^\dagger (\hat{n}_i + \hat{n}_{i+1}) \hat{a}_{i+1}$. The various DAT processes and their amplitudes are shown in Fig [2.5 b] as a function of V_0 . The amplitude of these processes is orders of magnitude smaller than J_1 and hence can be neglected.

In the next section, we calculate the Hubbard parameters for the Rydberg-dressed interaction and study their behavior as a function of V_0 and R_c . The tunability of the range of the interaction provided by Rydberg-dressed interaction changes the behavior of Hubbard parameters drastically compared to the contact interaction case. We also identify the dominant density-assisted tunneling process.

2.3.2 Rydberg-dressed potential: density-density interactions

The Rydberg-dressed interaction can be re-written as

$$W(r_{ij}) = \frac{W_{eff}}{[(r_{ij}/R_c)^6 + 1]}, \quad (2.17)$$

with $W_{eff} = \hbar\Omega^4/(8|\Delta|^3)$ being an effective interaction strength given by the light shift due to the Rydberg laser and $R_c = [C_6/2\hbar|\Delta|]^{1/6}$ provides the interaction range. Among the two parameters, R_c can be controlled independently of W_{eff} by changing the Rydberg state through $C_6(n)$, but any variation in Δ and Ω affects both simultaneously. The possibility of tuning the interaction range without affecting the

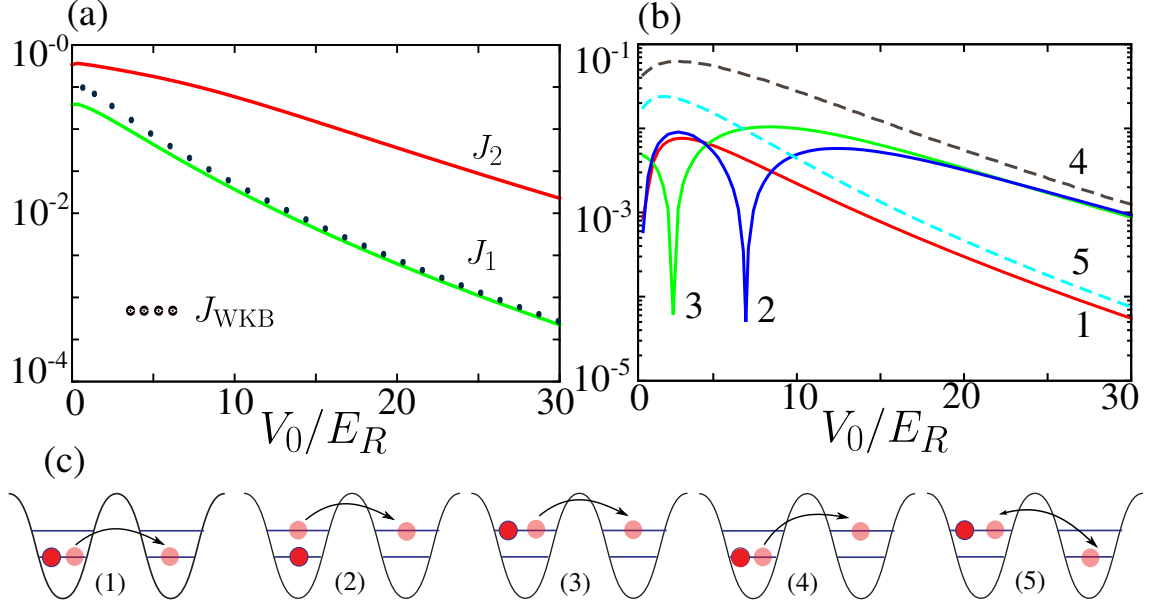


Figure 2.5: (a) The nearest neighbour hopping matrix element for particle in band 1 (solid green line) and band 2 (solid red line) as a function of lattice depth V_0 . The WKB approximation for band 1 (dotted line) (b) The amplitudes of the various density assisted tunneling processes depicted in (c) as a function of V_0 , scaled by $\tilde{g}$. The numbering corresponds to the respective process in (c)

effective strength can be pointed out as an elite feature of Rydberg-admixed atoms compared to other existing long-range systems. See section. 2.5 for the values of R_c as a function of $C_6(n)$ (or simply n) for Rubidium atoms.

With this, we estimate the Hubbard parameters for Rydberg-dressed interaction ($W_{ijij'}^{nmm'm'}$) using MLWFs, as a function of both lattice depth V_0 and R_c .

$$(W)_{ijij'}^{nmm'm'} = W_{eff} \iint d\mathbf{r} d\mathbf{r}' w_n^*(\mathbf{r}-\mathbf{R}_i) w_m^*(\mathbf{r}'-\mathbf{R}_j) \frac{1}{(r_{ij}/R_c)^6 + 1} w_{m'}(\mathbf{r}'-\mathbf{R}_{j'}) w_{n'}(\mathbf{r}-\mathbf{R}_{i'}). \quad (2.18)$$

We consider three cases of the density-density interaction, both the particles in either first band ($\tilde{W}_i^1 = W_{0i0i}^{1111}/W_{eff}$), both the particles in the second band ($\tilde{W}_i^2 = W_{0i0i}^{2222}/W_{eff}$) and other being both the particles in different bands ($\tilde{W}_i^{12} = W_{0i0i}^{1212}/W_{eff}$). The strength of these parameters depend upon both the nature of the potential (via R_c) and the depth of the lattice V_0 , (implicitly via WF). Hence we study the behavior of these parameters as a function of R_c and V_0

The results for the case in which two atoms occupy the lowest band ($\tilde{W}_i^1 = W_{0i0i}^{1111}/W_{eff}$) are shown in Fig [2.6]. For small values $R_c = d/2$, the behavior of density-density interaction Hubbard parameters is same as that of contact interac-

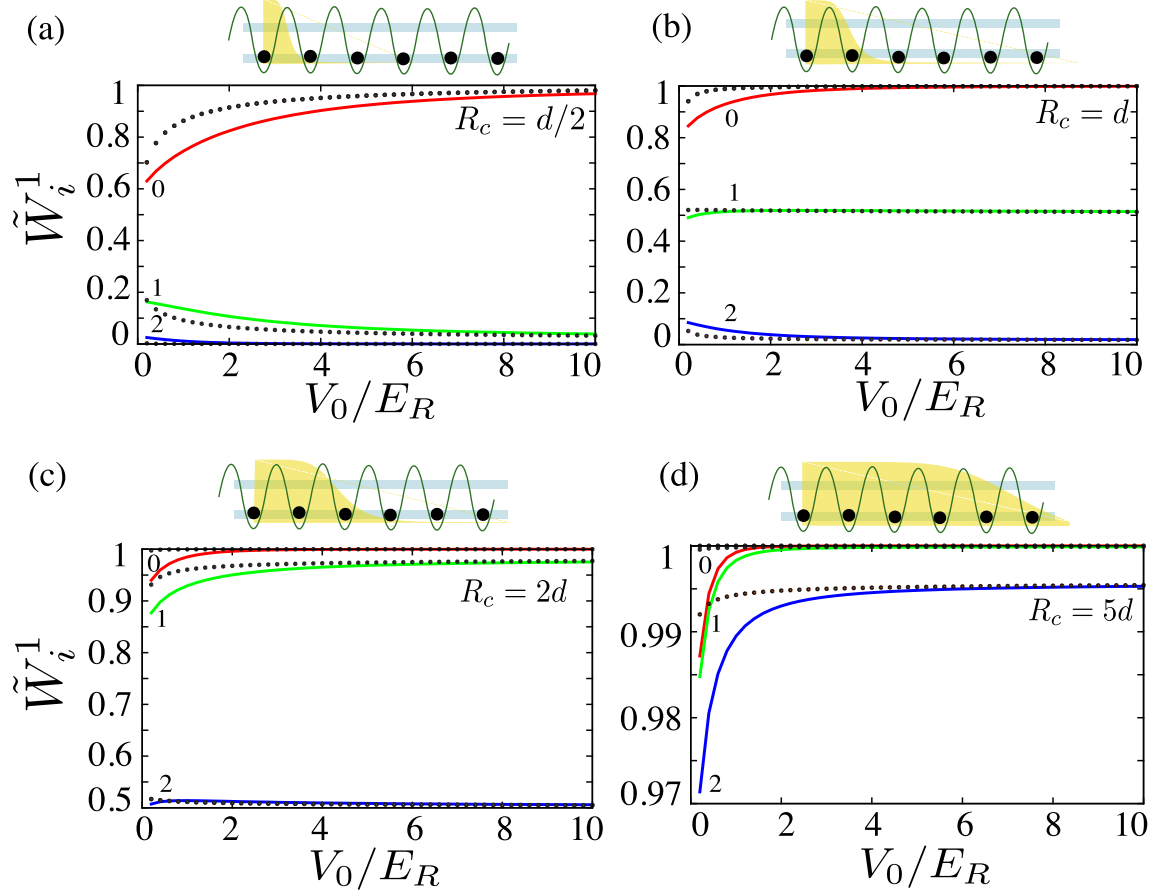


Figure 2.6: The Hubbard parameter for Rydberg-dressed interaction $\tilde{W}_i^1 = W_{0i0i}^{1111}/W_{eff}$ for both the particles in the lowest band ($n = m = 1$) as a function of the lattice depth V_0 for the range of the interaction (a) $R_c = d/2$, (b) $R_c = d$, (c) $R_c = 2d$ and (d) $R_c = 5d$. The numbers $i = 0, 1$ and 2 correspond to the onsite, nearest neighbor and the next nearest neighbor interaction parameters respectively. The dotted lines show the result from tight binding approximation. The schematic on top of each figure shows the nature of Rydberg dressed interaction potential.

tion such that onsite interaction parameter ($i = 0$) increases with increase in V_0 while the offsite parameters decrease with V_0 Fig [2.6 a]. This is because, for small values of R_c , the onsite interaction parameter is directly proportional to the localization of WF, which increases with an increase in V_0 . On the other hand, offsite matrix elements depend upon the overlap between the two WFs. Hence for small values of R_c , an increase in V_0 decreases the overlap between the WFs, leading to a decrease of offsite Hubbard parameters. With the increase in the R_c , we see the change in the behavior of offsite Hubbard parameters. For $R_c = d$, nearest neighbor matrix element ($i = 1$) starts to increase with increase in V_0 . This can be explained by looking at the shape of the Rydberg-dressed interaction for $R_c = d$ as shown

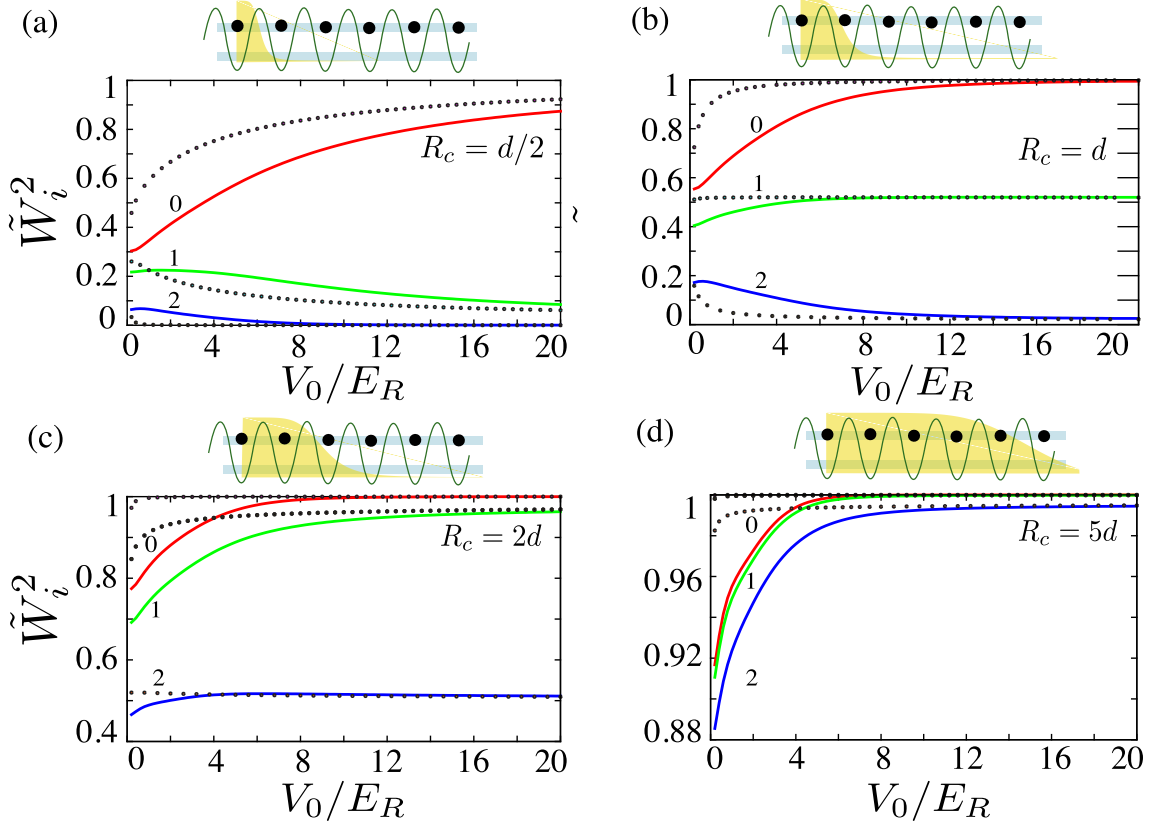


Figure 2.7: The Hubbard parameter for Rydberg-dressed interaction $\tilde{W}_i^1 = W_{0i0i}^{2222}/W_{eff}$ for both the particles in the lowest band ($n = m = 2$) as a function of the lattice depth V_0 for the range of the interaction (a) $R_c = d/2$, (b) $R_c = d$, (c) $R_c = 2d$ and (d) $R_c = 5d$. The numbers $i = 0, 1$ and 2 correspond to the onsite, nearest neighbor and the next nearest neighbor interaction parameters respectively. The dotted lines show the result from tight binding approximation. The schematic on top of each figure shows the nature of Rydberg dressed interaction potential.

in Fig [2.6 b]. For this case the range of Rydberg-dressed interaction is sufficient to affect the particle in the nearest neighbor site. This leads to the non-zero value of NN Hubbard parameter as shown in Fig [2.6 b] (solid green line). However, for $R_c = d$, the next nearest neighbor (NNN) interaction parameter still decreases with an increase in V_0 because the range of Rydberg-dressed interaction (R_c) is not sufficient to influence the NNN particle. However, with further increase in $R_c = 2d$, the NNN matrix element also starts to increase and obtains significantly non-zero value even at large V_0 . As shown in Fig [2.6 c] for $R_c = 2d$, the NN particle experiences almost a constant value of the Rydberg-dressed potential hence the NN matrix element saturates to its constant value W_{eff} . This can be explained by looking at the matrix element

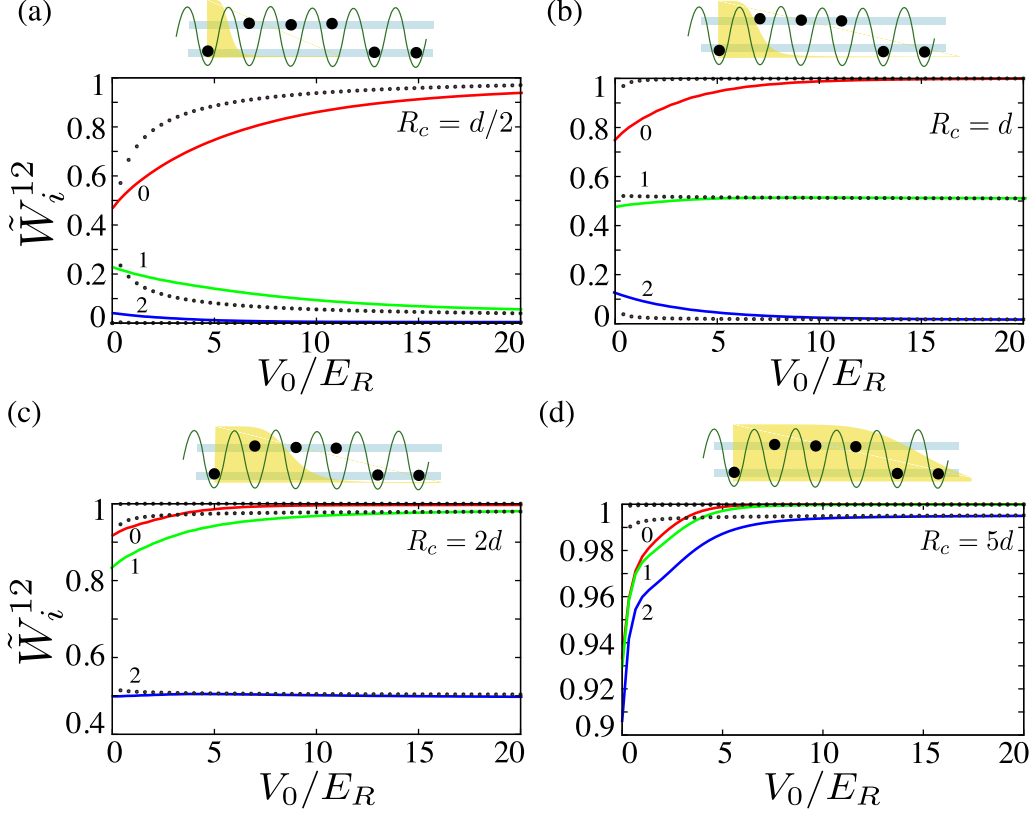


Figure 2.8: The Hubbard parameter for Rydberg-dressed interaction $\tilde{W}_i^1 = W_{0i0i}^{1212}/W_{eff}$ for both the particles in the lowest band ($n = 2$ and $m = 1$) as a function of the lattice depth V_0 for the range of the interaction (a) $R_c = d/2$, (b) $R_c = d$, (c) $R_c = 2d$ and (d) $R_c = 5d$. The numbers $i = 0, 1$ and 2 correspond to the onsite, nearest neighbor and the next nearest neighbor interaction parameters respectively. The dotted lines show the result from tight binding approximation. The schematic on top of each figure shows the nature of Rydberg dressed interaction potential.

$$W_{0101}^{nnnn} \simeq W(x - x') \int dx |w_n^*(x)|^2 \int dx' |w_m^*(x' - X_1)|^2 = W_{eff}. \quad (2.19)$$

when the value of potential is constant over the range in which particles are localized, the value of potential can be approximated by its maximum value W_{eff} and hence can be taken out of the integral leading to the result above. For the larger value of $R_c = 5d$ both the NN and the NNN particles are under the effect of soft-core potential and hence the corresponding matrix elements saturate to their maximum value W_{eff} as shown in Fig [2.6 d]. Hence R_c can be used to tune the strength of the off-site density-density Hubbard parameters. By increasing R_c , the off-site matrix elements can be made equal to each other. This results from the unique shape of the Rydberg-dressed interaction.

For the higher bands, the behavior of the Hubbard parameters as a function of R_c and V_0 remain qualitatively the same. However, the rate at which the Hubbard parameters saturate to their maximum value changes depending on the band. For the case of two particles in the second band, Hubbard parameter W_{0i0i}^{2222} , saturate at a much slower rate than the one in the first band Fig [2.7]. This is because higher bands require a larger lattice depth V_0 to localize the WF. For the case where, one particle is in band one and the other one is in band two W_{0i0i}^{1212} , has qualitatively same behavior Fig [2.8]. However, the strength of the interaction parameter lies in between the other two parameters.

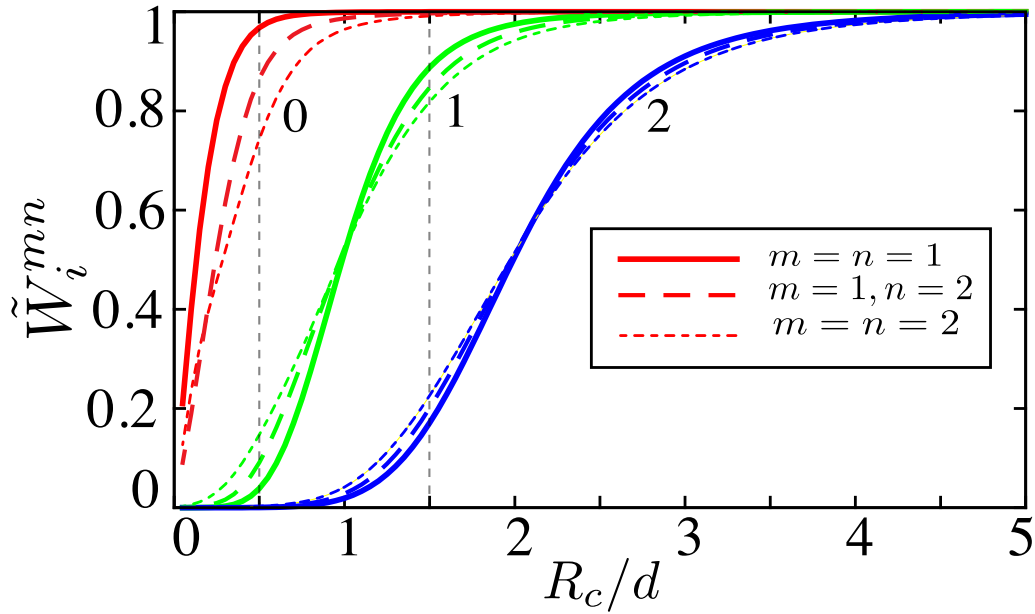


Figure 2.9: The onsite and off-site matrix elements ($\tilde{W}_i^{mn} = W_{0i0i}^{mnmn}/W_{eff}$) for the Rydberg admixed interactions as a function of R_c for $V_0 = 10E_R$. The numbering shown in the plots are for onsite ($i = 0$), nearest neighbour ($i = 1$) and next nearest neighbours ($i = 2$). For each of them the results are shown for the lowest band ($m = n = 1$), first excited band ($m = n = 2$) and between them ($m = 1, n = 2$).

The results shown above can be summarized by plotting all the matrix elements as a function of R_c Fig [2.9]. As we can see, for a fixed lattice depth V_0 , R_c provides us with the control over the off-site matrix elements which can be made of equal strength. Note that for off-site matrix elements, the lowest and the first excited bands cross each other at particular R_c . Consider the case of NN matrix elements for various bands in Fig [2.9] (green lines). For the value of R_c smaller than the separation between two particles, the strength of the matrix elements depend upon the overlap between two wavefunctions. Since the overlap is more for the particles

higher band, the corresponding matrix element has a higher value. In Fig [2.9], For $R_c = 0.5$, marked by dashed vertical line, the matrix element of band 2 ($m = n = 2$) lies above the band one matrix element ($m = n = 1$). The corresponding nature of the wavefunctions and Rydberg-dressed potential is shown in Fig [2.10 a,b]. For higher bands the overlap between the wavefunction is more hence the large value of the matrix element. On the other hand, when $R_c = 1.5 > d$ the strength of the matrix elements depend upon how well the two wavefunctions are localized under the soft-core potential. As shown in Fig [2.10 c,d], the Band 1 wavefunctions are more localized compared to the band 2, hence at $R_c = 1.5d$ (dashed vertical line in Fig [2.9]), the matrix element corresponding to band 1 ($m = n = 1$) has higher value than band 2 ($m = n = 2$).

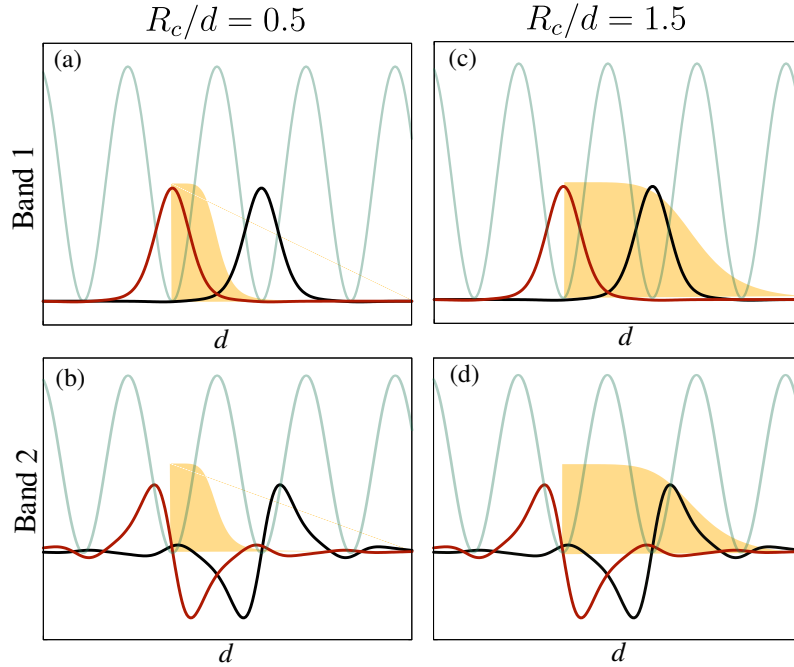


Figure 2.10: The Wannier functions for the particles in neighboring sites in band 1 (top panel) and band 2 (bottom panel). The yellow shaded region shows the form of the Rydberg dressed interaction for $R_c/d = 0.5$ and 1.5 . The blue colored curve represents the optical lattice potential

2.3.3 Rydberg admixed potential: Density Assisted Tunnelings

In this section, we look at the dominant DAT processes resulting from the Rydberg-dressed interaction. The dominant processes are represented schematically in Fig

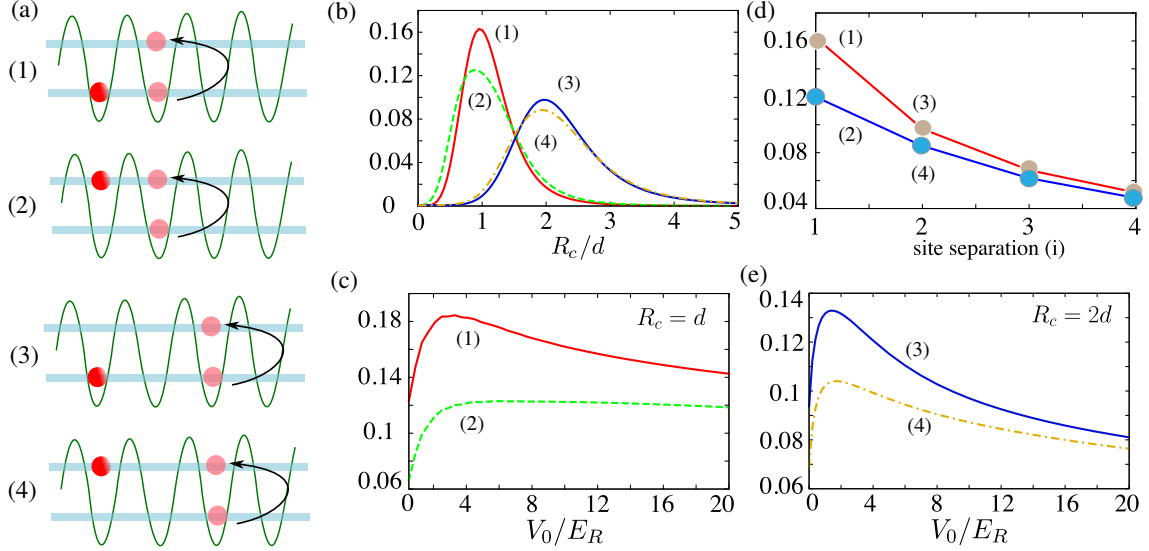


Figure 2.11: (a) The dominant off-site DAT inter-band processes due to the Rydberg admixed interactions. (b) The amplitudes of the processes as a function of R_c for $V_0 = 10E_R$. The same as a function of V_0 for (c) $R_c = d$ (e) $R_c = 2d$. (d) The maximum of the peak appearing in (b) as a function of inter-site separation for $V_0 = 10E_R$.

[2.11 a]. For process 1, one particle stays in band 1 while the other hops from band 1 to band 2. Similarly, for process 2, one particle stays in band 2 and another one hops from band 1 to band 2. The amplitude of these DAT processes depends upon the range of the Rydberg-dressed interaction, R_c . For processes 1 and 2, where particles are in the adjacent lattice sites, the amplitude of the process is peaked at $R_c = d$ Fig [2.11b]. Similarly for the process 3 and 4, for which particles are separated by two lattice sites ($d = 2$), the amplitude of the process is peaked at $R_c = 2d$ Fig [2.11b]. A similar trend would follow for the other processes with larger separation between the particles although the maximum amplitude will decrease with an increase in the site separation. As shown in Fig [2.11 d], the maximum of peak observed in Fig 2.11 b decreases with an increase in the separation between the particles.

The behavior of the above processes as a function of R_c can be understood as follows: for large values of R_c , the value of the Rydberg-dressed interaction is constant over the range of the particle separation. Which leads to the vanishing of the matrix elements dependent upon the integrals of the form $\sim \int w_0(x)w_1^*(x)$. The integral has zero value due to the orthogonality. On the other hand for values of R_c smaller than interparticle separation, the Rydberg dressed interaction between the particles is too weak to trigger the DAT processes. This leads to the small amplitude of these processes. For intermediate values of R_c , we observe a hump-like structure.

For a fixed value of R_c , all the processes have decreasing amplitude as a function of V_0 as shown in Fig [2.11 c,e]. Note that the amplitudes for all other DAT events are at least one order of magnitude lower than those shown in figure 2.11(a). The above processes introduces the following type of terms: $\sim \sum_{i,j} \hat{a}_{j2}^\dagger \hat{n}_{i1} \hat{a}_{j1}$ [process 1 and 2], $\sim \sum_{i,j} \hat{a}_{j2}^\dagger \hat{n}_{i2} \hat{a}_{j1}$ [process 2 and 4] within the two lowest-band EBHM for the Rydberg-admixed atoms in a 1D optical lattice.

2.4 Validity of our model

The results show above crucially depend upon the ability to trap the Rydberg atom and the ground state atom. One has to be careful while choosing the parameters of the setup in order for the model to be valid. The trapping lasers should be chosen in such a way that both ground and Rydberg state atoms are trapped in a magic wavelength optical lattice (MWOL) such that atoms occupying both states experience identical lattice potentials [68–71]. Large wavelength infrared MWOLs due to effective landscape polarizability, suitable for high lying alkali atom Rydberg states are also proposed [72]. If the Rydberg state trapping is neglected an additional time constraint arises due to the expansion of the atomic wave packet when atoms occupy the Rydberg state, details of which are given in the following subsection.

Rydberg state trapping:- As mentioned before, the calculations we provide above are based on the assumption that both ground and Rydberg state atoms experience the same lattice potential which requires MWOL. If it is not the case motional heating can occur during ground-Rydberg state transitions, which may lead to severe decoherence [73]. The Rydberg-Rydberg interactions can also induce mechanical effects at short distances and that can be safely neglected for Rydberg-dressed atoms [74]. In this section, we discuss what criteria in which the effective interactions calculated using Equation (2.6) are valid when no-trapping is provided for Rydberg atoms. It depends crucially on the timescale at which the free expansion of the atomic wave packet results in a considerable change of the Wannier state. It has to be shorter compared to the lifetime of Rydberg atoms and the timescales set by effective interaction strengths in the lattice. Assuming the harmonic oscillator (HO) states for the two lowest Wannier states (valid in the tight-binding case), we estimate the duration at which the wave-packets remain intact after excited to a trap-free Rydberg state. The time evolution of the standard deviation for the widths in the

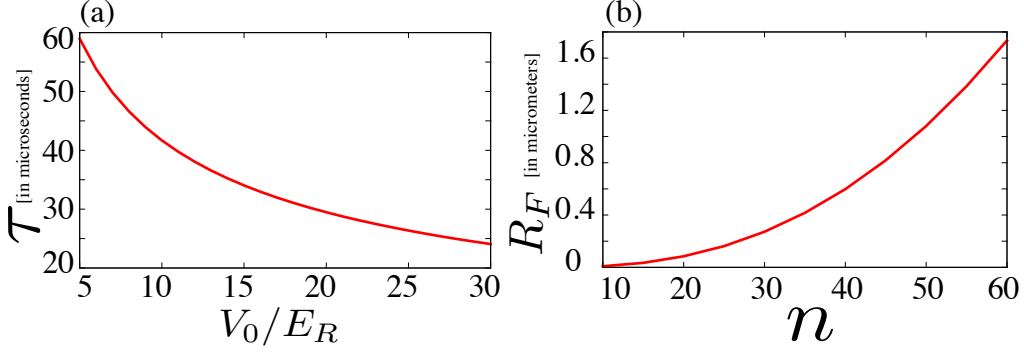


Figure 2.12: (a) The time (τ) taken for the atomic wave packet to increment 10% of its initial width during free expansion as a function of V_0 . (b) Numerical calculations for the critical distance at which the Förster and vdW regimes are separated as a function of n for Rubidium $nS_{1/2}$ states.

n^{th} state of the HO is given by

$$\Delta X_n(t)/\Delta X_n(0) = \sqrt{1 + \frac{\hbar^2 t^2}{m^2 l_0^4}}, \quad (2.20)$$

where $l_0 = \sqrt{\hbar/m\omega}$. The frequency ω of the HO in terms of the lattice depth V_0 and lattice spacing d is $\omega = (\pi/d)\sqrt{\frac{2V_0}{m}}$. Note that we are interested in a duration of time τ such that the wave packet hardly undergoes any expansion, i.e. when the criteria:

$$\frac{\hbar^2 \tau^2}{2m^2 l_0^4} \ll 1 \quad \text{or} \quad \frac{\tau^2 V_0 \pi^2}{m d^2} \ll 1 \quad (2.21)$$

is satisfied. For a given V_0 , above conditions can be satisfied by sufficiently large values of d and it is also highly desirable for us since we want to access the van der Waals regime for the interactions between the Rydberg atoms. The large lattice spacings of the order of micrometers can be accessed by adjusting the angle θ between the co-propagating lattice beams [75], given as $d = \lambda/[2 \sin(\theta/2)]$.

Rydberg-Rydberg interactions :- For two atoms occupying the same Rydberg state $|\alpha\rangle$ and far away from Förster resonance the second-order level shifts due to the dipole-dipole interactions to the pair state $|\alpha\alpha\rangle$ provide us the vdW interactions between the atoms. The Förster resonance is characterized by the Förster defect: $\delta_F = E_{\alpha\alpha} - E_{\beta\gamma}$, where the atomic states $|\beta\rangle$ and $|\gamma\rangle$ are dipole coupled to the state $|\alpha\rangle$. This introduces a cross-over between Förster regime at short distances and vdW regime at large separations between the atoms. The transition point R_F can be calculated as

$$R_F^3 = \sum_{\beta, \gamma} \left| \frac{\langle \beta\gamma | V_d(R) | \alpha\alpha \rangle}{\delta_F} \right|, \quad (2.22)$$

where $V_d(R)$ is the dipole-dipole interaction and hence, the lattice spacing has to be greater than R_F for our calculations to be valid. We estimate R_F for Rubidium $nS_{1/2}$ states in section 2.5.

2.5 An example: Rubidium atoms

In this section, we consider the state-of-the-art Rubidium (^{87}Rb) lattice setup. If the Rydberg state atoms are unconfined, as discussed in Section 2.4 the initial atomic wave packet for the ground state atoms undergoes free expansion resulting in the delocalization of the particle. This disturbs the picture of the localized Hubbard model. In order to preserve that, the experimental process has to be restricted within the time scale at which the spatial extension of the initial wave packet remains unchanged. The latter is determined by the Equation 5.8 and in figure 2.12(a) we plot the time taken in which the width of the wave packet is incremented by 10% from the initial value as a function of V_0 , for Rubidium atoms with a lattice spacing of $d = 4 \mu\text{m}$. The lattice spacing of $4 \mu\text{m}$ can be achieved with co-propagating laser beams, of wavelength $\lambda = 1064 \text{ nm}$, forming an angle of $\theta = 13.3$ degrees between them. As V_0 increases the initial width gets lesser and lesser and the wave packet carries more kinetic energy hence, takes lesser time to expand. This definitely restricts the study of the Hubbard-like model with un-trapped Rydberg states with large principal quantum numbers in deep optical lattices. For $V_0 = 10E_R$, the maximum value of n one can attain is ~ 35 . Therefore magic wavelength optical lattices are strongly recommended to explore the physics in the tight-binding regimes using Rydberg-dressed atoms involving large principal quantum numbers.

On the other hand for any given Rydberg state $nS_{1/2}$, the validity of the vdW picture in our lattice model requires that the lattice separation must be larger than R_F [see Equation (2.22)], the cross-over point between the Förster regime and vdW regime. In figure 2.12(b), we show the numerical results of R_F as a function of n for $nS_{1/2}$ Rubidium states. Though the main contributions from the dipole coupling are coming from the nearest $nP_{1/2}$, we also included $nP_{3/2}$. It shows that in order to access the vdW regime the lattice spacings are at least of about $2\mu\text{m}$ for $n > 60$.

As we have pointed out earlier in section 2.3.2, any change in detuning Δ or Ω affect R_c and W_{eff} simultaneously, but the interaction range R_c can be varied independently by changing the Rydberg states. Below we estimate realistic values for R_c as a function of $C_6(n)$ for Rubidium atoms weakly coupled to $nS_{1/2}$ states, in

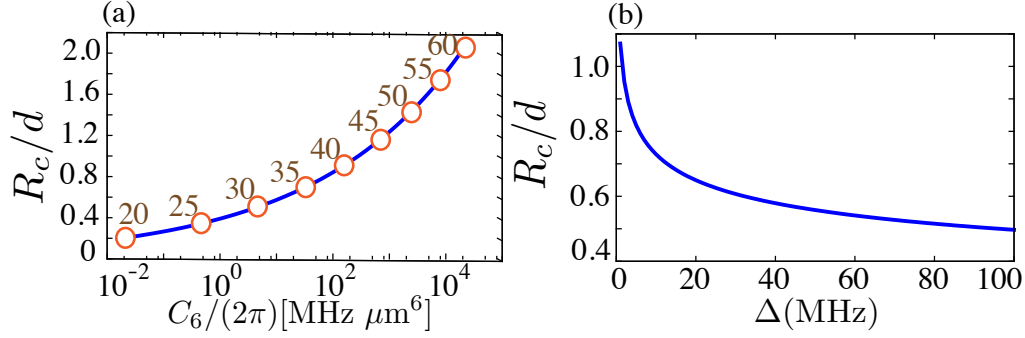


Figure 2.13: (a) The range of Rydberg admixed interaction (R_c) as a function of $C_6(n)$ for ^{87}Rb atoms in which the ground state is weakly admixed to $nS_{1/2}$ states with a detuning $\Delta = 100$ MHz and a lattice space of $d = 2\mu\text{m}$. The corresponding principal quantum numbers n are indicated by the empty bubbles. (b) R_c as a function of Δ for $30S_{1/2}$.

an 1D optical lattice [figure 2.13(a)]. We consider a lattice spacing of $d = 2\mu\text{m}$. It can be seen that the range of interactions can be extended over as many as 2 sites when considering a Rydberg state $60S_{1/2}$ with $\Delta = 100$ MHz. Note that for fixed C_6 the variation of R_c against Δ is relatively slow. With $\Omega/\Delta = 0.1$ and $\Delta = 100$ MHz, we can attain an effective interaction strength of $W_{\text{eff}} = 10$ kHz.

2.6 Summary

In conclusion, we have estimated *ab initio* the Hubbard parameters for Rydberg-dressed atoms in a one-dimensional sinusoidal optical lattice in the basis of maximally localized Wannier states. The finite range, soft-core nature of the Rydberg induced vdW interactions strongly modifies the nature of Hubbard parameters. In particular, in controlling the spatial extension of the soft-core barrier one can engineer the off-site interactions and make them the same magnitude as that of the onsite ones, hence making them position-independent. This may influence the many-body dynamics a great deal. In addition to the typical density-density interactions, we provide the information for the DAT coefficients in this system. Two dominant processes which depend crucially on the soft-core have been identified and discussed which will be highly relevant when studying non-standard multi-band Hubbard models. In the end, we have discussed realistic parameters for the state-of-the-art experimental Rydberg-dressed Rubidium lattice setup.

This work resulted in the following publication: *Ab initio* calculation of Hubbard parameters for Rydberg-dressed atoms in a one-dimensional optical lattice [76]

2.7 Appendix

2.7.1 Single particle energy bands and Bloch states in an 1D optical lattice

The Hamiltonian for a single particle in the presence of an 1D optical lattice potential $V(x)$ is

$$\hat{h}_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{OL}(x), \quad (2.23)$$

where $V_{OL}(x) = V_0 \sin^2(k_0 x)$ and the wave number $k_0 = \pi/d$ with d being the lattice spacing. The single particle energy band structure is obtained by solving the eigenvalue equation $\hat{h}_0 \psi_q^n(x) = E_q^n \psi_q^n(x)$ for a given quasi-momentum $q \in [-\pi/d, \pi/d]$ and n is the band index. According to the Bloch theorem, we have Bloch solutions $\psi_q^n(x) = e^{iqx} u_q^n(x)$ and $u_q^n(x)$ has the same periodicity as that of the lattice potential. The above eigen value equation is best tackled in the Fourier space, and by introducing the Fourier expansion for the lattice potential $V_{OL}(x) = (1/\sqrt{d}) \sum_k v_k e^{iG_k x}$ and for $u_q^n(x) = (1/\sqrt{d}) \sum_k c_{q,k}^n e^{iG_k x}$. With Fourier coefficients $c_{q,k}^n$ satisfying the normalization condition $\sum_k (c_{q,k}^n)^* c_{q,k}^n = \delta_{m,n}$, the periodic functions $u_q^n(x)$ is normalized over the primitive unit cell of the lattice in the real space. Finally we arrive at

$$\frac{\hbar^2}{2m} (G_k + q)^2 c_{q,k}^n + \frac{1}{\sqrt{d}} \sum_{k'} v_{k-k'} c_{q,k'}^n = E_q^n c_{q,k}^n. \quad (2.24)$$

We can write the above equation in a matrix form as $H_q c_q^n = E_q^n c_q^n$ with eigenvectors c_q^n and eigenvalues E_q^n . The matrix elements of H_q :

$$(H_q)_{ij} = \frac{\hbar^2}{2m} (G_i + q)^2 \delta_{ij} + \frac{1}{\sqrt{d}} v_{i-j}. \quad (2.25)$$

Diagonalizing H_q provides us the Fourier coefficients $c_{q,k}^n$ and they possess certain properties based on various symmetries. If inversion symmetry exists and together with time-reversal symmetry, they guarantee that $c_{q,k}^n$ are real apart from a common phase factor and also satisfies $c_{q,k}^n = (c_{-q,-k}^n)^*$. This property can considerably reduce the numerical cost in calculating the Bloch functions $\psi_q^n(x)$. We employ a LAPACK routine to obtain the eigenstates and eigenvalues of the Hamiltonian matrix given in equation 2.25 for $q \in [-\pi/d, \pi/d]$. The eigen vectors c_q^n are real-valued and the periodic Bloch function $u_q^n(x)$ is then obtained by its Fourier transform.

2.7.2 Maximally Localized Wannier functions

Consider a Wannier function localized in the unit cell such that $X_j = 0$, Eq. [2.8] becomes.

$$w_n(x) = \frac{d}{2\pi} \int_{BZ} dq e^{i\phi_q^n} e^{iqx} u_q^n(x). \quad (2.26)$$

We need to find the phase factor which minimizes the imaginary part of the Wannier functions.

$$w_n(x) = \frac{d}{2\pi} \int_{BZ} dq (\cos(qx + \phi_q^n) + i \sin(qx + \phi_q^n)) (\text{Re}[u_q^n(x)] + i * \text{Im}[u_q^n(x)]) \quad (2.27)$$

the imaginary part of the wave-function is given by,

$$\text{Im}[w_n(x)] = \frac{d}{2\pi} \int_{BZ} dq (\cos(qx + \phi_q^n) \text{Im}[u_q^n(x)] + \sin(qx + \phi_q^n) \text{Re}[u_q^n(x)])$$

Differentiating the imaginary part w.r.t ϕ_q^n and equating it to zero we get,

$$\frac{\partial \text{Im}[w_n(x)]}{\partial \phi} = -\sin(qx + \phi_q^n) \text{Im}[u_q^n(x)] + \cos(qx + \phi_q^n) \text{Re}[u_q^n(x)] = 0 \quad (2.28)$$

which gives us the condition on ϕ_q^n as,

$$\phi_q^n = -qx_0 + \tan^{-1} \left(\frac{\text{Re}(u_q^n)}{\text{Im}(u_q^n)} \right) \quad (2.29)$$

for the symmetric first band we choose $x_0 = 0$ whereas for the first band, x_0 is the point where the imaginary part of $u_q^n(x)$ is maximum

Chapter 3

Correlated Rabi Oscillations in a driven Rydberg atomic chain

The novel dynamical processes can lead to exotic phases in strongly correlated quantum many-body systems. The identification and characterization of such processes are crucial in understanding the physics of strongly correlated systems. One such type of process is Density Assisted Tunneling (DAT) processes, which arises due to interaction. In this process, particles make inter-site or inter-band hopping due to interaction. Such processes are also called bond charge interaction or correlated tunneling. These are different than the tunnelings occurring due to kinetic energy. These processes have been observed experimentally in the standard Bose-Hubbard model [77, 78]. For the extended Bose Hubbard model (EBHM) with dipolar interaction, the existence of DAT processes has a significant impact on the phase diagram [34]. For both cases, transition points from mott insulator to superfluid phase get modified due to DAT. Similar processes were observed in the EBHM with Rydberg-dressed interaction studied in the previous chapter. These processes involved particle making inter-band transition at the same site due to the presence of another particle.

In this chapter, we identify similar processes for a chain of two-level atoms in which the ground state is coupled to the Rydberg state by an external laser. DAT type of processes emerge in a chain of Rydberg atoms due to long-range nature of the vdW interaction when atoms are in the Rydberg state. We call these processes Correlated Rabi Oscillations. In these processes one atom makes a transition from the ground state to the Rydberg state while other atoms are in the Rydberg state. By using the Schrieffer-Wolf transformation, which gives a low energy description

of a strongly interacting quantum many-body system, we show the emergence of correlated Rabi oscillations. We introduce the periodic driving to the system by modulating the detuning from the Rydberg state sinusoidally in time and study its effect on Correlated Rabi oscillations. We quantify the behavior of correlated Rabi oscillations by calculating the effective Hamiltonian and correlation functions for various driving parameters.

This chapter is organized as follows: In section 3.1, we describe the model and the Hamiltonian. Section 3.2 calculates the effective Hamiltonian in different parameter regimes. In section 3.3 we mention the correlation functions. Using the effective Hamiltonian and correlation functions, we study the behavior of correlated Rabi Oscillation for two atoms in section 3.4 and more than two atoms in section 3.5.

3.1 Model

We consider a one-dimensional array of N two-level atoms trapped in an optical lattice. The two levels of the atoms being the ground state $|g\rangle$ and the Rydberg state $|r\rangle$. The Hamiltonian for the system in the frozen gas limit is given by,

$$\hat{H}(t) = -\Delta(t) \sum_{i=1}^N \hat{\sigma}_{rr}^i + \frac{\Omega}{2} \sum_{i=1}^N \hat{\sigma}_x^i + \sum_{i<j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \quad (3.1)$$

where, $\hat{\sigma}_{ab} = |a\rangle \langle b|$ with $[a, b] \in \{g, r\}$ and $\hat{\sigma}_x = \hat{\sigma}_{rg} + \hat{\sigma}_{gr}$ are the Pauli spin matrices. The first term in the Hamiltonian represents the time dependent detuning with periodic modulation of the form $\Delta(t) = \Delta_0 + \delta \sin \omega_0 t$, with Δ_0 is offset in detuning, $\delta > 0$ is the amplitude and ω_0 being the frequency of modulation. The second term represents the coupling of the ground state $|g\rangle$ to the Rydberg state $|r\rangle$ with coupling strength given by Rabi frequency Ω . The last term accounts for the van der Waals interaction between two atoms in the Rydberg state, $V_{ij} = C_6/r_{ij}^6$.

To get a better understanding of the effect of periodic driving on the dynamics we move to the rotating frame defined by the unitary transformation

$$\hat{U}(t) = \exp[i(\delta/\omega_0 \cos \omega_0 t - \Delta_0 t) \sum_j \hat{\sigma}_{rr}^j + it \sum_{j<k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k] \quad (3.2)$$

The new Hamiltonian in the rotating frame, $\hat{H}' = \hat{U} \hat{H} \hat{U}^\dagger - i\hbar \hat{U} \hat{U}^\dagger$, is given by (see 3.7.1),

$$\hat{H}'(t) = \frac{\Omega}{2} \sum_{j=1}^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) g(t) e^{i \sum_{k \neq j} V_{kj} \hat{\sigma}_{rr}^k t} \hat{\sigma}_{rg}^j + \text{H.c} \quad (3.3)$$

with $g(t) = e^{i(m\omega_0 - \Delta_0)t}$ and $J_m(\delta/\omega_0)$ is the m^{th} order Bessel function. Using this Hamiltonian, we calculate the effective Hamiltonians for different parameters in the next section.

3.2 Effective Hamiltonians

For a periodically driven Hamiltonian with $\hat{H}(t+T) = \hat{H}(t)$, at stroboscopic times ($t_n = nT$), the evolution is governed by unitary operator of the form $e^{-i\hat{H}_F T}$ [79]. The Floquet Hamiltonian, $\hat{H}_F$, can be calculated by using Magnus expansion as $\hat{H}_F = \sum_{n=0}^{\infty} \hat{H}_F^{(n)}$. The zeroth order Floquet Hamiltonian can be obtained by calculating the time average of a time dependent Hamiltonian. This gives an insight into the long time dynamics of the system. The effective Hamiltonian is given by,

$$H_{\text{eff}} = \hat{H}_F^{(0)} = \frac{1}{T} \int_0^T dt \hat{H}'(t) \quad (3.4)$$

where the time period of the oscillation T is defined by the highest energy scale. For small interactions, where $V_0 \ll \omega_0$, we have $T = 2\pi/\omega_0$ whereas for strong interactions, where $V_0 \gg \omega_0$, we have $T = 2\pi/V_0$. In order to simplify the calculations, we rewrite the Hamiltonian 3.3 using the identity, $e^{\pm i \sum_{k \neq j} V_{jk} \hat{\sigma}_{rr}^k t} = \prod_{k \neq j} \hat{\sigma}_{rr}^k (e^{\pm i t V_{jk}} - 1) + \mathcal{I}$, which leads to,

$$\begin{aligned} \hat{H}'(t) = \frac{\Omega}{2} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) \left[g(t) \hat{\sigma}_{rg}^j \left(\prod_{k \neq j} [\hat{\sigma}_{rr}^k (e^{i V_{jk}} - 1) + \mathcal{I}] \right) + \right. \\ \left. g^*(t) \hat{\sigma}_{gr}^j \left(\prod_{k \neq j} [\hat{\sigma}_{rr}^k (e^{i V_{jk}} - 1) + \mathcal{I}] \right) \right] \end{aligned} \quad (3.5)$$

with $g(t) = e^{i(m\omega_0 - \Delta_0)t}$. We truncate the RRI to the nearest neighbor such that $V_{i,i+1} = V_0$, which leads to the Hamiltonian

$$\begin{aligned} \hat{H}'_{NN}(t) = \frac{\Omega}{2} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) g(t) \hat{\sigma}_{rg}^j \left[1 + \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1} (e^{i V_{jk}} - 1)^2 + \right. \\ \left. + (\hat{\sigma}_{rr}^{j+1} + \hat{\sigma}_{rr}^{j-1}) (e^{i V_0 t - 1}) \right] + \text{H.c.} \end{aligned} \quad (3.6)$$

Now, substituting Equation 3.6 into Equation 3.4 and carrying out the integration, we get the effective Hamiltonian. Depending on the relative strength of the

interaction and driving frequency, the effective Hamiltonian can be written for two cases given by

Case 1 – $\omega_0 \gg V_0$

Here, $T = 2\pi/\omega_0$

$$\begin{aligned} \hat{H}_{eff}^{\omega_0 \gg V_0} = & \frac{\Omega}{2iT} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) \left[\frac{e^{-i\Delta_0 T} - 1}{m\omega_0 - \Delta_0} (1 - \hat{\sigma}_{rr}^{j+1} - \hat{\sigma}_{rr}^{j-1} + \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}) + \right. \\ & \left. \frac{e^{-i(\Delta_0 - 2V_0)T} - 1}{m\omega_0 - \Delta_0 + 2V_0} \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1} + \frac{e^{-i(\Delta_0 - V_0)T} - 1}{m\omega_0 - \Delta_0 + V_0} (\hat{\sigma}_{rr}^{j+1} + \hat{\sigma}_{rr}^{j-1} - 2\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}) \right] \hat{\sigma}_{rg}^j + \text{H.c} \end{aligned} \quad (3.7)$$

which, in the case of $\Delta_0 = 0$ reduces to

$$\begin{aligned} \hat{H}_{eff}^{\omega_0 \gg V_0} = & \frac{\Omega}{2iT} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) \left[\frac{e^{i2V_0 T} - 1}{m\omega_0 + 2V_0} \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1} + \frac{e^{iV_0 T} - 1}{m\omega_0 + V_0} \hat{\sigma}_{rr}^{j+1} + \right. \\ & \left. \hat{\sigma}_{rr}^{j-1} - 2\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1} \right] \hat{\sigma}_{rg}^j + \frac{J_0(\delta/\omega_0)\Omega}{2} \sum_{j=1}^N \hat{\sigma}_{rg}^j (1 - \hat{\sigma}_{rr}^{j+1} - \hat{\sigma}_{rr}^{j-1} + \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}) + \text{H.c.} \end{aligned} \quad (3.8)$$

Case 2 – $V_0 \gg \omega_0$

Here, $T = 2\pi/V_0$

$$\begin{aligned} \hat{H}_{eff}^{V_0 \gg \omega_0} = & \frac{\Omega}{2iT} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) (g(T) - 1) \left[\frac{(1 - \hat{\sigma}_{rr}^{j+1} - \hat{\sigma}_{rr}^{j-1} + \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1})}{m\omega_0 - \Delta_0} + \right. \\ & \left. \frac{\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}}{m\omega_0 - \Delta_0 + 2V_0} + \frac{\hat{\sigma}_{rr}^{j+1} + \hat{\sigma}_{rr}^{j-1} - 2\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}}{m\omega_0 - \Delta_0 + V_0} \right] \hat{\sigma}_{rg}^j + \text{H.c.} \end{aligned} \quad (3.9)$$

$$\begin{aligned} \hat{H}_{eff}^{V_0 \gg \omega_0} = & \frac{\Omega}{2iT} \sum_j^N \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) (e^{im\omega_0 T} - 1) \left[\frac{(1 - \hat{\sigma}_{rr}^{j+1} - \hat{\sigma}_{rr}^{j-1} + \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1})}{m\omega_0} + \right. \\ & \left. \frac{\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}}{m\omega_0 + 2V_0} + \frac{\hat{\sigma}_{rr}^{j+1} + \hat{\sigma}_{rr}^{j-1} - 2\hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}}{m\omega_0 + V_0} \right] \hat{\sigma}_{rg}^j + \text{H.c.} \end{aligned} \quad (3.10)$$

We make use of these effective Hamiltonians along with correlation functions defined in the next section to understand the behavior of correlated Rabi oscillations in different parameter regimes.

3.3 Correlation functions

The correlation functions can also be used to study the dynamics of the system. Two-body correlation functions have been widely used to study the non-equilibrium dynamics of the system. Behavior of these correlation functions with respect to time gives us an idea about propagation of correlations, particle-hole pairs in the system [48, 80, 81]. For our case we use two-body and three-body correlation functions to characterize various correlated Rabi oscillation processes. The correlation functions are defined as

$$C_{x2}(t) = \langle \sum_{j=1}^N (\hat{\sigma}_x^j \hat{\sigma}_{rr}^{j+1} + \hat{\sigma}_x^j \hat{\sigma}_{rr}^{j-1}) \rangle / N \quad (3.11)$$

$$C_{x3}(t) = \langle \sum_{j=1}^N (\hat{\sigma}_x^j \hat{\sigma}_{rr}^{j+1} \hat{\sigma}_{rr}^{j-1}) \rangle / N \quad (3.12)$$

where C_{x2} and C_{x3} are two-body and three-body correlation functions respectively. $\langle \dots \rangle$ represents the expectation with respect to state $|\psi(t)\rangle$. The behaviour of these correlation functions as a function of driving parameters and interaction strength gives information about correlated Rabi oscillations. In the next section, we first study the correlated Rabi oscillations using effective Hamiltonian and correlation functions for the case of two atoms and then extend to the case of ten atoms.

3.4 $N = 2$

We first study the emergence of correlated Rabi oscillations in the simplest case of two atoms. we write Equation 3.3 for the case of two atoms ($N = 2$), (see 3.7.1)

$$\hat{H}'^{(2)}(t) = \frac{\Omega}{2} \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) g(t) \left(\sum_{j=1}^2 \hat{\sigma}_{rg}^j + \hat{X}(e^{iV_0 t} - 1) \right) + \text{H.c.} \quad (3.13)$$

with $\hat{X} = \hat{\sigma}_{rg}^1 \hat{\sigma}_{rr}^2 + \hat{\sigma}_{rg}^2 \hat{\sigma}_{rr}^1$. The term $\hat{X}$ represents the correlated Rabi Oscillations. The process $\hat{X}$ is represented pictorially in Fig [3.1 a]

We see that the correlated Rabi oscillations are present because of the Rydberg-Rydberg interaction. It represents an atom making a transition from the ground state $|g\rangle$ to the Rydberg state $|r\rangle$ when the other atom is already in the Rydberg

state. Fig [3.1 a] pictorially represents the correlated Rabi oscillation process for the case of two atoms. The effect of periodic driving on correlated Rabi oscillations can be understood by the effective Hamiltonian and also by calculating various correlation functions.

Lets first consider the limit $\omega_0 \gg V_0$ and restrict to the case of two atoms $N = 2$, Equation 3.8 reduces to,

$$H_{\text{eff}}'^{(2)} = \frac{\Omega}{2iT} \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) \frac{(e^{iV_0 T} - 1)}{m\omega_0 + V_0} \hat{X} + \frac{J_0(\delta/\omega_0)\Omega}{2} \left(\sum_{j=1}^2 \hat{\sigma}_{rg}^j - \hat{X} \right) + \text{H.c.} \quad (3.14)$$

Now if we take the small interaction limit $V_0 \rightarrow 0$ we get the following expression for the Hamiltonian,

$$\hat{H}_{\text{eff}}^{V_0 \gg \omega_0} \simeq J_0(\delta/\omega_0) \frac{\Omega}{2} \sum_j \hat{\sigma}_{rg}^j + \frac{i\Omega J_0(\delta/\omega_0)T}{4} V_0 \hat{X} + \mathcal{O}(V_0^2) \quad (3.15)$$

which implies that for small interaction strengths, the correlated Rabi oscillations increase linearly with the interaction strength V_0 . We shall see this when we calculate the average correlation functions in the next section.

On the other hand, in the strong interaction limit where $V_0 \gg \omega_0$, we get the effective Hamiltonian for two atoms from Equation 3.10,

$$\begin{aligned} \hat{H}_{\text{eff}}^{V_0 \gg \omega_0} &= \frac{\Omega}{2iT} \sum_{m=-\infty}^{\infty} i^m J_m(\delta/\omega_0) (e^{im\omega_0 T} - 1) \\ &\times \left[\sum_{j=1}^2 \frac{\hat{\sigma}_{rg}^j}{m\omega} + \left(\frac{1}{m\omega_0 + V_0} - \frac{1}{m\omega_0} \right) \hat{X} \right] \end{aligned} \quad (3.16)$$

Now if we take the limit where the amplitude of the driving $\delta \rightarrow 0$, we get the case of non-driven system with strong interactions. In such limit, the effective Hamiltonian becomes,

$$\hat{H}_{\text{eff}}^{V_0 \gg \omega_0} \simeq \frac{\Omega J_0(\delta/\omega_0)}{2} \left(\sum_{j=1}^2 \hat{\sigma}_{rg}^j - X \right) \quad (3.17)$$

The negative sign in front of the correlated Rabi oscillation term plays a crucial role. If we take the matrix element of the effective Hamiltonian between the states

$|+\rangle = (|gr\rangle + |rg\rangle)/\sqrt{2}$ and $|gg\rangle$ we get $\langle +|\hat{H}_{\text{eff}}^{V_0 \gg \omega_0}|rr\rangle = 0$. This represents that the transition from the singly excited state $|+\rangle$ to a doubly excited state $|rr\rangle$ is forbidden. This is true because of the Rydberg blockade effect in strong interaction limit. Hence the correlated Rabi oscillations provide an alternative explanation for the Rydberg blockade.

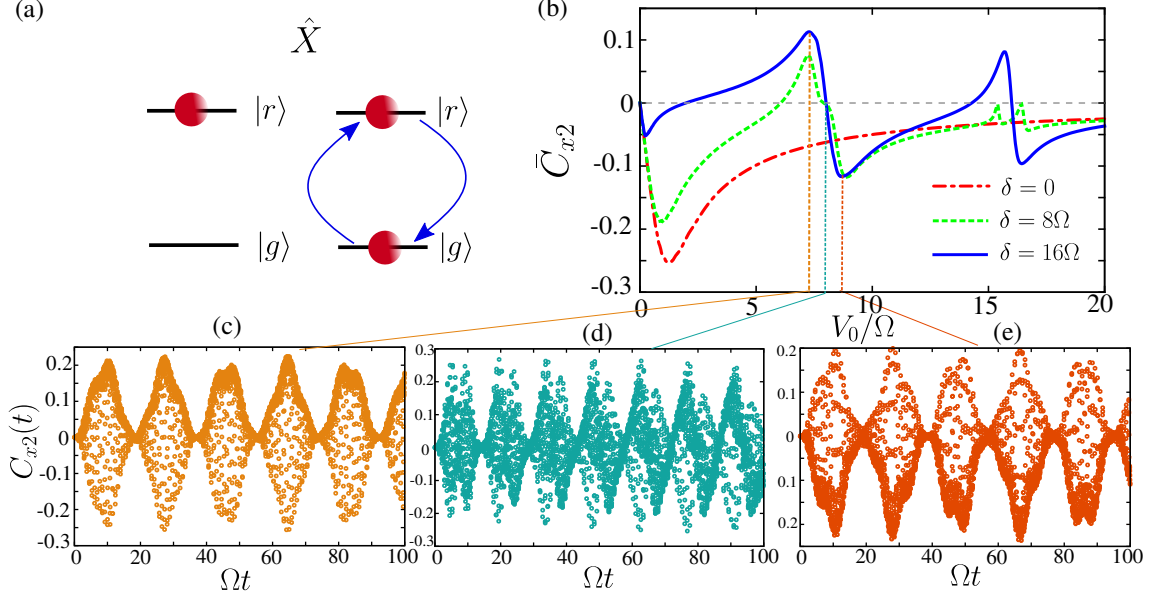


Figure 3.1: (a) A schematic representation of correlated Rabi oscillations represented by $\hat{X}$ (b) An average value of correlation function, $\bar{C}_{x2}$ vs V_0 for $\Delta_0 = 0$, $\omega_0 = 8\Omega$ and $\Omega T_f = 150$, three subplots show the time evolution of correlation function C_{x2} for a positive, negative and zero value of $\hat{C}_{x2}$ respectively

To support the calculations of the effective Hamiltonian and to characterize the dynamics of correlated Rabi oscillations, we calculate the correlation function and study their time evolution as well as the average behavior as a function of driving parameters and interaction. Firstly, for the case of two atoms we define the average two-body correlation function as,

$$\bar{C}_{x2} = \frac{1}{2T_f} \int_0^{T_f} C_{x2}(t) dt \quad (3.18)$$

with $C_{x2}(t)$ given by Equation 3.11. It quantifies the correlation between the two events in which one atom stays in the Rydberg state while the other makes a transition from the ground state to the Rydberg state. As shown above, for small values of interactions the correlation increases linearly with an increase in V_0 . Fig [3.1 b] shows the variation of the average correlation function for different value of driving

amplitude δ . For the non-driven case, $\delta = 0$, the correlation increase linearly with increase in V_0 at small values of V_0 . For large values of V_0 , correlations decrease with an increase in V_0 as $1/V_0$ due to the Rydberg blockade effect. For the case of driven atoms, with driving amplitude $\delta/\Omega = 8, 16$, we observe oscillations due to the competing effect of the Rydberg blockade and the resonances. The Rydberg blockade tries to suppress the transition to $|rr\rangle$ state resulting in suppression of two-body correlations. However at a particular value of V_0 , where the resonance condition for population transfer from $|gg\rangle \rightarrow |+\rangle$, $|+\rangle \rightarrow |rr\rangle$ and $|gg\rangle \rightarrow |rr\rangle$ at $n_1\omega_0 = \Delta_0$, $n_2\omega_0 = \Delta_0 - V_0$ and $n_3\omega_0 = \Delta_0 - V_0/2$ are satisfied, the population gets transferred from both $|gg\rangle$ and $|+\rangle$ to the $|rr\rangle$ state. Hence at these points, the behavior of the system on average is equivalent to that of a non-interacting system. The bottom middle plot in Fig [3.1 d] shows the behavior of $C_{x2}(t)$ as a function time at the resonance point. As we can observe, at the resonance point, the correlations on average are zero because of equally positive and negative values. This is similar to the non-interacting case, $V_0 = 0$, where, population makes the transition from the ground state to all the excited states. However, we observe such dynamics at large interaction values ($V_0 \sim 8\Omega$) for a particular value of driving parameters. Whereas on either side of the resonance point, the correlations attain the maximum value in both positive and negative directions. This can be explained based on the time evolution of the correlation function at each extreme point. As shown in Fig [3.1 c,e], correlation function has accumulated values in either positive or negative direction. This leads to the non-zero value of the correlation function on average. Hence a choice of the periodic driving parameters and interaction strength parameter V_0 give us control over the correlations in the system.

3.5 $N > 2$

We now study the two-body and three-body correlations for the chain of ten atoms, $N = 10$. To quantify the three-body correlation we calculate the following quantity,

$$\bar{C}_{x3} = \frac{1}{T_f} \int_0^{T_f} C_{x3}(t) dt \quad (3.19)$$

where $C_{x3}(t)$ is given by Equation 3.12. Fig [3.2 a] schematically represents the process quantified by C_{x3} . It calculates the probability of an atom making transition from the ground state to the Rydberg state when its neighboring atoms are in the

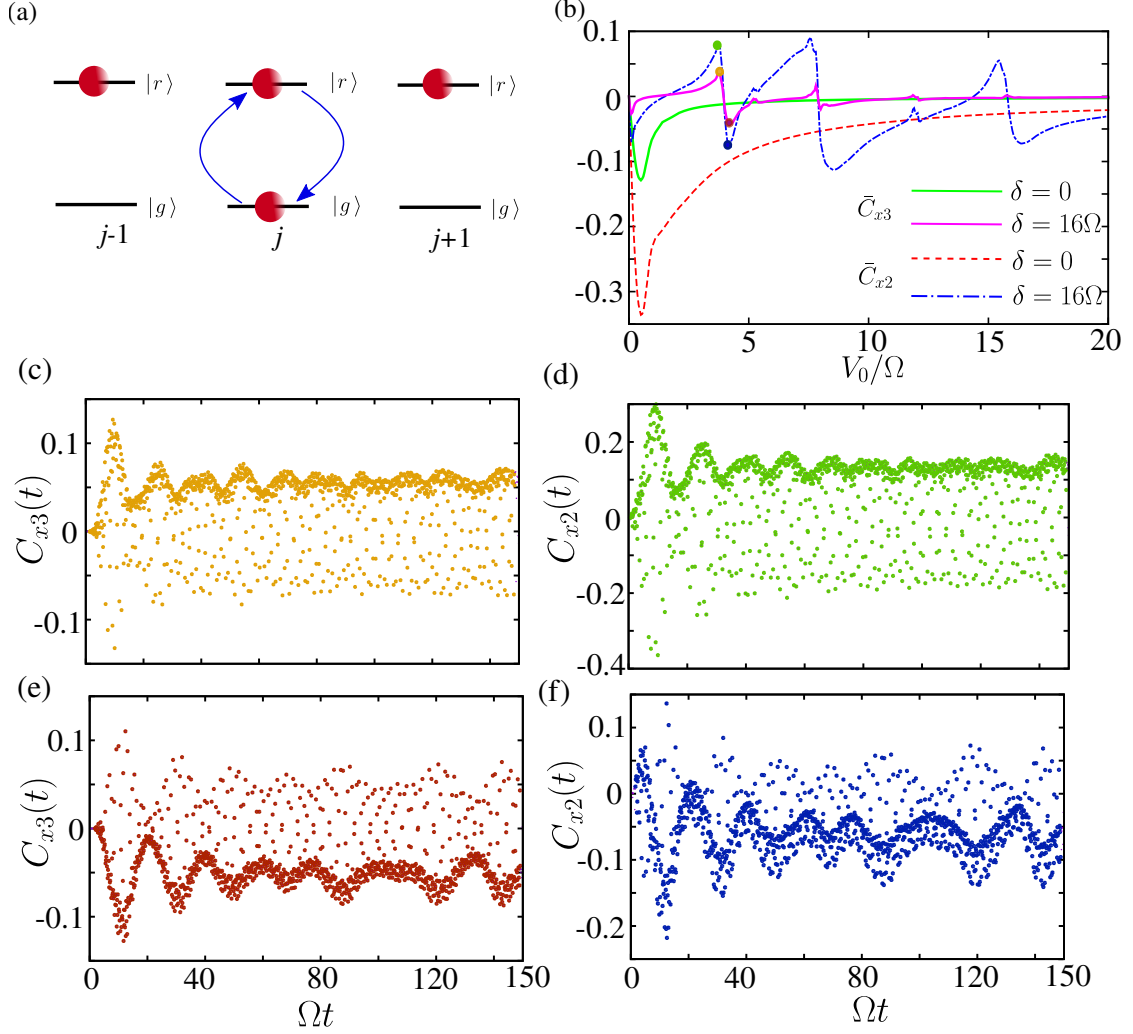


Figure 3.2: (a) A schematic representation of three body correlated Rabi oscillation process (b) An average value two body $\hat{C}_{x2}$ and three body $\hat{C}_{x3}$ correlators as function of V_0 for a chain of ten atoms ($N = 10$) for $\Delta_0 = 0$, $\omega_0 = 8$ and $\Omega T_f = 150$. (c)-(f) The time evolution of two-body $C_{x2}(t)$ and three-body $C_{x3}(t)$ correlation functions at their extreme values marked by respective colored circle in (b).

Rydberg state.

As shown in the Fig [3.2 b] for the non-driven case ($\delta = 0$), both $\bar{C}_{x2}$ and $\bar{C}_{x3}$ behave qualitatively same as that of two atom case. For small vales of interaction strengths, both the correlation functions increase linearly and for large values decrease algebrically. However the amplitude of the three body correlator $\bar{C}_{x3}$ is significantly smaller than the two body correlator $\bar{C}_{x2}$. This implies that the events represented by the two body correlators are more probable than the three body events. For the driven case ($\delta = 16\omega$), we observe the similar periodic behaviour of correlators as a function of V_0 . The Fig [3.2 c-f] shows the time evolution of $C_{x2}(t)$

and $C_{x3}(t)$ for their extreme values marked by colored circles in Fig [3.2 b]. For both the correlation functions, we observe the accumulation of points on positive and negative side similar to the two atom case. Hence on average we observe the positive or negative value of correlation functions.

3.6 Summary

To summarize, we showed the emergence of Correlated Rabi oscillations in a chain of Rydberg atoms using Schrieffer-Wolf transformation. The behavior of correlated Rabi oscillation is studied for various driving parameters using effective Hamiltonian and correlation functions. The effective Hamiltonian revealed that in the strong interaction limit, correlated Rabi oscillations are responsible for the Rydberg blockade. Also, in the presence of periodic driving, average correlation functions showed oscillatory behavior as a function of interaction strength. By appropriately choosing the driving parameters we could control the dynamics of correlated Rabi oscillations.

This work is a part of following publication: Periodically driven array of single Rydberg atoms [82]

3.7 Appendix

3.7.1 Hamiltonian in Rotating frame

In order to obtain the Hamiltonian in rotating frame, we start with the many body Hamiltonian given by

$$H = -\hbar\Delta(t) \sum_{j=1}^N \hat{\sigma}_{rr}^j + \frac{\hbar\Omega}{2} \sum_j^N (\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j) + \sum_{i<j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \quad (3.20)$$

Using the following unitary transformation we obtain the Hamiltonian in the rotating frame.

$$U(t) = e^{if(t) \sum_j \hat{\sigma}_{rr}^j + it \sum_{i<j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \quad (3.21)$$

with $f(t) = \delta/\omega_0 \cos \omega_0 t - \Delta_0 t$. The Hamiltonian in the rotating frame, H' , can be calculated using,

$$H'(t) = U(t)H(t)U^\dagger(t) - i\hbar U \dot{U}^\dagger \quad (3.22)$$

We now consider each term separately, the first term is given by,

$$e^{if(t) \sum_j \hat{\sigma}_{rr}^j + it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \left(-\hbar \Delta(t) \sum_{j=1}^N \hat{\sigma}_{rr}^j + \frac{\hbar \Omega}{2} \sum_j^N (\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j) + \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \right) e^{-if(t) \sum_j \hat{\sigma}_{rr}^j - it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \quad (3.23)$$

The first and third term in the Hamiltonian will commute with unitary transformation operator, leading to

$$e^{if(t) \sum_j \hat{\sigma}_{rr}^j + it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \left(\frac{\hbar \Omega}{2} \sum_j^N (\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j) \right) e^{-if(t) \sum_j \hat{\sigma}_{rr}^j - it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} - \hbar \Delta(t) \sum_{j=1}^N \hat{\sigma}_{rr}^j + \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \quad (3.24)$$

Now consider the first term the equation above,

$$e^{if(t) \sum_j \hat{\sigma}_{rr}^j + it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \left(\frac{\hbar \Omega}{2} \sum_j^N (\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j) \right) e^{-if(t) \sum_j \hat{\sigma}_{rr}^j - it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \quad (3.25)$$

First taking single body terms together

$$\frac{\hbar \Omega}{2} \sum_j^N e^{if(t) \sum_j \hat{\sigma}_{rr}^j} \left(\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j \right) e^{-if(t) \sum_j \hat{\sigma}_{rr}^j}$$

It can be shown that,

$$e^{if(t) \hat{\sigma}_{rr}^i} (\hat{\sigma}_{rg}^i) e^{-if(t) \hat{\sigma}_{rr}^i} = e^{if(t)} \hat{\sigma}_{rg}^i$$

and

$$e^{if(t) \hat{\sigma}_{rr}^i} (\hat{\sigma}_{gr}^i) e^{-if(t) \hat{\sigma}_{rr}^i} = e^{-if(t)} \hat{\sigma}_{gr}^i$$

$$\frac{\hbar \Omega}{2} \sum_j^N e^{if(t) \sum_j \hat{\sigma}_{rr}^j} \left(\hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j \right) e^{-if(t) \sum_j \hat{\sigma}_{rr}^j} = \frac{\hbar \Omega}{2} \sum_j^N e^{if(t)} \hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j e^{-if(t)}$$

substituting above equations in Eqn 3.19, we get,

$$e^{it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \left(\frac{\hbar \Omega}{2} \sum_j^N (\hat{\sigma}_{rg}^j e^{if(t)} + \hat{\sigma}_{gr}^j e^{-if(t)}) \right) e^{-it \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \quad (3.26)$$

To do further calculations, let's first simplify following term,

$$\begin{aligned}
e^{\frac{it}{2} \sum_{i,j}^{i \neq j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} &= \left(e^{\frac{it}{2} \sum_{j \neq 1} V_{1j} \hat{\sigma}_{rr}^1 \hat{\sigma}_{rr}^j} \right) \left(e^{\frac{it}{2} \sum_{j \neq 2} V_{2j} \hat{\sigma}_{rr}^2 \hat{\sigma}_{rr}^j} \right) \dots \left(e^{\frac{it}{2} \sum_{j \neq N} V_{1N} \hat{\sigma}_{rr}^N \hat{\sigma}_{rr}^j} \right) \\
&= \left(\prod_{j \neq 1} e^{\frac{it}{2} V_{1j} \hat{\sigma}_{rr}^1 \hat{\sigma}_{rr}^j} \right) \left(\prod_{j \neq 2} e^{\frac{it}{2} V_{2j} \hat{\sigma}_{rr}^2 \hat{\sigma}_{rr}^j} \right) \dots \left(\prod_{j \neq 1} e^{\frac{it}{2} V_{Nj} \hat{\sigma}_{rr}^N \hat{\sigma}_{rr}^j} \right)
\end{aligned}$$

From every product, which contains sum over j , only one term will not commute with $\hat{\sigma}_{rg}^k$, i.e. when $j = k$. All other terms will commute with $\hat{\sigma}_{rg}^k$ and cancel the term on the other side of $\hat{\sigma}_{rg}^k$

$$\begin{aligned}
&\left(e^{\frac{it}{2} V_{1k} \hat{\sigma}_{rr}^1 \hat{\sigma}_{rr}^k} \right) \left(e^{\frac{it}{2} V_{2k} \hat{\sigma}_{rr}^2 \hat{\sigma}_{rr}^k} \right) \dots \left(e^{\frac{it}{2} V_{Nk} \hat{\sigma}_{rr}^N \hat{\sigma}_{rr}^k} \right) \hat{\sigma}_{rg}^k \left(e^{-\frac{it}{2} V_{1k} \hat{\sigma}_{rr}^1 \hat{\sigma}_{rr}^k} \right) \left(e^{-\frac{it}{2} V_{2k} \hat{\sigma}_{rr}^2 \hat{\sigma}_{rr}^k} \right) \dots \left(e^{-\frac{it}{2} V_{Nk} \hat{\sigma}_{rr}^N \hat{\sigma}_{rr}^k} \right) \\
&\prod_{j, j \neq k} \left(e^{\frac{it}{2} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \right) \hat{\sigma}_{rg}^k \prod_{j, j \neq k} \left(e^{-\frac{it}{2} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \right) \\
&e^{\frac{it}{2} \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \hat{\sigma}_{rg}^k e^{-\frac{it}{2} \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k}
\end{aligned}$$

Here we have reduced double summation to a summation over single index.

$$e^{it \sum_{i,j}^{i \neq j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} \hat{\sigma}_{rg}^k e^{-it \sum_{i,j}^{i \neq j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j} = e^{it \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \hat{\sigma}_{rg}^k e^{-it \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k}$$

Using this in Eqn 3.20 we get,

$$e^{it \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \left(\frac{\hbar \Omega}{2} \sum_k^N (\hat{\sigma}_{rg}^k e^{if(t)} + \hat{\sigma}_{gr}^k e^{-if(t)}) \right) e^{-it \sum_j^{j \neq k} V_{jk} \hat{\sigma}_{rr}^j \hat{\sigma}_{rr}^k} \quad (3.27)$$

Define a new operator

$$\hat{M} = \sum_{k \neq l} V_{lk} \hat{\sigma}_{rr}^k$$

Consider first term in Eqn 3.21

$$e^{it \hat{M} \hat{\sigma}_{rr}^k} \hat{\sigma}_{rg}^k e^{-it \hat{M} \hat{\sigma}_{rr}^k}$$

Using Baker-Hausdorff property

$$e^{itM\hat{\sigma}_{rr}^k}\hat{\sigma}_{rg}^ke^{-itM\hat{\sigma}_{rr}^k} = \hat{\sigma}_{rg}^k + it[M\hat{\sigma}_{rr}^k, \hat{\sigma}_{rg}^k] + \frac{(it)^2}{2!} \left[M\hat{\sigma}_{rr}^l, [M\hat{\sigma}_{rr}^k, \hat{\sigma}_{rg}^k] \right] + \dots$$

Calculating all the commutators first,

$$[M\hat{\sigma}_{rr}^k, \hat{\sigma}_{rg}^k] = M[\hat{\sigma}_{rr}^k, \hat{\sigma}_{rg}^k] = M\hat{\sigma}_{rg}^k$$

$$\left[M\hat{\sigma}_{rr}^l, [M\hat{\sigma}_{rr}^k, \hat{\sigma}_{rg}^k] \right] = \left[M\hat{\sigma}_{rr}^l, M\hat{\sigma}_{rg}^k \right] = M^2\hat{\sigma}_{rg}^k$$

Therefore,

$$e^{itM\hat{\sigma}_{rr}^k}\hat{\sigma}_{rg}^ke^{-itM\hat{\sigma}_{rr}^k} = \hat{\sigma}_{rg}^k + itM\hat{\sigma}_{rg}^k + \frac{(it)^2}{2!}M^2\hat{\sigma}_{rg}^k + \dots = \hat{\sigma}_{rg}^ke^{itM}$$

and similarly,

$$e^{itM\hat{\sigma}_{rr}^k}\hat{\sigma}_{gr}^ke^{-itM\hat{\sigma}_{rr}^k} = \hat{\sigma}_{gr}^k - itM\hat{\sigma}_{gr}^k + \frac{(it)^2}{2!}M^2\hat{\sigma}_{gr}^k + \dots = \hat{\sigma}_{gr}^ke^{-itM}$$

Substituting all this in Eqn 3.18 we get,

$$\begin{aligned} U(t)H(t)U^\dagger(t) &= \frac{\hbar\Omega}{2} \sum_j^N e^{if(t)+it\sum_{k \neq j} V_{jk}\hat{\sigma}_{rr}^k} \hat{\sigma}_{rg}^j + \hat{\sigma}_{gr}^j e^{-if(t)-it\sum_{k \neq j} V_{jk}\hat{\sigma}_{rr}^k} \\ &\quad - \hbar\Delta(t) \sum_{j=1}^N \hat{\sigma}_{rr}^j + \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j \end{aligned} \quad (3.28)$$

and

$$i\hbar U\dot{U}^\dagger = \hbar(\Delta_0 + \delta \sin \omega_0 t) \sum_j \hat{\sigma}_{rr}^j - \sum_{i < j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j$$

Therefore, $H'(t) = U(t)H(t)U^\dagger(t) - i\hbar U\dot{U}^\dagger$ becomes,

$$H'(t) = \frac{\hbar\Omega}{2} \sum_j^N \left[\hat{\sigma}_{rg}^j e^{if(t)+it\sum_{k \neq j} V_{jk}\hat{\sigma}_{rr}^k} + \hat{\sigma}_{gr}^j e^{-if(t)-it\sum_{k \neq j} V_{jk}\hat{\sigma}_{rr}^k} \right] \quad (3.29)$$

After resubstituting for $f(t)$ and using the Jacobi-Anger expansion $e^{\pm iz \cos \omega_0 t} = \sum_{m=-\infty}^{\infty} J_m(z) e^{\pm im[\omega_0 t + \pi/2]}$ we get the Equation 3.3 in the main text.

In order to obtain Equation 3.13 of the main text, we first simplify the equation for N particles and then write it for the two-particle case. For that, we simplify the following term as

$$\begin{aligned}
e^{it \sum_{k \neq j} V_{jk} \hat{\sigma}_{rr}^k \hat{\sigma}_{rr}^j} &= \prod_{k \neq j} e^{it V_{jk} \hat{\sigma}_{rr}^k \hat{\sigma}_{rr}^j} = \prod_{k \neq j} \sum_{n=0}^{\infty} \frac{(it V_{jk} \hat{\sigma}_{rr}^k \hat{\sigma}_{rr}^j)^n}{n!} \\
&= \prod_{k \neq j} [\hat{\sigma}_{rr}^k \hat{\sigma}_{rr}^j (e^{it V_{jk}} - 1) + 1]
\end{aligned}$$

Substituting this into Equation 3.23 and doing further simplification we get the Hamiltonian in the following format,

$$H'(t) = \frac{\hbar\Omega}{2} \sum_j^N \left[\hat{\sigma}_{rg}^j e^{if(t)} \left(\prod_{k \neq j} [\hat{\sigma}_{rr}^k (e^{it V_{jk}} - 1) + 1] \right) + \hat{\sigma}_{gr}^j e^{-if(t)} \left(\prod_{k \neq j} [\hat{\sigma}_{rr}^k (e^{-it V_{jk}} - 1) + 1] \right) \right] \quad (3.30)$$

Writing this Hamiltonian for the case of two atoms , i.e. $N = 2$ we get,

$$H'^{(2)}(t) = \frac{\hbar\Omega}{2} [\hat{\sigma}_{rg}^1 e^{if(t)} (\hat{\sigma}_{rr}^2 (e^{it V_0} - 1) + 1) + \hat{\sigma}_{gr}^1 e^{-if(t)} (\hat{\sigma}_{rr}^2 (e^{-it V_0} - 1) + 1) +$$

$$\hat{\sigma}_{rg}^2 e^{if(t)} (\hat{\sigma}_{rr}^1 (e^{it V_0} - 1) + 1) + \hat{\sigma}_{gr}^2 e^{-if(t)} (\hat{\sigma}_{rr}^1 (e^{-it V_0} - 1) + 1)]$$

Rearranging the terms we get,

$$\begin{aligned}
H'^{(2)}(t) &= \frac{\hbar\Omega}{2} [(\hat{\sigma}_{rg}^1 \hat{\sigma}_{rr}^2 + \hat{\sigma}_{rg}^2 \hat{\sigma}_{rr}^1) e^{if(t)} (e^{it V_0} - 1) + (\hat{\sigma}_{gr}^1 \hat{\sigma}_{rr}^2 + \hat{\sigma}_{gr}^2 \hat{\sigma}_{rr}^1) e^{-if(t)} (e^{-it V_0} - 1) \\
&\quad + (\hat{\sigma}_{rg}^1 + \hat{\sigma}_{rg}^2) e^{if(t)} + (\hat{\sigma}_{gr}^1 + \hat{\sigma}_{gr}^2) e^{-if(t)}] \quad (3.31)
\end{aligned}$$

Here, the first two terms correspond to the process in which any one of the atoms remains in the excited state and the other atom makes the transition from ground to excited state or vice versa. The last two terms correspond to single atom terms representing the Rabi oscillations.

Chapter 4

Single excitation dynamics in an atomic chain coupled to a PCW

4.1 Introduction

The hybrid quantum systems consisting of dielectric structures such as nanofibers, nanowires, photonic crystal waveguides (PCW) in combination with atomic systems such as ultracold atoms, plasmons have emerged as an effective tool to engineer strong light-matter interaction [83–86]. The dielectric structures used in these systems allow one to control and modify the propagation of light which is crucial for engineering the strong light-matter interaction. This strong coupling between light and matter has application in quantum information protocols where it's used to achieve entanglement between different nodes of a quantum information network [87]. The logic gates implemented using cavity-assisted interaction have also been demonstrated [88]. On the more fundamental side, these hybrid systems are used to explore the physics of quantum many-body systems. These systems have been shown to demonstrate strongly correlated effects such as quantum phase transitions of Hubbard models or spin models, Dicke quantum phase transition [89–92]. Also, the spin models where the range and the strength of the interaction can be controlled, giving rise to interesting phenomena such as topological order, frustrated magnetism are implemented using these hybrid systems[93, 94]. Recently, the atoms trapped near photonic crystal waveguides (PCW) have shown to give rise to effective long-range spin Hamiltonian with long-range interactions mediated by photons [95]. The range and the strength of this long-range interaction can be tuned by varying the external laser parameters or by varying the properties of PCW.

In this chapter, we look at the dynamics of excitation in a chain of single atoms coupled to a PCW. The excitations are exchanged with other ground-state atoms via locally induced cavity modes. The strength of the exchange interaction decay exponentially over distance, with a high tunability over the range of interactions [95]. An initially localized single excitation undergoes quantum diffusion, and the properties of the excitation dynamics depend crucially on the range of the exchange interaction. For instance, for short-range exchange couplings, the long-time probability distribution (LTPD) for the position of an excitation exhibits the features of a continuous-time quantum walk (CTQW) [96–102]. In contrast, for the long-range, LTPD displays quasi-localization and tailing behavior. A better understanding of the excitation dynamics is accessed through excess kurtosis and inverse participation ratio (IPR). Interestingly, IPR reveals to us that the single excitation dynamics is super-ballistic at the very initial stage of the quantum diffusion due to the initially localized state of the excitation, whereas, at longer times, it is ballistic. The initially localized excitation being a source of entangled pairs of quasi-particles with opposite momenta, correlates different parts of the atomic array during the time evolution. We quantify the correlation via the bipartite entanglement entropy for which the system is divided into two equal parts. Interestingly, we found that the entanglement entropy generated by a single excitation is globally bounded, independently of the system size. The single excitation scenario we discuss here can be related to an impurity in a quantum spin chain, with its relevance in entanglement or quantum state transfer [103]. On the other hand, the photon transport is studied using an identical setup [104, 105].

4.2 Setup and Model

Our work is motivated by the recent developments in coupling atoms to a PCW, and in particular, based on the setup described in Ref. [95]. We consider a one-dimensional setup, which consists of an array of N two-level atoms with a ground state $|g\rangle$ and an excited $|e\rangle$, trapped near a PCW and arranged along waveguide longitudinal z -axis as shown in Fig. [4.1(a)]. The combination of forces arising from the Casimir-Polder effect and far off-resonant trap (FORT) gives rise to electric field intensity minima which can be used for trapping the atoms near PCW [10]. Additionally, an external optical lattice can also be used for trapping the atom as proposed in ref [94]. We assume deep potential wells so that the center of mass

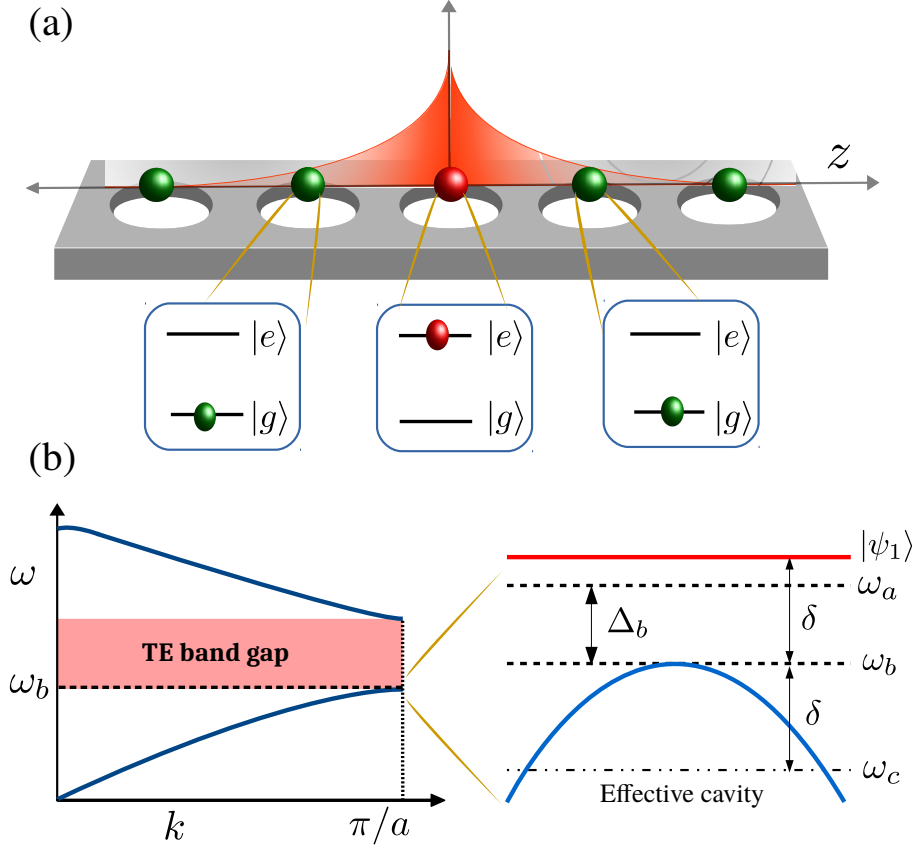


Figure 4.1: (Color online) (a) Atomic lattice and PC setup. An exponentially decaying single-photon profile is depicted at the position of the central atom and mediated by it, the excitation can be exchanged to other ground state atoms. (b) Band structure of a PC, with the atom-band edge detuning $\Delta_b = \omega_a - \omega_b$ where ω_a is the atomic resonance frequency, and ω_b provides the lowest band edge. ω_c is the effective cavity mode frequency with an effective detuning δ . The eigenfrequency ω of the atom-photon bound state $|\psi_1\rangle$ lies in the bandgap.

motion of the atoms can be neglected, and they remain in their respective lattice sites $j = 1, \dots, N$.

The atomic resonant frequency ω_a lies in the bandgap of the PCW, with a detuning $\Delta_b = \omega_a - \omega_b$ from the lowest band edge ω_b Fig. [4.1(b)]. Other band edges are assumed very far from ω_a , and therefore, only the modes close to ω_b play an important role. The dispersion can then be approximated as $\epsilon_k \approx \epsilon_b[1 - \alpha(k - k_0)^2/k_0^2]$, where k_0 is the band edge wave number, and α determines the band curvature. These modes are of Bloch form due to the periodic structure of the PCW, with electric field $E_{k_0}(z) = e^{ik_0z}u_{k_0}(z)$. The Hamiltonian that describes a single two-level

atom trapped at $z = 0$ coupled to the PCW reads,

$$\hat{H} = \hbar\epsilon_a\hat{\sigma}_{ee} + \hbar \int dk \epsilon_k \hat{a}_k^\dagger \hat{a}_k + \hbar g \int dk (\hat{\sigma}_{eg} \hat{a}_k E_k(0) + h.c.), \quad (4.1)$$

where the atomic operators $\hat{\sigma}_{\alpha\beta} = |\alpha\rangle\langle\beta|$ with $\alpha, \beta \in \{e, g\}$ and $\hat{a}_k$ ($\hat{a}_k^\dagger$) is an annihilation (creation) operator of a photon in the k^{th} mode. The atom-light coupling constant is $g = d_{eg}\sqrt{\epsilon_b/4\pi\hbar\epsilon_0 A}$ with d_{eg} being the atomic dipole moment, and A is the mode cross-sectional area [10]. The first term in the Hamiltonian describes the atomic energy of the atom. The second term represents the energy of the photonic mode while the third term is the interaction between atom and electric field mode.

In the single excitation sector of the system, there exists a bound eigenstate ($\hat{H}|\psi_1\rangle = \hbar\omega|\psi_1\rangle$) in which the atom is dressed by a localized excitation of the photonic mode. The eigenfrequency ω lies at the bandgap with a detuning $\delta = \omega - \epsilon_b$, and it has been shown that the eigenenergy can be approximately obtained from the positive root of $(\delta - \Delta)\sqrt{\delta} = \beta^{3/2}$ with $\beta = (\pi g^2 |u_{k_0}(0)|^2 k_0 / \sqrt{4\alpha\epsilon_b})^{2/3}$ [95]. The single excitation bound state is of the form: $|\psi_1\rangle = \cos\theta|e\rangle|0\rangle + \sin\theta|g\rangle|1\rangle$, where the atom is dressed by a localized photon: $|1\rangle = \int dk c_k \hat{a}_k^\dagger |0\rangle$ around the atomic position and has the spatial wave function

$$\phi_K(z) = \sqrt{\frac{2\pi}{L}} e^{-|z|/L} E_{k_0}(z). \quad (4.2)$$

The length scale, $L = \sqrt{\alpha\epsilon_b/(k_0^2\delta)}$ quantifies the exponential decay of the photon probability from the atomic position. Interestingly, one can map this scenario to that of an atom-cavity system with a cavity length L , cavity mode frequency $\omega_c = \omega_b - \delta$, effective atom-cavity coupling $g_c = g\sqrt{2\pi/L}$, and an effective detuning $\Delta_c = \Delta_b + \delta$ Fig. [4.1(b)]. With all these, the state $|\psi_1\rangle$ is mapped onto the corresponding dressed state in the Jaynes-Cummings model. Now extending to an array of atoms with positions z_j , and assuming the far-detuned limit: $\Delta_c \gg \beta$, the weakly populated photonic modes can be adiabatically eliminated. This leads to a dipole-dipole exchange Hamiltonian for the atomic excitations of the form,

$$\hat{H}_{ex} = J \sum_{j,l}^N \hat{\sigma}_{eg}^j \hat{\sigma}_{ge}^l f(z_j, z_l), \quad (4.3)$$

where the exchange coupling strength reads $J = \hbar g_c^2 / \Delta_c$. We take J as a constant and explore the effect of L on the excitation dynamics, which appears in the exponential function, $f(z_j, z_l) = \exp(-|z_j - z_l|/L) E_{k_0}^*(z_j) E_{k_0}(z_l)$. Taking lattice spacing as twice the length of the PCW unit cell, we have $E_{k_0}(z_j) = 1$ at atomic locations

[106]. As we can see that the range of the exchange interactions, L , can be controlled by tuning the band structure of the PCW.

In the following sections, we analyze the coherent dynamics induced by the exchange Hamiltonian in Eq. 4.3, for a single excitation. We analyze the effect of L on the dynamics of excitation. To characterize the changes in the dynamics we use various parameters such as IPR, kurtosis, Shannon entropy, and population imbalance.

4.3 Excitation Dynamics & Characterization

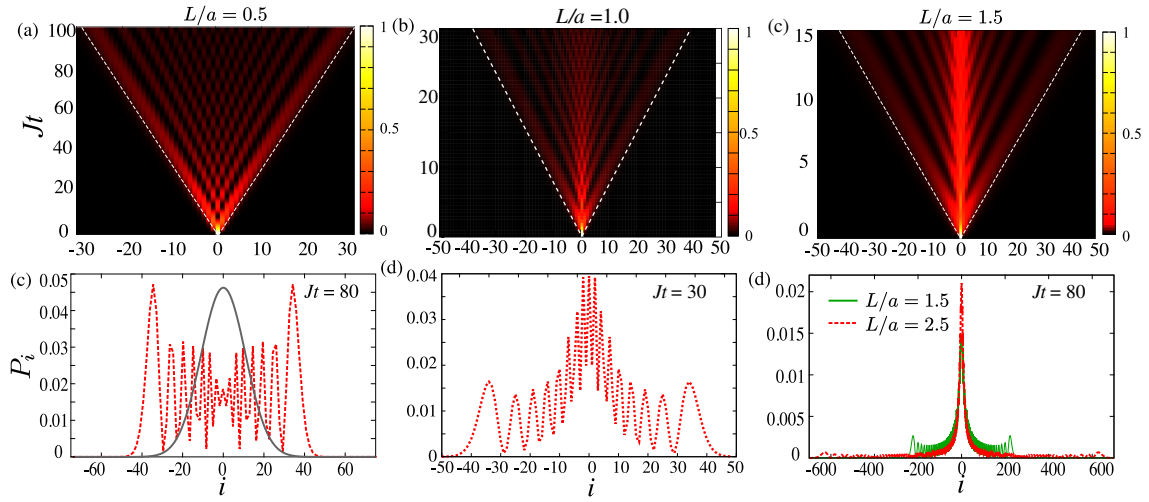


Figure 4.2: (Color online) (a-c) The probability density P_i as a function of lattice index i and time t for $L/a = 0.5, 1.0$ and 1.5 . Dashed white lines mark the region bounded by $|i|a/v_g^{max}$. (c-e) Dashed red line shows P_i vs i for respective L values. The solid grey line shows the Gaussian probability distribution of a classical random walker.

We study the single excitation dynamics by numerically solving the Schrödinger equation: $i\partial|\psi(t)\rangle/\partial t = H_{ex}|\psi(t)\rangle$ ($\hbar = 1$). We assume the excitation is initially localized at the center of the lattice, and evolve the system up to various times before the excitation probability hits the boundary of the lattice. The Hamiltonian H_{ex} preserves the number of excitations, and we can truncate the Hilbert space to the subspace of N singly excited states $\{|i\rangle \equiv |\dots g^{i-1} e^i g^{i+1} \dots\rangle, i = 1, 2, \dots, N\}$. The probability of finding an excitation at site i is given by $P_i(t) = |\langle i|\psi(t)\rangle|^2$. The single excitation spectrum ϵ_k of the Hamiltonian $\hat{H}_{ex}$ Eq. 4.3 is obtained as [4.6.1]

$$\epsilon_k = J \frac{(\cos ka - e^{-a/L})}{\cosh(a/L) - \cos ka}, \quad (4.4)$$

From which, the group velocity is obtained as $v_g = \partial\epsilon_k/\partial k$. The maximum of the group velocity and the momentum (q) values corresponding to it is given by

$$v_g^{max} = \left(\frac{d\epsilon_k}{dk} \right)_{max} = -Ja \frac{\sinh(a/L) \sin(qa)}{[\cosh(a/L) - \cos(qa)]^2}, \quad (4.5)$$

where

$$q = \frac{1}{a} \cos^{-1} \left[\frac{1}{2} \left(\sqrt{\cosh^2(a/L) + 8} - \cosh(a/L) \right) \right].$$

Fig.[4.2] shows the dynamics of the excitation for various values of exchange interaction range L . For small values of L , the exchange interaction beyond the nearest neighbor can be neglected. Hence the Hamiltonian is the same as that with only the nearest neighbor exchange. For such a case, we can see the spreading of the excitation across the lattice captured by the probability distribution $P_i(t)$ in Fig.[4.2 a]. For a given instance of time, the probability distribution is the same as that of CTQW, with the maximum value at the edge of the distribution Fig.[4.2 c] [98, 99, 101]. This is drastically different from the classical random walk for which the probability distribution is a Gaussian wavefunction with the maximum at the center of the distribution Fig.[4.2 c] (grey line). This fundamental difference in the probability distribution can be attributed to the properties such as superposition and quantum interference which are inherent to CTQW. The spreading of the excitation is bounded the lines given by $t = |i|a/v_g^{max}$, where v_g^{max} is the maximum group velocity for a given L obtained from the Eq. 4.5. Beyond this region, the probability of finding an excitation decays exponentially.

4.3.1 Quasi-localization and Tailing

Interestingly, as L increases, especially when $L > a$, the LTPD gets modified drastically as shown in Fig.[4.2(b-d)]. For large L , the excitation can get exchanged at a larger distance. Hence we expect the faster diffusion of the excitation. But surprisingly it exhibits a quasi-localization behavior, in which there is a higher probability of finding an excitation at the center of the lattice (initial position). This indicates slower diffusion of the excitation with a long tail at all times. At a given instant, an increment in L makes the central peak sharper with higher values and makes the tail longer Fig. [4.2 d]. The speed of propagation of the tail increases with an increase in L . Despite having a qualitative change in the shape of LTPD for large L , the probability distribution is still bounded by the straight lines of the form $t = |i|a/v_g^{max}$ (dashed white lines in Fig. [4.2 (a-c)]). Although for the large L values, the value

of maximum group velocity increases monotonously as shown in Fig. [4.3 d], unlike the power-law hoppings of the form $1/r^\alpha$, the group velocity never diverges at any value of L , confirming the presence of bounds on the excitation propagation.

This quasi-localization and fast-moving tail observed at large L can be understood with the help of energy spectrum ϵ_k . For large values of L , the spectrum gets flatter near the end of the Brillouin zone Fig. [4.3 c]. Which results in a vanishingly small group velocity for the modes near the end of the Brillouin zone. Since the initial state is an equal superposition of all the modes, these slow group velocity modes reduce the rate of diffusion, resulting in the peak at the initial position, also called quasi-localization. The fast-moving tail is due to the modes at the center of the Brillouin zone with the higher group velocity. As shown in Fig. [4.3 d], the k value of the mode corresponding to the highest group velocity tends to zero with increasing L , indicating that the tailing behavior is due to large wavelength modes.

For all the values of L , the spread of the probability distribution Δz remains a linear function of time such that $\Delta z = \beta(L)t$. The function $\beta(L)$ can be obtained from the dispersion relation in large N limit [107] as,

$$(\Delta z)^2 = \langle z^2 \rangle(t) = \left[\frac{a}{2\pi} \int_{BZ} \left(\frac{d\epsilon_k}{dk} \right)^2 dk \right] t^2 \quad (4.6)$$

where BZ stands for the first Brillouin zone. As shown in Fig. [4.3 b], $\beta(L)$ increases monotonously with L , indicating the ballistic diffusion of excitation for all the values of L . Results obtained from the numerics are in excellent agreement with analytical expression for $\beta(L)$ given by,

$$\beta(L) = aJ \sqrt{\frac{\coth(a/L)}{2 \sinh^2(a/L)}}, \quad (4.7)$$

4.3.2 Kurtosis and Inverse participation ratio

To gain a comprehensive picture of the excitation dynamics, and to characterize the behavior of the LTPD as a function of L , we look at both the excess kurtosis of the probability distribution and the inverse participation ratio (IPR).

Kurtosis:—In probability theory, the excess kurtosis (κ) is used to characterize the “tailedness” of the probability distribution. It is defined as

$$\kappa = \frac{\langle (z - \langle z \rangle)^4 \rangle}{\langle (z - \langle z \rangle)^2 \rangle^2} - 3. \quad (4.8)$$

The first term in Eq. (4.8) is the normalized 4-th central moment of the probability distribution while the factor of 3 comes from the Kurtosis value of the standard

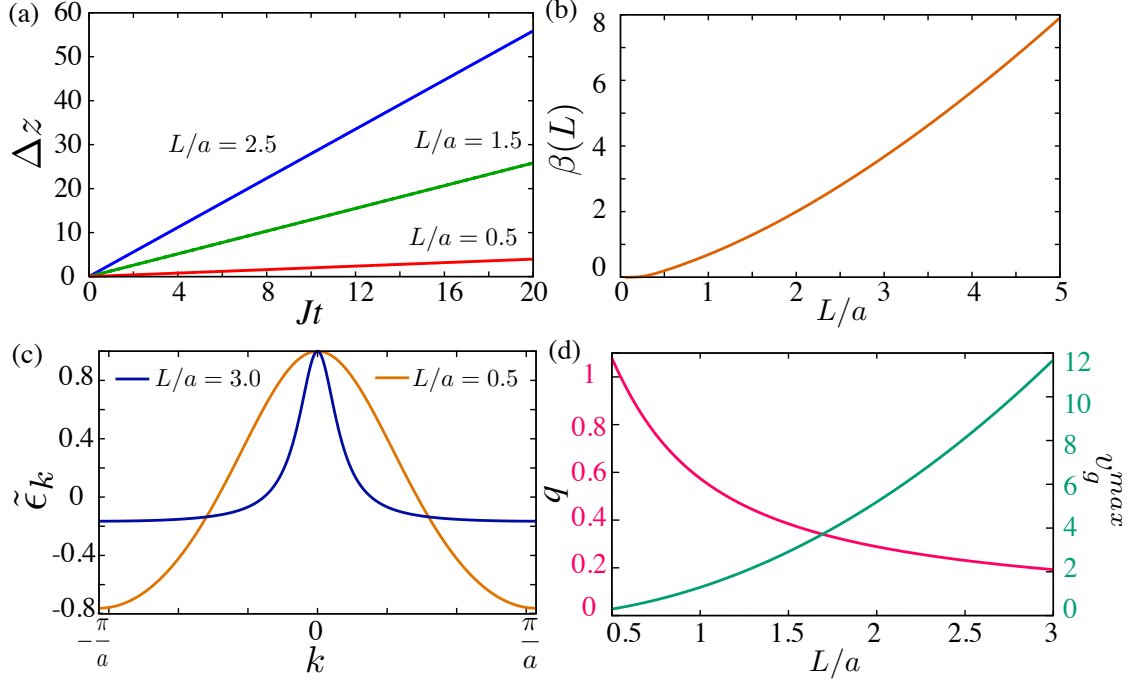


Figure 4.3: (Color online) (a) The spread Δz of the distribution as a function of time for different L values. (b) The $\beta(L)$, the rate at which the spread of the distribution increases in time, as a function of L . (c) The spectrum $\tilde{\epsilon}_k = \epsilon_k/|\epsilon_{k=0}|$ vs k in the first Brillouin zone for different L . For large L , the energy band becomes increasingly flat near the edges of the Brillouin zone and steeper at very low momenta, giving rise to quasi-localization and tailing behavior in LTPD. (d) maximum group velocity and corresponding k values as a function of L . Increase in L increases v_g^{max} monotonously and the corresponding k tends to the center of the Brillouin zone

normal distribution. A positive-valued κ implies that distribution has a longer tail as compared to a standard normal distribution for which $\kappa = 0$. Similarly, $\kappa < 0$ corresponds to distributions having a fast decaying tail compared to a standard normal distribution. In the context of single excitation dynamics discussed above, a significantly large and positive κ implies a (quasi) localized state with a longer tail, whereas a negative κ signifies a typical CTQW profile with a fast decaying tail. Fig. [4.4 a] shows the time dependence of κ for different values of L . κ decreases in time after an initial transient, and asymptotically ($t \rightarrow \infty$) approaches a constant value (κ_a) when the probability distribution has properly evolved. A constant κ_a at longer times indicates that the shape of the probability distribution remains intact even though its spread increases in time. Hence we can use κ_a to quantify the characteristic change in the probability distribution as a function of L . The excess kurtosis κ_a exhibits a smooth crossover (around $L/a \sim 1.3$) from a negative to a

positive value as a function of L Fig. [4.4 b]. For large L , it increases linearly with L . An analytic expression for the kurtosis is obtained in the large N limit using the relation,

$$\langle z^4 \rangle(t) = \frac{a}{2\pi} \int_{BZ} \left[t^2 \left(\frac{d^2 \epsilon_k}{dk^2} \right)^2 + t^4 \left(\frac{d\epsilon_k}{dk} \right)^4 \right] dk, \quad (4.9)$$

and we get,

$$\kappa(t) = \frac{2[2 + \cosh^2(a/L)] \tanh(a/L)}{(Jt)^2} + \frac{3[1 + 2 \cosh^2(a/L)]}{\sinh(2a/L)} - 3, \quad (4.10)$$

The first term is a transient term responsible for higher values of k at short times. This term disappears in a long time limit, which gives us,

$$\lim_{t \rightarrow \infty} \kappa(t) = \kappa_a = \frac{3[1 + 2 \cosh^2(1/L)]}{\sinh(2/L)} - 3$$

and it agrees exactly with the numerical results for sufficiently large N . For a large L , the asymptotic kurtosis, $\kappa_a \approx 9L/(4a) - 3$, depends linearly on L as expected. The derivation for the analytical results for the kurtosis and the eigenspectrum are given in Appendix 4.6.1.

IPR:— Interestingly, the inverse participation ratio (IPR),

$$\Pi_1(t) = \frac{1}{\sum_i P_i^2} - 1 \quad (4.11)$$

captures some finer details of the dynamics, especially at the initial stage of the diffusion, which are not captured by other parameters. For a completely localized excitation at the center of the lattice, we have $P_{N/2} = 1$ and $\{P_i = 0, i \neq N/2\}$ making $\Pi_1 = 0$ and for a completely delocalized case, we get the uniform distribution with $P_i = 1/\sqrt{N}$ making $\Pi_1 = N - 1$, which suggests that Π_1 can be interpreted as a sort of a length scale over which the excitation is delocalized. As previously discussed, the linear dependence of the width of the probability distribution with time ($\Delta z \propto t$) indicates that the diffusion is ballistic at any instant of time. However, IPR predicts that at the very initial stage of the time evolution, i.e., for times $Jt \leq 1$, we have $\Pi_1(t) \propto t^2$, indicating a super ballistic diffusion Fig. [4.4 c]. At larger times, $\Pi_1(t) \propto t$, the diffusion is ballistic. The transient super-ballistic nature of IPR is due to the initially localized state of the excitation [108]. Further, at a given instant of time, IPR is larger for large L in the super ballistic regime, but in the ballistic regime, IPR increases with L and then decreases for large L due to the quasi-localization. This can be observed in Fig [4.4 c], where for $L/a = 5$, in superballistic regime, IPR is higher than $L/a = 1.5$ values, however in the ballistic regime it is less than $L/a = 1.5$.

4.3.3 Population imbalance and Shannon entropy

Population imbalance :- We define another parameter named edge-center population imbalance to quantify the characteristic change in the single excitation LTPD occurring for a large value of L . For small values of L , the maximum of the probability distribution is closer to the edge of the distribution. For increasing L , the maximum of the distribution shifts to the center of the distribution at the initial position of excitation. This characteristic change in the population at the center and at the edge of the distribution can be quantified using the edge-center population imbalance defined as,

$$\zeta(L) = \frac{1}{\tau_d} \int_{\tau_{min}}^{\tau_{max}} \frac{P_c(t) - P_e(t)}{P_c(t) + P_e(t)} dt \quad (4.12)$$

where we define $\tau_d = \tau_{max} - \tau_{min}$ with $\tau_{min} = 1/(J \exp(-1/L))$ and $\tau_{max} = 20/(J \exp(-1/L))$. $P_e(t)$ is the probability at the first maximum from the left/right of the distribution and $P_c(t)$ is the probability at the center of the distribution at time t . The integration time scales $\tau_{min} = 1/(J \exp(-1/L))$ is set up by the nearest neighbor exchange coupling strength. For small values of L , the maximum of the probability distribution is at the edge of the distribution during the entire time evolution, resulting in $P_c(t) < P_e(t)$ and hence negative ζ . For large values of L , the population is maximum at the center of the lattice due to quasi-localization making $P_c(t) \gg P_e(t)$ and hence $\zeta \approx 1$. The crossover from the negative to positive values of $\zeta(L)$ indicates the change in the likelihood of finding the excitation from the edge to center respectively. Fig [4.4 d] shows the variation of ζ as a function of L . ζ changes sign from negative to positive around $L/a = 1$.

Shannon entropy :- The temporal growth of the Shannon entropy defined as,

$$S_{Shannon}(t) = - \sum_{i=1}^N P_i(t) \ln P_i(t) \quad (4.13)$$

provides insight into the diffusion dynamics of excitation in the lattice. Similar to IPR, it measures the extent of delocalization of excitation over the lattice. At $t = 0$, excitation is completely localized at the center of the lattice making $P_{N/2}(0) = 1$ and $P_i(0) = 0$ for $i \neq N/2$ and hence leading to $S_{Shannon}(0) = 0$. For $t > 0$ excitation delocalizes over the lattice sites making other P_i 's non-zero. This leads to the temporal growth of the Shannon entropy as shown in Fig.[4.5 a]. For $L/a < 1$, the exchange coupling is short-range, leading to slow delocalization of excitation

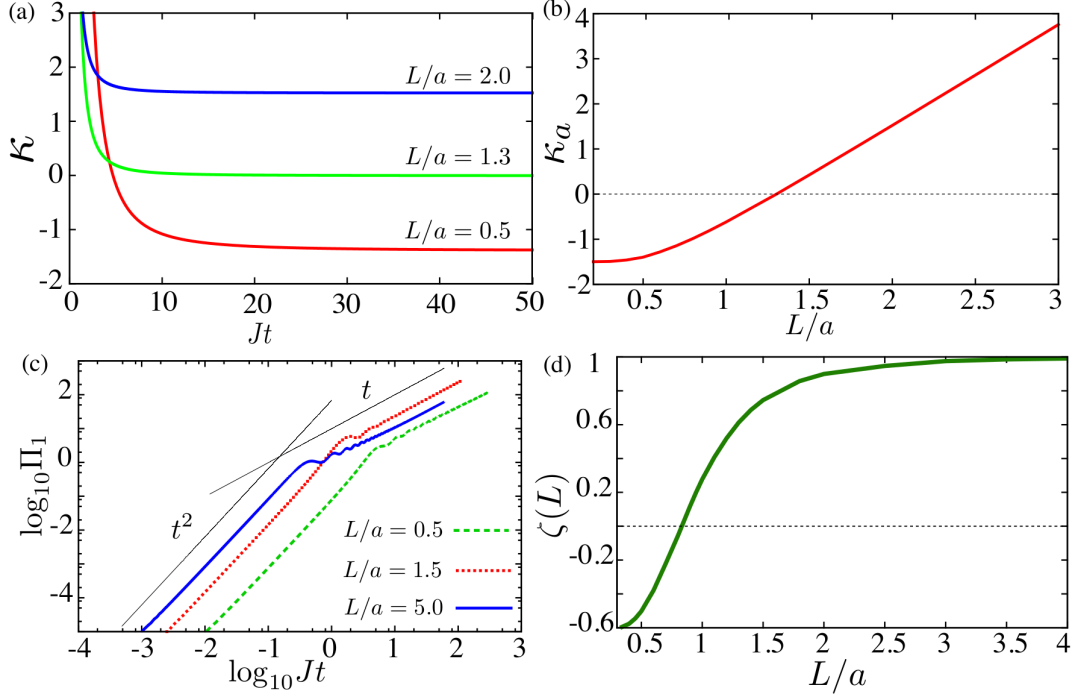


Figure 4.4: (Color online) (a) The time evolution of excess kurtosis κ for $L/a=0.5, 1.3$ and 2.0 for $N = 2001$. (b) Shows the asymptotic behavior of the excess kurtosis κ_a as a function of L . The positive κ_a for $L/a > 1.33$ characterizes the quasi-localization, and negative κ_a implies CTQW dynamics. (c) IPR $[\Pi_1(t)]$ vs time for different L . The solid thin lines symbolically show the t^2 and t behavior, indicating the super-ballistic at short times and ballistic diffusion at longer times, respectively. (d) The edge-center population imbalance parameter as function of L . The crossover from positive to negative values quantifies the change in the shape of the probability distribution.

and hence the slower growth of the Shannon entropy. For an intermediate value of L , excitation delocalizes rapidly leading to the faster growth of Shannon entropy. For large values of L , at small t , entropy grows faster due to the fraction of modes with the high group velocity. At larger t , due to slow propagating modes, the quasi-localization takes place leading to the suppression of delocalization and hence the suppression of the Shannon entropy. As shown in Fig.[4.5 b], the value of Shannon entropy at a fixed time $Jt = 15, 20$, and 30 as a function of L . As we can see, after a certain value of L , the value of Shannon entropy decreases with an increase in L for all times due to quasi-localization.

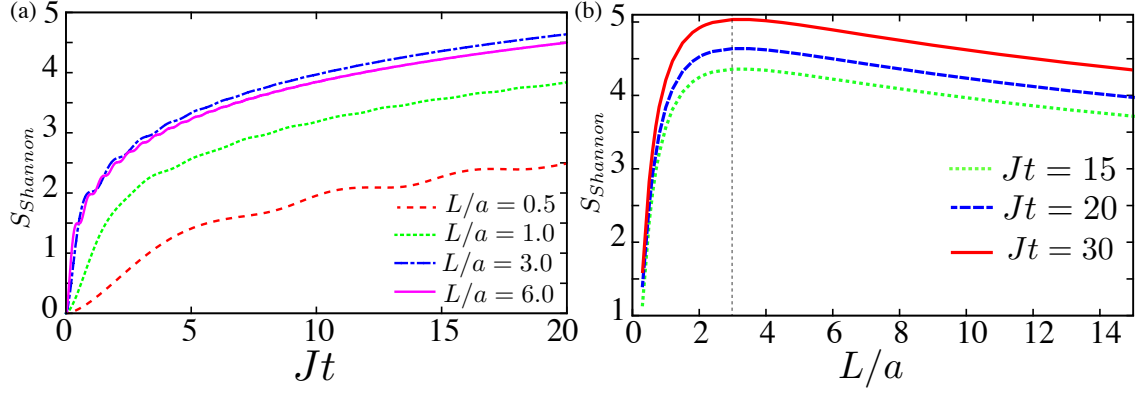


Figure 4.5: (Color online) (a) The temporal growth of Shannon entropy for different values of L . (b) The value of Shannon entropy as a function of L for a fixed time of $Jt = 15, 20$ and 30 .

4.3.4 Bipartite Entanglement entropy

As we have seen, the excitation which is localized at the center of the lattice at an initial time gets delocalized over the lattice. This diffusion of excitation from one part of the system to another part makes the different parts of the lattice get correlated [77]. To quantify this effect, we use the bipartite entanglement entropy. We divide the atomic array into two parts, A and B , in which A constitutes the left half, and B represents the right half with the number of lattice sites $N/2$ each. The Hilbert spaces for the subsystems, each having a dimension of $N/2 + 1$, are spanned by $\mathcal{H}_A \in \{|0\rangle_A, |i\rangle_A\}$ for A and $\mathcal{H}_B \in \{|0\rangle_B, |i\rangle_B\}$ for B . The state $|0\rangle_A$ ($|0\rangle_B$) represents all $N/2$ atoms in the subsystem A (B) are in the ground state $|g\rangle$ and $|i\rangle_A$ ($|i\rangle_B$) is a singly excited state of the sub-system A (B) in which only the atom in the i^{th} site is in the excited state $|e\rangle$. As far as the excitation is concerned, each subsystem can be visualized as an effective two-level system with two states that stand for the presence and absence of the excitation. Note that the position of the excitation in a given subsystem is irrelevant.

Now, we write the generalized state in term of states of the sub-system A and B . $|\psi(t)\rangle = \sum_{i=1}^{N/2} c_i(t) |i\rangle_A |0\rangle_B + \sum_{i=N/2+1}^N c_i(t) |0\rangle_A |i\rangle_B$, and the density matrix of the total system is $\rho_{AB} = |\psi(t)\rangle \langle \psi(t)|$. Thus, $P_A(t) = \sum_{i=1}^{N/2} |c_i(t)|^2$ and $P_B(t) = \sum_{i=N/2+1}^N |c_i(t)|^2$ provide us the probability of finding the excitation in the subsystem A and B , respectively. The entanglement entropy of subsystem A is $\mathcal{S}_A = -\text{Tr}(\rho_A \log_2 \rho_A)$ where

$$\rho_A(t) = P_A(t) |E(t)\rangle \langle E(t)| + P_B(t) |0\rangle \langle 0| \quad (4.14)$$

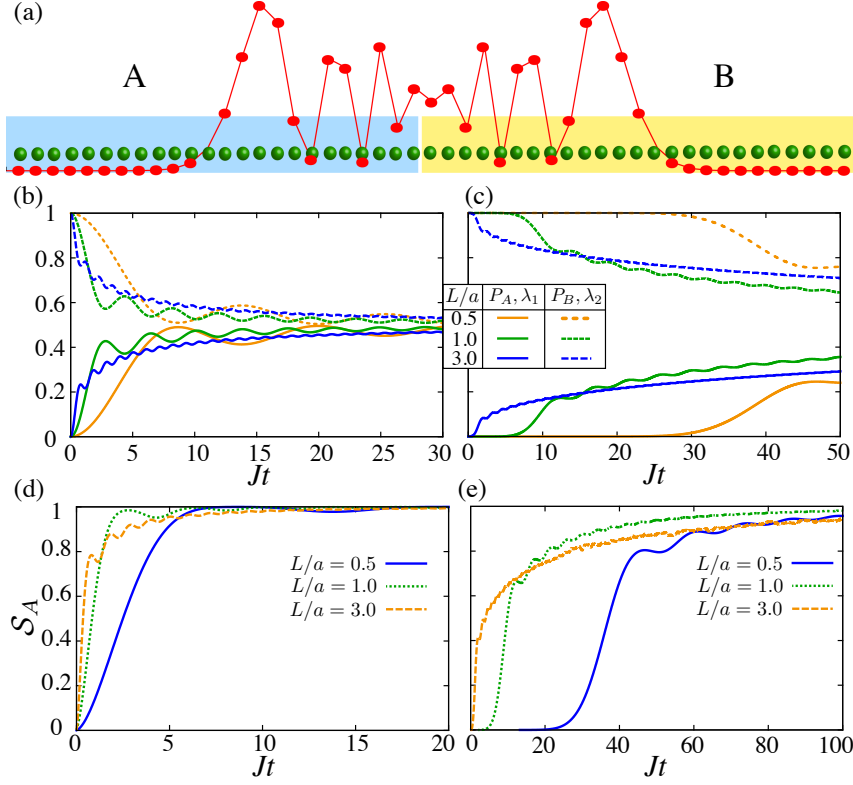


Figure 4.6: (a) The partition of the system into two identical subsystems (A and B) and the excitation is delocalized over the atomic array. (b) and (c) show the eigenvalues of the density operator ρ_A which provide us the probability of finding the excitation in the subsystems A and B where initially the excitation is placed in the subsystem B . For (b) $|\psi(t=0)\rangle = |0\rangle_A |N/2+1\rangle_B$ and for (c) $|\psi(t=0)\rangle = |0\rangle_A |N/2+10\rangle_B$. The growth of entanglement entropy $\mathcal{S}_A$ in time for different L , for the parameters in (b) and (c) are respectively shown in (d) and (e).

is the reduced density matrix of the subsystem A obtained by the partial trace of ρ_{AB} . The state $|E(t)\rangle = \left[1/\sqrt{P_A(t)}\right] \sum_i^{N/2} c_i(t)|i\rangle_A$ is a general single excitation state of the subsystem A . In Eq. (4.14) we removed subscript A from the state vectors for convenience. Note that, the form of ρ_A implies that in general, subsystem A is in a statistical mixture of two pure states: a single excitation state ($|E(t)\rangle$) and a state with no excitations ($|0\rangle$). Diagonalizing ρ_A , we get two non-zero eigenvalues (λ_1 and λ_2) in complying with the two-level description, which corresponds to the probability of finding the excitation in two subsystems A and B Fig. [4.6(b-c)]. The latter also indicates that the entropy $\mathcal{S}_A$ will be bounded by a maximum value of one and is independent of system size N and exchange interaction range L . $\mathcal{S}_A = 1$ corresponds to a maximally mixed state with equal probabilities to find the excitation either in A or B . Note that the density matrix ρ_A has the dimension of $N/2 + 1$ but the

diagonalization of ρ_A leads to only two non-zero eigenvalues (λ_1 and λ_2).

We assume that the excitation is initially localized in subsystem B , but at the edge with subsystem A i.e., $|\psi(t=0)\rangle = |0\rangle_A |N/2+1\rangle_B$. Thus, we have $\rho_A = |0\rangle\langle 0|$ and consequently both $P_A = 0$ and $\mathcal{S}_A(t=0) = 0$. As the excitation diffuses from the subsystem B to A , we observe the increase in the probability of finding an excitation in subsystem A (P_A), Fig. [4.6b], which leads to the rise in the entanglement entropy $\mathcal{S}_A(t)$ and Fig. [4.6d]. After a sufficiently long time, the single excitation probability distribution evolves in such a way that there is almost equal probability to find the excitation in each subsystem ($P_A \approx P_B$) Fig. [4.6b], resulting in $\mathcal{S}_A(t)$ approaching the value very close to one. Since the excitation was initially localized in B , we always have $P_B > P_A$, and the initial position of the excitation in block B determines how close P_A and P_B get. The entanglement dynamics depend only on the initial separation between the excitation and the boundary between the subsystems l_0 .

Now, to study the effect of separation l_0 , consider the initial state, $|\psi(t=0)\rangle = |0\rangle_A |N/2+l_0\rangle_B$, i.e., the excitation is initially localized in subsystem B , but slightly away from the partition boundary. We see that it requires a finite time to build up the correlation between A and B and that time corresponds to the time taken by the excitation to cross the partition boundary. Fixing l_0 , the time required to generate the correlation between A and B decreases with an increase in L , as shown in Fig. [4.6(d-e)]. Also, for larger l_0 , the probability of finding the excitation in A at longer times gets smaller and, consequently, the correlations. A physical interpretation of the entanglement growth between A and B can be made based on quasiparticles [77, 109, 110]. The initially localized excitation in the block B is a source of quasiparticles with dispersion ϵ_k , as given in Eq. (4.4). A pair of entangled quasiparticles with quasi momenta $\pm\hbar k$, propagates on either side of the lattice from the initial position of the excitation, eventually making subsystems A and B correlated.

As expected, for large values of L , faster diffusion of the excitation results in the increased rate of growth of $\mathcal{S}_A(t)$ Fig. [4.6 d]. But for a very large value of $L/a \sim 3.0$ and at a later time, the effect of quasi-localization is apparent in the time evolution of $\mathcal{S}_A$. As shown in Fig. [4.6(d-e)] although the initial growth of $\mathcal{S}_A$ for $L/a = 3$ is faster than small L cases, it takes longer to saturate to max value due to suppressed delocalization happening because of quasi-localization.

4.4 Dissipative dynamics

In this section, we briefly outline the effect of dissipation on the dynamics observed in the previous sections. Any realistic setup consisting of atoms coupled to a PCW will have dissipation arising from the spontaneous emission to the free space from the excited state with a decay rate γ and the photon loss from the photonic crystal [95]. The photon loss from the photonic crystal can be neglected since the photonic modes are weakly populated. In the presence of atomic spontaneous emission, the state of the atomic chain must be described by a density matrix $\rho(t)$, whose dynamics in the Markovian approximation is governed by the master equation,

$$\dot{\rho} = -\frac{i}{\hbar}[H_t, \rho] + \mathcal{L}_\gamma \rho \quad (4.15)$$

with a Lindblad term of the form,

$$\mathcal{L}_\gamma \rho = -\frac{\gamma}{2} \sum_j (\{\sigma_{ee}^j, \rho\} - 2\sigma_{ge}^j \rho \sigma_{eg}^j). \quad (4.16)$$

In Fig. [4.7(a-b)], we show the single excitation dynamics for different values of γ with $L/a = 0.5$ and $L/a = 3.0$. As we can see, even though the excitation probability decays drastically, the features of the coherent dynamics are intact for a decay rate of 5% of the hopping strength. For instance, the quasi-localization behavior at large values of L is visible, as shown in Fig. [4.7b]. After a sufficiently long time ($t \gg 1/\gamma$), the excitation decays completely, and that halts the dynamics. We verified that CTQW for small L has survived up to a decay rate of 20%, i.e., for $\gamma = 0.2J$ whereas the quasi-localization at large L is visible even for $\gamma \sim J$ despite having a small excitation probability.

4.5 Summary

To summarize, we analyzed in detail the dynamics of a single excitation in an atomic array coupled to a photonic crystal waveguide. For an initially localized single excitation, we observed quantum diffusion, which exhibits a typical CTQW for short-range exchange interaction. For long-range interaction, we observed quasi-localization and tailing behavior. The change in the dynamics as a function of interaction range was captured by parameters such as kurtosis, IPR, population imbalance, and Shannon entropy. The dynamics of IPR revealed the transition from super-ballistic at the initial stage to ballistic at longer times. In addition, we

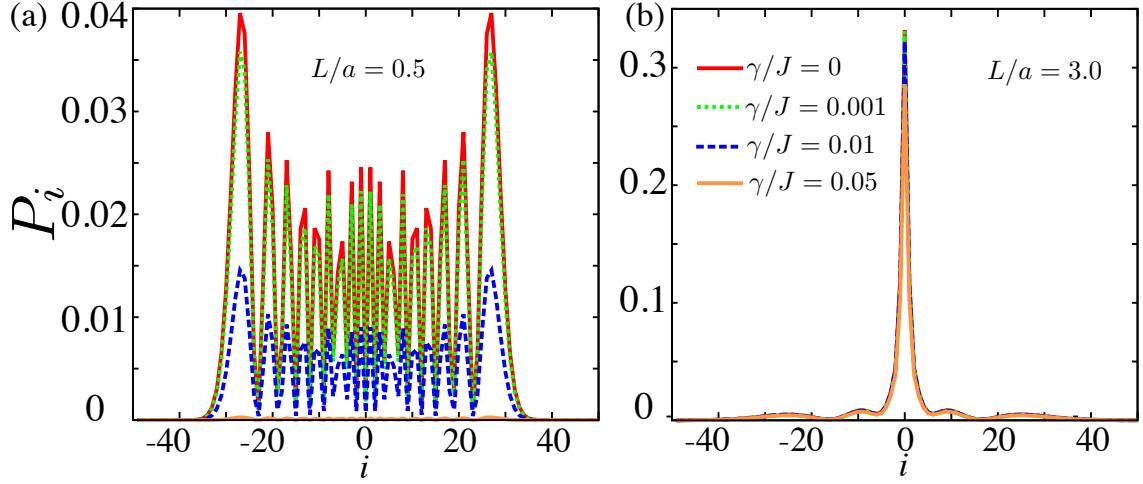


Figure 4.7: The dissipative single excitation dynamics for (a) $L/a = 0.5$, and (b) $L/a = 3$ with different values of γ . The dynamics in (a) resemble that of a CTQW and in (b) shows the quasi-localization behavior. The times at which each of the snapshots are taken (a) $Jt = 100$, and (b) $Jt = 3$.

studied the dynamics of the bipartite entanglement entropy of the system which was found to be globally bounded for the case of a single excitation. The effect of spontaneous emission was also studied. In the next chapter, we study the effect of the presence of other excitation on the dynamics. When the excitations are Rydberg excitation, they interact strongly via van der Waals (vdW) interaction. We study the interplay between the exchange coupling, vdW interaction, and separation between two excitations in the next chapter.

This work is a part of following publication: Dynamics of Rydberg excitations and quantum correlations in an atomic array coupled to a photonic crystal waveguide [111]

4.6 Appendix

4.6.1 Single excitation dispersion, Width and Kurtosis

The Hamiltonian of the system is given by,

$$\hat{H}_{ex} = J \sum_{j \neq l} e^{-|x_j - x_l|/L} \hat{\sigma}_{eg}^j \hat{\sigma}_{ge}^l \quad (4.17)$$

and the corresponding Schrödinger equation is,

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle. \quad (4.18)$$

Taking $|\psi(t)\rangle = \sum_i c_i(t) |i\rangle$ where $\{|i\rangle \equiv |\dots g^{i-1} e^i g^{i+1} \dots\rangle\}$ provides the single excitation basis, we can rewrite the Schrödinger equation as,

$$i \frac{dc_j}{dt} - J \sum_{l \neq j}^N e^{-|j-l|a/L} c_l = 0. \quad (4.19)$$

with $\hbar = 1$. To get the dispersion relation for the plane waves, we take the ansatz of the form $c_j(t) = A e^{i(jka + \epsilon_k t)}$. Substituting this into Eq. (4.19) we get,

$$A \epsilon_k e^{i(jka + \epsilon_k t)} = \sum_{l \neq j}^N e^{-|l-j|a/L} A e^{i(lka + \epsilon_k t)} \quad (4.20)$$

Let $d = l - j$ and

$$\begin{aligned} \epsilon_k &= \sum_{d=-\infty}^{\infty} -J e^{-da/L} e^{ikd} \\ \epsilon_k &= \sum_{d=1}^{\infty} -2J e^{-da/L} \left[\frac{e^{ikd} + e^{-ikd}}{2} \right] \\ \epsilon_k &= -2J \sum_{d=1}^{\infty} e^{-da/L} \cos(kad). \end{aligned} \quad (4.21)$$

After the summation,

$$\epsilon_k = \frac{J(\cos ka - e^{-a/L})}{(\cosh(a/L) - \cos ka)}. \quad (4.22)$$

Using the dispersion relation, below we obtain the width and the Kurtosis of the probability distribution.

The second moment of the probability distribution is given by $\langle z^2 \rangle = a^2 \sum_{n=-\infty}^{\infty} n^2 p_n(t)$ where $p_n(t) = |u_n(t)|^2$ with $u_n(t) = \frac{a}{2\pi} \int_{BZ} \exp(i[kna - \epsilon_k t]) dk$. Using the integration by parts, we can rewrite the $u_n(t)$ as,

$$u_n(t) = \frac{1}{2\pi n} \int_{BZ} e^{ikna - \epsilon_k t} \frac{d\epsilon_k}{dk} t$$

substituting this in the expression of $p_n(t)$ we get

$$p_n(t) = \left(\frac{1}{2\pi n} \right)^2 \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' e^{ina(k-k') + i(\epsilon_k - \epsilon_{k'})t} \frac{d\epsilon_k}{dk} \frac{d\epsilon_{k'}}{dk'} t^2$$

Using this expression for probability in the expectation value we get,

$$\langle z^2 \rangle = \left(\frac{a}{2\pi} \right)^2 \sum_{n=-\infty}^{\infty} n^2 \frac{1}{n^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' e^{ina(k-k') + i(\epsilon_k - \epsilon_{k'})t} \frac{d\epsilon_k}{dk} \frac{d\epsilon_{k'}}{dk'} t^2$$

$$\begin{aligned}
&= \frac{a^2}{2\pi} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' \left(\frac{1}{2\pi} \sum_{-\infty}^{\infty} e^{ina(k-k')} \right) e^{i(\epsilon_k - \epsilon_{k'})t} \frac{d\epsilon_k}{dk} \frac{d\epsilon_{k'}}{dk'} t^2 \\
&= \frac{a^2}{2\pi} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' \frac{\delta(k-k')}{|a|} e^{i(\epsilon_k - \epsilon_{k'})t} \frac{d\epsilon_k}{dk} \frac{d\epsilon_{k'}}{dk'} t^2 \\
\langle z^2 \rangle &= \left[\frac{a}{2\pi} \int_{BZ} \left(\frac{d\epsilon_k}{dk} \right)^2 dk \right] t^2.
\end{aligned} \tag{4.23}$$

Using the dispersion in Eq. (4.22) we get,

$$\begin{aligned}
\langle z^2 \rangle &= \frac{J^2 a^3 \sinh^2(a/L) t^2}{2\pi} \int_{-\pi/a}^{\pi/a} \frac{\sin^2 ka}{(\cosh(a/L) - \cos(ka))^2} dk \\
&= \frac{J^2 a^2 \sinh^2(a/L) t^2}{2} \frac{\cosh(a/L)}{(\sinh(a/L))^5} \\
\langle z^2 \rangle &= \frac{J^2 a^2}{2} \frac{\coth(a/L)}{\sinh(a/L)^2} t^2,
\end{aligned} \tag{4.24}$$

which then gives us

$$\alpha(L) = aJ \sqrt{\frac{\coth(a/L)}{2 \sinh^2(a/L)}}. \tag{4.25}$$

Similarly, the excess kurtosis κ of the distribution is given by,

$$\kappa = \frac{\langle z^4 \rangle}{(\langle z^2 \rangle)^2} - 3 \tag{4.26}$$

The fourth moment of the distribution $\langle z^4 \rangle = a^4 \sum_{n=-\infty}^{\infty} n^4 p_n(t)$ in terms of dispersion can be computed using the integration by parts twice in the expression of $u_n(t)$,

$$u_n(t) = \frac{1}{2\pi n^2 a} \int_{-\pi/a}^{\pi/a} e^{i(kna - \epsilon_k t)} \left[\frac{d^2 \epsilon_k}{dk^2} t + i \left(\frac{d\epsilon_k}{dk} \right)^2 t^2 \right]$$

which gives,

$$\begin{aligned}
p_n(t) &= \left(\frac{1}{2\pi} \right)^2 \frac{1}{a^2 n^4} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' e^{ina(k-k') + i(\lambda(k) - \lambda(k'))t} \\
&\quad \left[\frac{d^2 \lambda}{dk^2} t - i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \left[\frac{d^2 \lambda}{dk'^2} t + i \left(\frac{d\lambda}{dk'} \right)^2 t^2 \right]
\end{aligned} \tag{4.27}$$

substituting this into the expression for the fourth moment we get,

$$\begin{aligned}
\langle z^4 \rangle &= \left(\frac{a}{2\pi} \right)^2 \sum_{-\infty}^{\infty} n^4 \frac{1}{n^4} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' e^{ina(k-k') + i(\lambda(k) - \lambda(k'))t} \\
&\quad \left[\frac{d^2 \lambda}{dk^2} t - i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \left[\frac{d^2 \lambda}{dk'^2} t + i \left(\frac{d\lambda}{dk'} \right)^2 t^2 \right]
\end{aligned}$$

$$\begin{aligned}
&= \frac{a^2}{2\pi} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' \left(\frac{1}{2\pi} \sum_{-\infty}^{\infty} e^{ina(k-k')} \right) e^{i(\lambda(k)-\lambda(k'))t} \\
&\quad \left[\frac{d^2\lambda}{dk^2} t - i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \left[\frac{d^2\lambda}{dk'^2} t + i \left(\frac{d\lambda}{dk'} \right)^2 t^2 \right] \\
&= \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk \left[\frac{d^2\lambda}{dk^2} t - i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \left[\frac{d^2\lambda}{dk^2} t + i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \\
&= \frac{a^2}{2\pi} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk dk' \frac{\delta(k-k')}{|a|} e^{i(\lambda(k)-\lambda(k'))t} \\
&\quad \left[\frac{d^2\lambda}{dk^2} t - i \left(\frac{d\lambda}{dk} \right)^2 t^2 \right] \left[\frac{d^2\lambda}{dk'^2} t + i \left(\frac{d\lambda}{dk'} \right)^2 t^2 \right] \\
\langle z^4 \rangle &= \frac{a}{2\pi} \int_{BZ} dk \left[\left(\frac{d^2\epsilon_k}{dk^2} \right)^2 t^2 + \left(\frac{d\epsilon_k}{dk} \right)^4 t^4 \right] \tag{4.28}
\end{aligned}$$

From the dispersion relation we get the first integration as

$$\begin{aligned}
\frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} \left(\frac{d^2\epsilon_k}{dk^2} \right)^2 dk &= \frac{(\cosh(a/L) - e^{-a/L})^2 a^5}{2\pi} \\
&\quad \int_{-\pi/a}^{\pi/a} \frac{(\cosh(a/L) \cos ka - \sin^2 ka - 1)^2}{(\cosh(a/L) - \cos ka)^6} dk \\
\frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \left(\frac{d^2\epsilon_k}{dk^2} \right)^2 dk &= J^2 a^4 \frac{\cosh(1/L)(1 + \cosh^2(1/L)/2)}{\sinh^5(1/L)} \tag{4.29}
\end{aligned}$$

Similarly for the other term

$$\begin{aligned}
\frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} \left(\frac{d\omega}{dk} \right)^4 dk &= \frac{(\cosh(a/L) - e^{-a/L})^4 a^4}{2\pi} \\
&\quad \int_{-\pi/a}^{\pi/a} \frac{\sin^4 ka}{(\cosh(a/L) - \cos ka)^8} dk \\
\frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \left(\frac{d\omega}{dk} \right)^4 dk &= \frac{3J^4 a^4 \cosh(a/L)(1 + 2 \cosh^2(a/L))}{16 \sinh^7(a/L)} \tag{4.30}
\end{aligned}$$

Finally substituting eq[4.39] and eq[4.40] into Eq[4.38] we get,

$$\begin{aligned}
\langle z^4 \rangle &= J^2 a^4 \frac{\cosh(a/L) [1 + \frac{1}{2} \cosh^2(a/L)]}{\sinh^5(a/L)} t^2 \\
&\quad + \frac{3J^4 a^4 \cosh(a/L) [1 + 2 \cosh^2(a/L)]}{16 \sinh^7(a/L)} t^4 \tag{4.31}
\end{aligned}$$

Substituting equation 4.31 and 4.24 in 4.26 and after simplification we obtain,

$$\kappa(t) = 4 \left[1 + \frac{1}{2} \cosh^2(a/L) \right] \frac{1}{(Jt)^2} + \frac{3}{2} \frac{[1 + 2 \cosh^2(a/L)]}{\sinh(2a/L)} - 3. \quad (4.32)$$

The asymptotic value ($t \rightarrow \infty$) of kurtosis is given by

$$\kappa_a = \lim_{t \rightarrow \infty} \kappa(t) = \frac{3}{2} \frac{[1 + 2 \cosh^2(a/L)]}{\sinh(2a/L)} - 3 \quad (4.33)$$

Further in the large L limit where $L/a \gg 1$, we can use $\cosh(a/L) \approx 1$ and $\sinh(a/L) \approx a/L$ to obtain $\kappa_a \approx 9L/(4a) - 3$.

Chapter 5

Rydberg excitation Dynamics: Two excitations

The single excitation dynamics studied in the previous chapter can be made even more interesting by the addition of one more excitation in the system. The presence of another excitation gives rise to various control parameters in the system such as the interaction between excitations, the relative separation between excitations. The combination of all these effects results in the exciting two excitation dynamics. In recent times Rydberg excitations have been successfully coupled to nanophotonic structures such as hollow-core photonic crystal fibers and optical nanofibers [112–114]. The properties of Rydberg atoms near these structures have been studied recently which will pave the way for upcoming hybrid quantum systems involving Rydberg atoms and nanophotonic structures. Taking motivations from these developments we study the dynamics of Rydberg excitations coupled to a photonic crystal waveguide (PCW).

When atoms are excited to Rydberg state, Rydberg-Rydberg interactions (RRIs) emerge as a competitive interaction to exchange interaction. In order to study the effect of these two separately, we first look at the dynamics of two non-interacting excitations kept in the adjacent lattice sites as a function of exchange interaction range L . We observe the anti-bunching effects at short-range coupling whereas, for long-range couplings, we observe the quasi-localization of excitations. For an intermediate range of L , we observe the dynamics in which one excitation stays at its initial position while the other propagates away from it. For other initial separations, we observe different correlation dynamics due to quantum interference. The inclusion of RRI creates a competition with exchange interaction and in the

case of strong RRI gives rise to two excitations bound state. A similar bound state dynamics has been observed for fermions, hardcore bosons and anyons trapped in optical lattice [115–126]. Due to controllability over the strength of RRI and range of exchange interaction we observe the coexistence of bound state and anti-bunching dynamics. For a different initial separation, we observe an interesting interplay between RRI and exchange interaction. We explain all the results with the help of two excitation spectrum and overlap of the initial state onto the energy eigenstates. Further, we also study the entanglement dynamics as a function of exchange interaction range, RRI strength, and initial separation between excitations. Finally, we look at the effect of decoherence arising from spontaneous emission from the Rydberg state. We show that for small decay rates, all the interesting features survive making it possible to observe experimentally in near future.

5.1 Two Excitations Hamiltonian

The single excitation exchange Hamiltonian H_{ex} can be augmented to incorporate two excitation interactions due to RRI. Two atoms in the Rydberg state interact via van der Waals interaction potential which is given by $V_{ij} = C_6/r_{ij}^6$, where r_{ij} is the separation between the two excitations, and C_6 is the vdW coefficient. Together with the RRIs, the total Hamiltonian becomes

$$\hat{H}_t = \hat{H}_{ex} + \sum_{i < j} V_{ij} \hat{\sigma}_{ee}^i \hat{\sigma}_{ee}^j, \quad (5.1)$$

with $\hat{H}_{ex}$ given in Eq. (4.3). The Hamiltonian $\hat{H}_t$ preserves the number of excitations, and therefore we can restrict the dynamics to the subspace of two excitation states. In such case, $N(N-1)/2$ basis states of the form $\{|ij\rangle \equiv |\dots g, e^i, g, \dots g, e^j, g, \dots\rangle\}$, span the entire Hilbert space. A state $|ij\rangle$ represents the state in which excitations are at site i and j . A general state of the system can be written as a superposition of two excitation states as $|\psi(t)\rangle = \sum_{i < j} c_{ij}(t) |ij\rangle$, $|c_{ij}|^2$ is the probability of finding excitations at site i and j , such that $\sum_{i < j} |c_{ij}(t)|^2 = 1$. The time-dependent probability amplitudes $c_{ij}(t)$ are obtained by solving the corresponding Schrödinger equations. We use scaled two-body distribution $\Gamma_{ij}(t) = |c_{ij}(t)|^2 / \text{Max}(|c_{ij}(t)|^2)$ to characterize the dynamics, where $\text{Max}(\dots)$ is the maximum value of $|c_{ij}(t)|^2$ at the instant t .

Similar to the case of a single excitation, the energy spectrum of $\hat{H}_t$ plays an important role in determining the dynamics of the two initially localized excitations

[115, 121, 127]. To obtain the two excitation spectrum, we introduce the center of mass $R = (i + j)a/2$ and the relative $r = (j - i)a$ coordinates. Using $c_{ij} = \exp(iKR)\phi_K(r)$ in the Schrödinger equation with $\phi_K(r) = \phi_K(-r)$ and $\phi_K(0) = 0$ (hard-core constraint), we obtain the eigenspectrum by solving the set of coupled equations see [4.6.1],

$$\sum_{d>1}^{N-1} J_d^K \phi_K(r + da) + \sum_{d \neq r/a} J_d^K \phi_K(r - da) + \frac{C_6}{r^6} \phi_K(r) = \epsilon_{K,k} \phi_K(r) \quad (5.2)$$

where $J_d^K = 2Je^{-da/L} \cos(Kda/2)$ and d an integer. Let k_1 and k_2 be the quasi-momentum associated with the first and second excitations, and then we have the center of mass momentum $K = k_1 + k_2$ and the relative coordinate momentum as $k = (k_1 - k_2)/2$. Due to the exponential term ($\sim e^{-da/L}$) in the expression of J_d^K , the parameter L determines not only the range of the exchange interaction but also the strength of the exchange interaction. In other words, the larger the value of L , the higher the hopping matrix elements. When $C_6 = 0$, the states $\phi_K(r)$ are solely scattering states and the energy eigenvalues are the sum of the single-particle ones ($\epsilon_{K,k}^0 = \epsilon_{k_1} + \epsilon_{k_2}$),

$$\epsilon_{K,k}^0 = -J \frac{2AB - 2(A + B) \cos(Ka/2) \cos(ka) + \cos Ka + \cos 2ka}{B^2 - 2B \cos(Ka/2) \cos(ka) + \frac{1}{2}(\cos(Ka) + \cos(2ka))} \quad (5.3)$$

where $A = e^{-a/L}$, $B = \cosh(a/L)$, K and k are center of mass and relative coordinate momentum respectively. A non-zero C_6 can significantly modify the features of the spectrum, in particular, the bound states emerge. The eigenspectrum is obtained by diagonalizing the Hamiltonian:

$$H_K^{(2)} = \begin{bmatrix} V_1 + J_2^K & J_1^K + J_3^K & J_2^K + J_4^K & \dots \\ J_1^K + J_3^K & V_2 + J_4^K & J_1^K + J_5^K & \dots \\ J_2^K + J_4^K & J_1^K + J_5^K & V_3 + J_6^K & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

with $V_d = C_6/(da)^6$ and $d = 1, 2, \dots, N - 1$. In upcoming sections, we study the dynamics of two excitations for various parameters and explain the results using the two excitation spectrum calculated in this section.

5.2 Non-interacting case ($C_6 = 0$)

5.2.1 Excitation dynamics

For non-interacting excitations ($C_6 = 0$) the initial separation between the excitations plays a crucial role in determining the dynamics. When the excitations are well separated from each other, they evolve as independent excitations. Fig [5.1](top panel) shows the Γ_{ij} for different values of L , for the excitations separated by 50 lattice sites at $t = 0$. The bottom panel shows the single-particle probability distribution. For small values of $L/a = 0.5$, we observe LTPD of two excitations to be the same as two independent excitations doing CTQW Fig [5.1(a-b)]. With an increase in exchange interaction range to $L/a = 1$ and 1.5 the quasi-localization and tailing behavior starts to emerge in both the excitations 5.1(c-f). Hence for all values of L as long as the initial separation between two excitations is large and probability distributions don't overlap, two excitations can be considered independent.

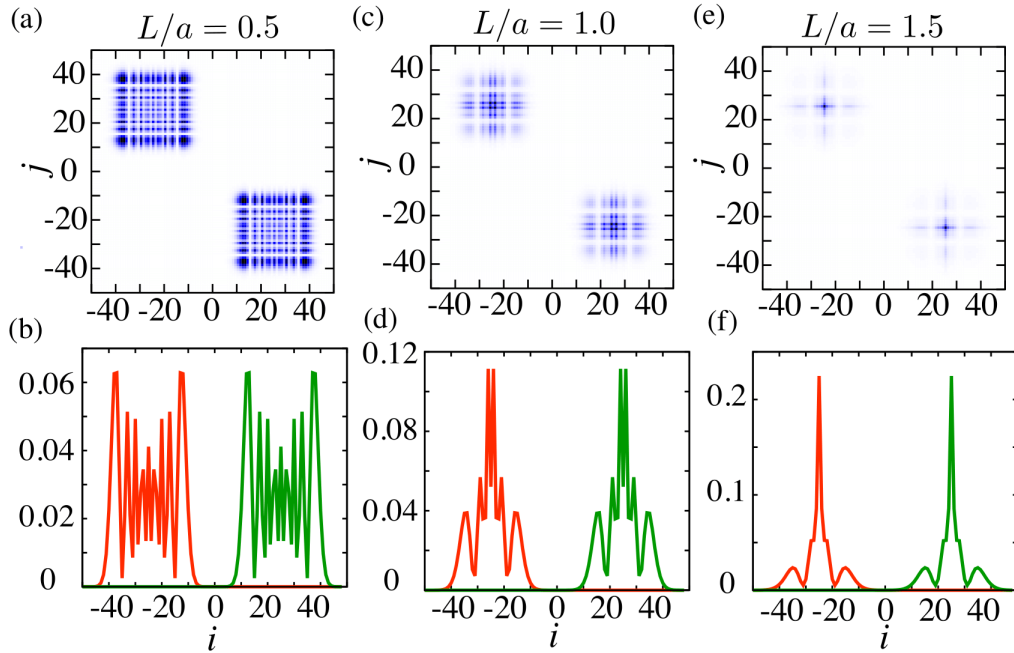


Figure 5.1: (Top panel) The scaled probability distribution for excitations separated by 50 lattice sites with initial state $|N/2 - 25, N/2 + 25\rangle$ for $L/a = 0.5, 1.0$ and 1.5 at $Jt = 50, 10$ and 5 respectively. (Bottom panel) A single particle probability distribution obtained from Γ_{ij} by taking the projection onto one the axis of figures in the top panel.

On the other hand, when the excitations are placed closed to each other in adjacent lattice sites, we observe the maximum effect of the presence of one excitation

onto another. The Fig.[5.2(a-d)] shows the scaled LTPD (Γ_{ij}) for the initial condition $c_{i=N/2, j=N/2+1} = 1$ in which the excitations are localized initially in adjacent sites ($d_0 = 1$) at the center of the lattice. For small values of L , since the exchange interaction is predominantly nearest neighbor, excitation can only get exchanged with the nearest neighbor ground state atom. But the presence of other excitation in the nearest site hinders the exchange due to hardcore constraint. This leads to the dynamics in which two excitations move away from each other resulting in the anti-bunching effect Fig [5.2(a-b)]. The anti-bunching effect observed here is similar to the anti-bunching of non-interacting fermions, hardcore bosons and anyons [115–121, 128].

With the increase in the L , we observe the deviation from the anti-bunching dynamics. For very large values of L , we observe the quasi-localization behavior similar to the case of single excitation discussed in Sec. 4.3. As shown in Fig. [5.2d], for $L/a = 3$ there is a high probability of finding excitations at their initial positions. The stripes appearing in the probability distribution are due to the high group velocity modes. For an intermediate value of $L \approx 1$, we observe the dynamics in which one excitation gets quasi-localized while the other propagates away from the initial position Fig. [5.2c]. This can be attributed to the combined effect of hardcore constraint and quantum interference. Similar to the single excitation case the effect observed here can be explained in terms of modification of two excitation spectrum $\epsilon_{K,k}^0$.

As L increases, $\epsilon_{K,k}^0$ gets modified as shown in Fig. [5.2(e-h)], where $\epsilon_{K,k}^0$ is plotted in the $k_1 - k_2$. The quasi-localization at large L is attributed to those modes having both $\partial\epsilon_{K,k}^0/\partial k_1 \sim 0$, and $\partial\epsilon_{K,k}^0/\partial k_2 \sim 0$. They appear as flat modes near $k_1, k_2 \sim \pm\pi/a$, and the local maxima of the emerging energy stripes, as shown in Fig. [5.2h]. For the intermediate value of L , we have a scenario in which one of the two excitations experiences a quasi-localization, and the other one propagates towards the edge of the array, as seen in Fig. [5.2c]. The latter arises from those modes in the stripes with either $\{\partial\epsilon_{K,k}^0/\partial k_1 \sim 0, \partial\epsilon_{K,k}^0/\partial k_2 \neq 0\}$ or vice versa. The modes near $k_1, k_2 \sim 0$ have large value of group velocity which leads to the tailing behavior in Fig.[5.2d], with almost horizontal and vertical probability tails in the LTPD.

As shown in the bottom panel of Fig. [5.2i], for small values of $L/a = 0.2$, at the edge of the Brillouin zone $K = \pm\pi/a$, the energy eigenvalues converge to one value leading to degenerate eigenvalues. With increasing L , the degeneracy in the

spectrum gets lifted due to the inclusion of a long-range hopping terms. The top of the spectrum for any K value can be obtained from Eqn. 5.3 by putting $k = 0$. This quantity will play a crucial role in the next section when two excitations can interact with each other.

As the initial separation between the two excitations (d_0) increases, the LTPD reveals non-trivial patterns due to the quantum interference, especially at small values of L . For $L/a = 0.5$, as shown in Fig. [5.3], a slight change in the initial position to $d_0 = 2, 3$ destroys the anti-bunching effect. With increasing initial separation, probability distribution pattern becomes more and more uniform Fig. [5.3(c-d)]. Similar effects can be seen for intermediate values of $L \sim 1$ as shown in Fig. [5.3(e-h)]. For a large value of $L/a = 3$ quasi-localization dominates at all separations. Although for large d_0 tailing behavior reduces Fig. [5.3(i-l)].

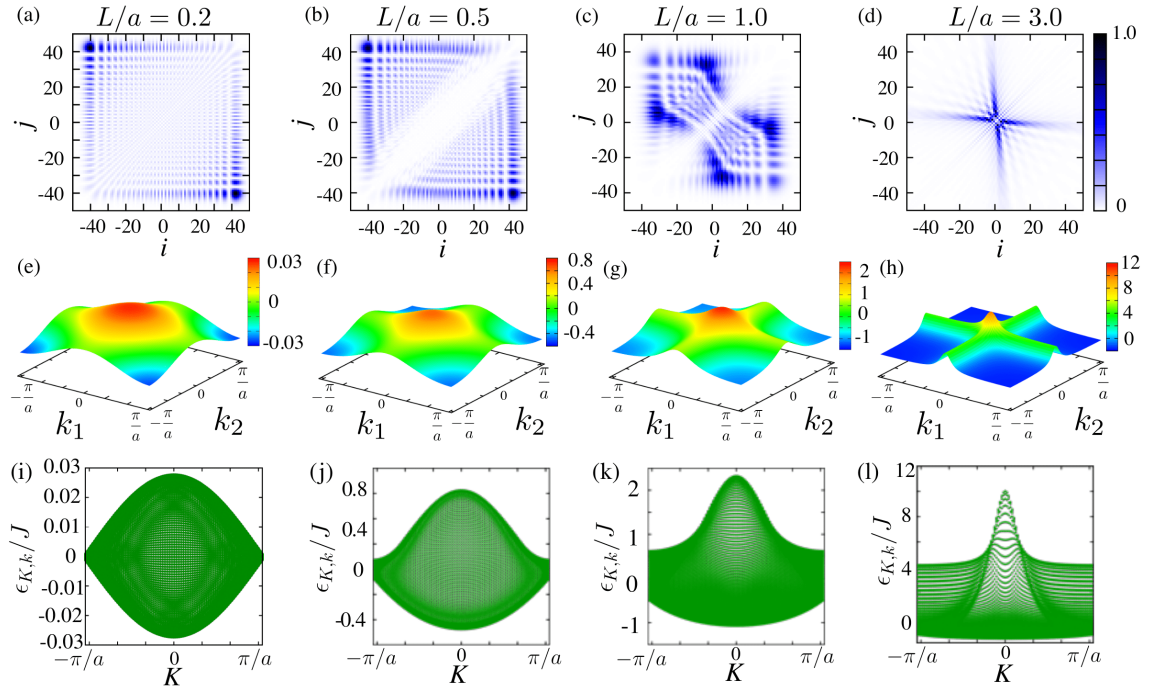


Figure 5.2: (a)-(d) The scaled two excitation distribution Γ_{ij} for $C_6 = 0$ and different values of L . Each column is for $L/a = 0.2, 0.5, 1.0$ and 3.0 shown at time $Jt = 3200, 150, 30$, and 15 respectively. (e)-(h) The energy spectrum $\epsilon_{K,k}^0$ in $k_1 - k_2$ plane for the corresponding L values of (a)-(d) respectively. (i)-(l) The two excitation spectrum as a function of center of mass momentum K for corresponding L .

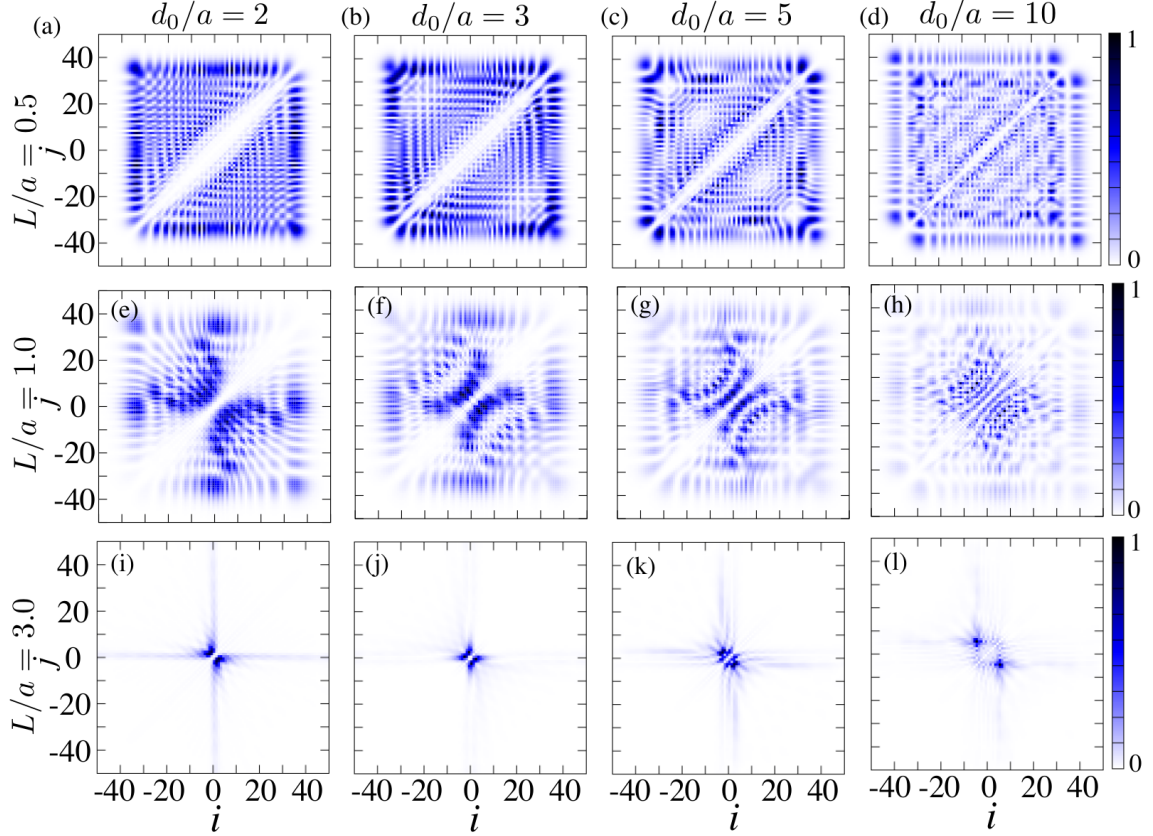


Figure 5.3: The scaled probability distribution Γ_{ij} for different initial separations $d_0 = 2, 3, 5$ and 10 and for different values of exchange coupling range $L/a = 0.5, 1$ and 3.0 .

5.2.2 Entanglement entropy

Here we study the effect of the presence of the second excitation on the entanglement generated by diffusion of one excitation. Similar to the single excitation case, we divide the system into two parts A and B . Compared to the single excitation case, the Hilbert space of each subsystem has three types of states $\{|0\rangle, |i\rangle, |ij\rangle\}$ with zero, one and two excitations respectively. Hence the Hilbert space of two subsystems is given by, $\mathcal{H}_A \in \{|0\rangle_A, |i\rangle_A, |ij\rangle_A\}$ and $\mathcal{H}_B \in \{|0\rangle_B, |i\rangle_B, |ij\rangle_B\}$, where i and j are the positions of two excitations in the subsystem. The general state of the system can then be written in terms of basis states of each sub system as

$$|\psi\rangle = \sum_{i < j}^{N/2} c_{ij} |ij\rangle_A |0\rangle_B + \sum_{i=1}^{N/2} \sum_{j=N/2+1}^N c_{ij} |i\rangle_A |j\rangle_B + \sum_{N/2 < i < j}^N c_{ij} |0\rangle_A |ij\rangle_B. \quad (5.4)$$

The first and the last term corresponds to both the excitations being in either the subsystem A and B respectively. The second term represents the states in which each subsystem has one excitation. From this, the density matrix of the total system given by ρ , the subsystem A given by ρ_A can be calculated. The entanglement entropy

S_A can be calculated in a similar way to the single excitation case as discussed in the previous chapter. The time evolution of the entanglement entropy depends on the initial separation between the excitations and their distance from the boundary of the two subsystems.

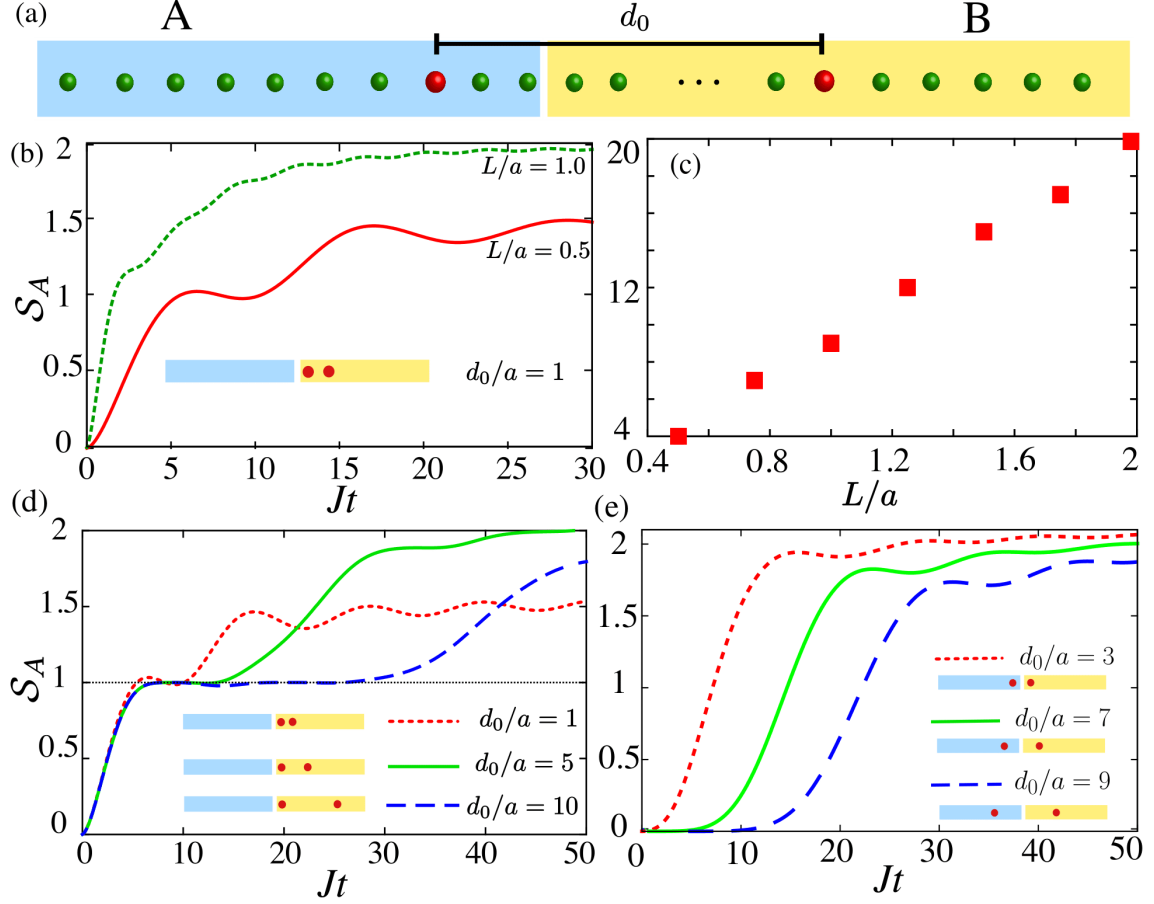


Figure 5.4: (a) The schematic of the initial state in which the two excitations (red spheres) that are separated by d_0 . (b) The dynamics of S_A for $d_0 = a$ with $L/a = 0.5$ (solid line) and $L/a = 1$ (dashed line). (c) The number of non-zero eigenvalues of ρ_A as a function of L at $Jt = 15$. (d) The dynamics of S_A for $L/a = 0.5$ with different d_0 such that both the excitations are in B . The thin horizontal line stands for $S_A = 1$. (e) The dynamics of S_A for $L/a = 0.5$ with different d_0 such that each sub system has one excitation.

First, we look at the time evolution of S_A for the case in which at $t = 0$ two excitations are in the subsystem B such that $d_0 = 1$ and one of the excitations is just outside the boundary of the of subsystem A as shown in the inset of Fig. [5.4b]. Since at $t = 0$, both the excitations are in the subsystem B we have $\rho_A = |0\rangle_A \langle 0|_A$ making $S_A = 0$. As time increases and excitations diffuse across the boundary leading to an increase in S_A . Unlike the single excitation case, S_A saturates to the value greater than 1. With the increase in L , both the rate of increase of S_A and the

saturation value of S_A increases Fig. [5.4b]. This implies that the two-level picture of a single excitation case is no longer valid for the case of two excitations. The different states of the subsystem A , $\{|ij\rangle_A\}$, are no longer degenerate, giving rise more than two non-zero eigenvalues of ρ_A . As shown in Fig. [5.4c], the number of non-zero eigenvalues of ρ_A at $Jt = 15$, increases linearly with L . This results in the growth of S_A which is not globally bounded by 1 and is dependent on both L and d_0 .

Next, we look at the effect of d_0 on entanglement dynamics. First, we consider the case in which both the excitations are in the sub-system B see inset of Fig. [5.4d]. In Fig. [5.4d], the entanglement dynamics for different values of d_0 is shown. For large d_0 only one excitation is closer to the system boundary hence S_A saturates to its single excitation values of 1, until the other excitation affects the dynamics. The timescales up to which the dynamics are similar to the single excitation case depend upon the values of L and d_0 . The lesser the separation between the excitation more will be the effect of one excitation onto the other, leading to an increase in the saturation value of S_A . However for $d_0 = 1$, due to antibunching dynamics of excitations, we observe partial suppression of S_A . Similarly, we look at the case in which each subsystem has one excitation separated by d_0 at $t = 0$ see inset of Fig. [5.4e]. As shown in Fig. [5.4e], at large d_0 it takes longer to generate the entanglement due to finite time taken by excitations to reach the subsystem boundary. The saturation value of S_A also decreases with an increase in d_0 due to less amplitude of two excitation wavefunction crossing the boundary. Hence by controlling the exchange interaction range L and the initial separation between the excitations relative to the subsystem boundary, we can coherently control the bipartite entanglement and its saturation value.

5.3 Rydberg interacting case ($C_6 \neq 0$)

5.3.1 Bound and Scattering States

In this section, we study the effect of sufficiently large RRI interaction strength $V_1 = C_6/a^6$ onto the two excitation spectrum. From here onwards we consider repulsive RRI interaction such that $V_1 > 0$. Fig. [5.5 (a-d)] show the spectrum for increasing value of V_1 for a fixed value of $L/a = 0.5$. For the non-interacting case of $V_1/J = 0$, the green region represents the free/scattering state solutions

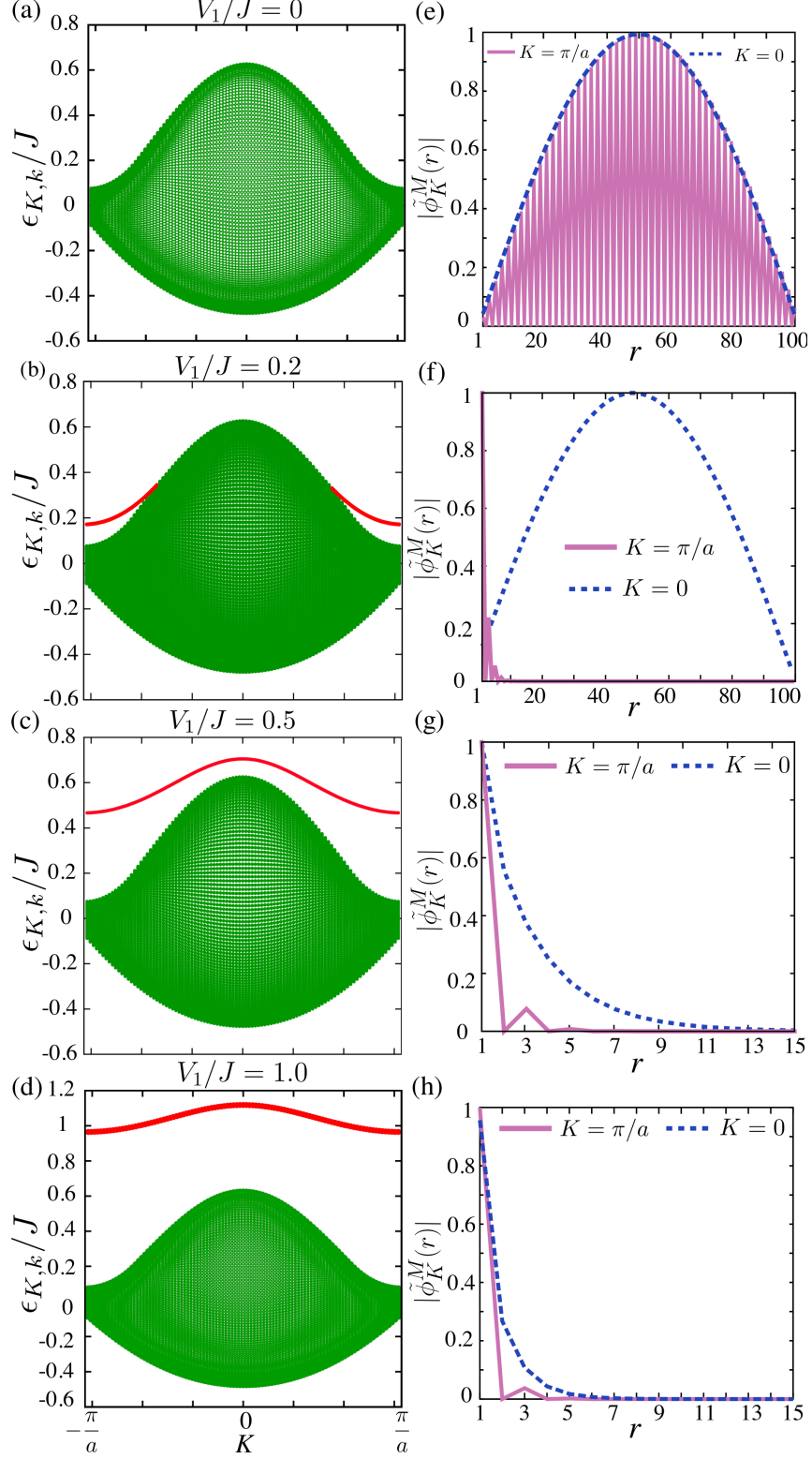


Figure 5.5: (Color online) The two excitation spectrum for $L/a = 0.5$ and RRI (a) $V_1/J = 0$ (b) $V_1/J = 0.2$ (c) $V_1/J = 0.5$ and (d) $V_1/J = 1$. The solid (red) line in (b)-(d) shows the isolated band for the bound states. (e)-(h) show the highest radial eigenfunctions (scaled by its maximum value) for $K = 0$ (dashed line) and $K = \pi/a$ (solid line), respectively for the excitation spectrum shown in (a)-(d).

of Equation 5.2. For scattering states, the wavefunctions are delocalized over entire lattice sites as shown in [Fig. 5.5e]. The wavefunctions of the states corresponding to maximum energy (top of the band) at $K = 0$ and $K = \pi/a$ are shown. The wavefunctions are scaled by their maximum value. With the increase in V_1 , an energy band starts to separate from the scattering states. The states in this isolated band are called bound states. These bound states are identical to the magnon bound states in spin models [118, 127] or the particle bound states in Hubbard models [122–126]. They are characterized by an exponentially decaying wavefunction $\phi_K(r)$. For small values of interaction ($V_1 = 0.2$), the bound states band is partially separated from the scattering states Fig. [5.5b]. The states near the end of the Brillouin zone ($K = \pm\pi/a$) are separated from the scattering states while the states at $K = 0$ are still part of the scattering states. This is reflected in the wavefunction at the corresponding K value. As shown in Fig.[5.5f] At $K = \pm\pi/a$ (solid line) the wavefunctions are localized with exponential decay while at $K = 0$ (dashed line) the wavefunctions are delocalized. Further increase in the value of V_1 completely separates the bound state band from the scattering states. For $V_1/J = 0.5$, the states at both $K = 0$ and $K = \pm\pi$ are separated from the scattering states and have exponentially decaying wavefunctions see Fig. [5.5g]. The wave function at $K = \pm\pi$ is more localized than $K = 0$ due to fewer hopping terms at $K = \pm\pi$. Hence it takes a large V_1 to localized the wavefunction at $K = 0$. Further increase in V_1 separates the bound state band even more from the scattering states. The curvature of the bound state band decreases with an increase in V_1 5.5(d). The corresponding wavefunctions also get more and more localized with an increase in V_1 see Fig. [5.5(g)]. Hence we can conclude that an increase in RRI interaction strength favors the formation of bound states in the spectrum.

On the other hand, for a fixed value of V_1 , an increase in L has the opposite effect. As shown in Fig. [5.6 (a,d)], For $V_1/J = 0.5$ and $L/a = 0.4$ we have a completely separated bound state band and localized wavefunctions at $K = 0$ and $K = \pm\pi$. Increasing L changes the scattering states in such a way that the bound state band gets partially merged with the scattering states Fig. [5.6b]. This, as expected makes the wavefunctions at $K = 0$ delocalized Fig. [5.6e]. Further increase in L modifies the spectrum such that the entire bound state band becomes the part of the scattering state and the wavefunctions become delocalized for all K values. Hence increase in L eliminates the bound states from the spectrum.

To characterize the competition between the RRIs (V_1) and exchange couplings

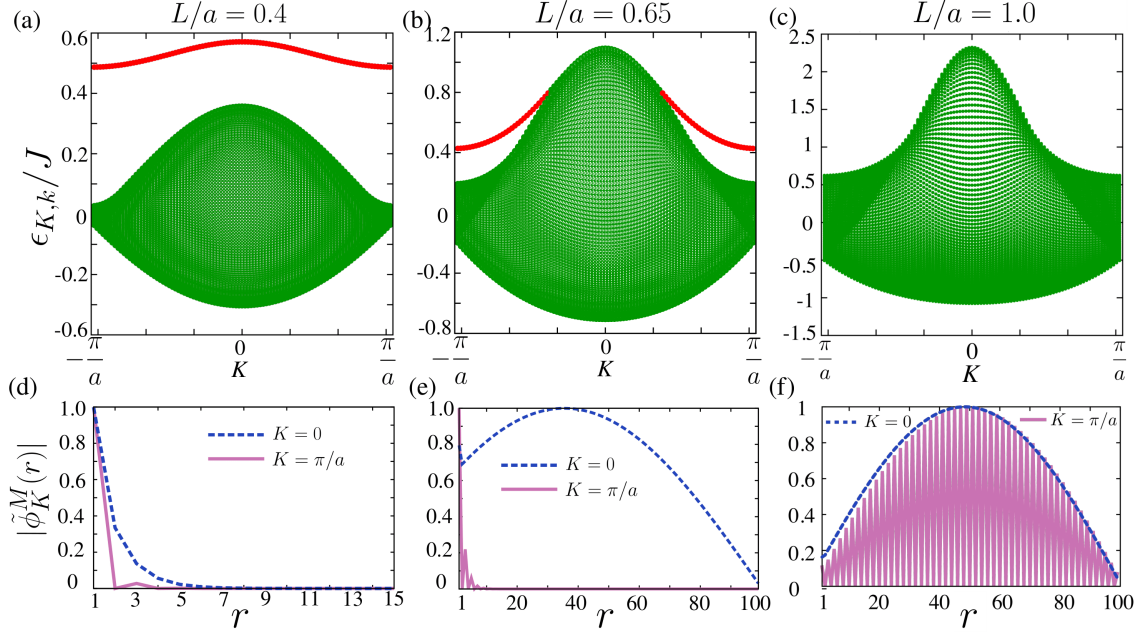


Figure 5.6: (Color online) The two excitation spectrum for $V_1/J = 0.5$, and For (a) $L/a = 0.4$, (b) $L/a = 0.65$ and (c) $L/a = 1.0$. The solid (red) line in (b) shows the isolated band for the bound states. (d)-(f) show the highest radial eigenfunctions (scaled by its maximum value) for $K = 0$ (dashed line) and $K = \pi/a$ (solid line), respectively for the excitation spectrum shown in (a)-(c).

L , we introduce a new parameter, the scaled radial width of the functions $\phi_K^M(r)$, and averaged over K ,

$$\Delta r = \frac{a}{2\pi N} \int_{-\pi/a}^{\pi/a} \Delta r_K dK, \quad (5.5)$$

where $\Delta r_K = \sqrt{\langle r^2 \rangle_K - \langle r \rangle_K^2}$, and the symbol $\langle \dots \rangle_K$ indicates that the average is taken over the state $\phi_K^M(r)$. In Fig. [5.7a], we show Δr as a function of V_1 and L , which identifies three different regions R1, R2, and R3. For sufficiently small values of L and large values of V_1 (region R1), we have $\Delta r \sim 0$. This implies that the radial states $\phi_K^M(r)$ are purely bound states, highly localized, and the energy spectrum has an isolated band of bound states, as shown in Fig. [5.5b]. At the other end, in region R3, the width Δr takes the maximum value (~ 0.2). It means that $\phi_K^M(r)$ are purely scattering states and the energy spectrum has no bound states, as shown in Fig. [5.5c]. The intermediate region R2 stands for an energy spectrum similar to the one shown in Fig. [5.5a], i.e., a partially separated bound state band that consists of scattering states as well.

Now we focus on obtaining analytical expressions for the boundaries separating the regions R1, R2, and R3. To simplify the analysis, we truncate the exchange

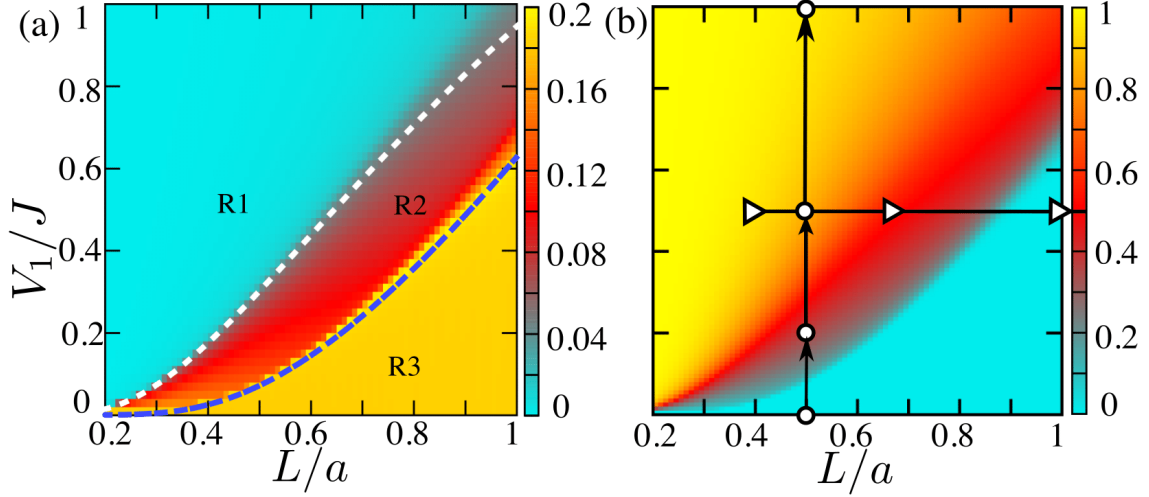


Figure 5.7: (a) The scaled, K -averaged Δr as a function of V_1 and L . In region R1, the excitation spectrum $\epsilon_{K,k}$ is characterized by an isolated band of bound states, in region R2 spectrum consists of at least one bound state, but there is no isolated band for bound states [see Fig. 5.5a], and in R3 region, $\epsilon_{K,k}$ has only scattering states. The dashed line between regions R1 and R2 is obtained from a truncated model whereas the same between regions R2 and R3 is provided by the criteria $V_1^{cr} = \epsilon_{\pi/a, \pi/2a}^0$. (b) The K -integrated overlap $\mathcal{O}_1^M$ of $\phi_K^M(r)$ on the initial state in which the two excitations are localized at the nearest neighbor sites ($d_0 = 1$).

couplings up to the next nearest neighbor and the RRI's up to the nearest neighbor terms. We obtain the energy of scattering and bound states as [127],

$$\epsilon_{K,k}^0 \simeq 2 \left(J_1^K \cos(ka) + J_2^K \cos(2ka) \right), \quad (5.6)$$

$$\epsilon_K^b \simeq 2J_2^K + \frac{(J_1^K)^2}{V_1} + \frac{(J_1^K)^2 J_2^K}{V_1^2} + \frac{V_1^2}{V_1 + J_2^K}, \quad (5.7)$$

respectively. The term J_d^K is given below Eq. (5.2) and the bound-state energy is independent of k . A bound state exists if

$$\epsilon_K^b - (\epsilon_{K,k}^0)_{max} > 0, \quad (5.8)$$

where $(\epsilon_{K,k}^0)_{max}$ is the maximum eigenvalue among the scattering states for a given K . Since the bound state first appears at $K = \pi/a$, the boundary between the regions R2 and R3 in Fig. [5.7a] is given by $\epsilon_{\pi/a}^b - (\epsilon_{\pi/a,k}^0)_{max} = 0$. The latter provides us the critical RRI strength V_1^{cr} above which we have at least a single bound state in the energy spectrum. Analytically, we have $V_{cr}^1 = 4Je^{-2a/L}$ and also using the truncated model, we have $\epsilon_{\pi/a, \pi/2a}^0 \simeq 4Je^{-2a/L}$. Therefore we assume that the critical value, $V_{cr}^1 = \epsilon_{\pi/a, \pi/2a}^0$ is valid beyond the truncated model and this is found to be in

good agreement with the numerical results even for sufficiently large L . Similarly, by taking $K = 0$ in Eq. (5.8), we can estimate a second critical RRI strength V_{cr}^2 above which we have a bound state at $K = 0$ or equivalently to have an isolated band of bound states. The truncated model gives us $V_{cr}^2 \simeq \left[J_1^0 + \sqrt{(J_1^0)^2 + 4J_1^0 J_2^0} \right] / 2$ with $J_1^0 = 2Je^{-a/L}$ and $J_2^0 = 2Je^{-2a/L}$, and this value separates the regions R1 and R2 in Fig. [5.7a], At large values of L , the analytical estimation of V_{cr}^2 from the truncated model starts to deviate from the exact numerical results since the long-range nature of the interactions become non-negligible. Henceforth, we restrict to $L/a \in [0, 1]$ with no restrictions on V_1 .

5.3.2 Dynamics

The dynamics of excitations under $\hat{H}_t$ crucially depends upon the interaction parameters L and V_1 and the overlap of the initial state onto the eigenstates of the Hamiltonian. When the initial state has a large overlap onto the scattering state we observe the dynamics in which the delocalization of excitations is favored. On the other hand, if the initial state has complete overlap with the bound state band, we observe the bound state dynamics. For the case where there is finite overlap with the bound and scattering states, we observe both bound state and delocalization dynamics. First, we study the dynamics in detail for the initial state in which two excitations are placed in the adjacent lattice sites ($d_0 = 1$) at the center of the lattice. To quantify the overlap of this initial state onto the eigenstates we define an overlap function

$$\mathcal{O}_{d_0}^M = \int_{-\pi/a}^{\pi/a} |\langle \phi_K^M | \psi(t=0) \rangle|^2 dK, \quad (5.9)$$

which measures the overlap of the initial state $|\psi(t=0)\rangle$ onto the eigenstates $|\phi_K^M\rangle$ corresponding to the topmost eigenstates at each K . In the state $|\psi(t=0)\rangle$, excitations are separated by d_0 lattice sites. We define n th-order bound states as those having the radial wave functions $\{\phi_K^{M-n}(r)\}$ with a peak at $r = (n+1)a$. With this the first band that separates from the scattering state is called the zeroth order bound state band. We calculate the overlap of the initial state onto the zeroth order bound state band. The Fig.[5.7b] shows $\mathcal{O}_1^M$ as a function of V_1 and L . For small values of $V_1 < \epsilon_{\pi/a, \pi/2a}^0$, in the region R3, the zeroth-order band is a part of the scattering states. Hence the contribution to $\mathcal{O}_1^M$ from the zeroth-order band is negligible, resulting in smaller $\mathcal{O}_1^M$ in R3. For the parameters in the region R3, an

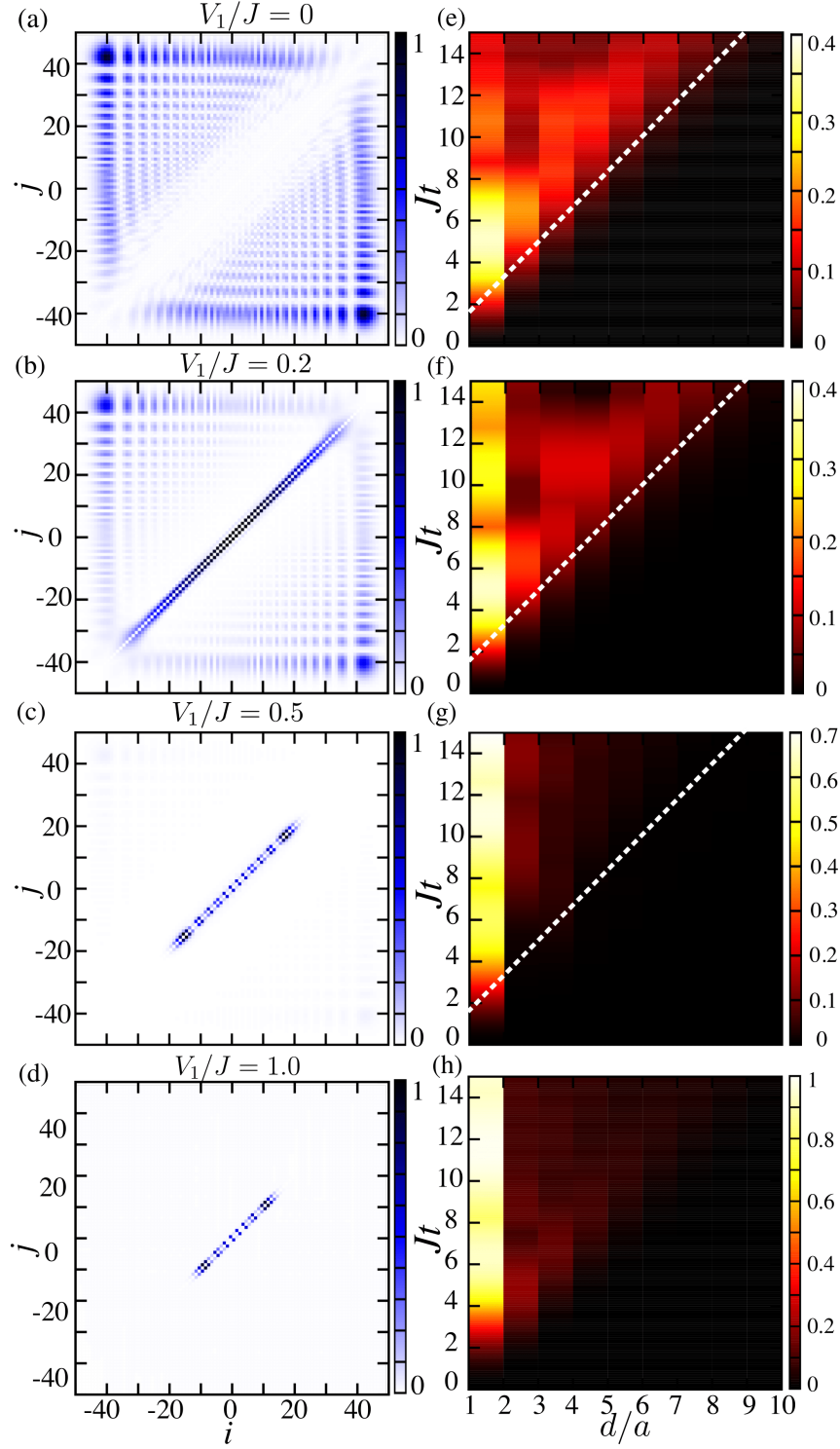


Figure 5.8: (a)-(d) The two-excitation dynamics $[\Gamma_{ij}(t)]$ for the initial state in which the two excitations are localized in the nearest neighbor sites ($d_0 = 1$) at the center of the lattice at $Jt = 150$. The interaction parameters are given above each plot, and the excitation spectrum for the same parameters are shown in Fig. 5.5(a)-5.5(d). The plots (e)-(h) show the corresponding correlations $C(d, t)$ for the dynamics shown in (a)-(d), respectively. The dashed line in (e)-(g) shows the theoretical estimate of maximum group velocity from the single excitation spectrum.

initial state with $d_0 = 1$ will have a major overlap with the scattering states. On the other hand for $V_1 \gg V_{cr}^2$, in region R1, the zeroth-order bound state band is completely separated from the scattering states with each eigenfunction localized at $r = a$. Hence the initial state with $d_0 = 1$ has complete overlap onto this band, resulting in the maximum value of $\mathcal{O}_1^M \approx 1$. Hence in region R1, the initial state has major overlap with the bound states. For an intermediate value of L and V_1 , the zeroth-order bound state band is partially separated from the scattering state hence the initial state with $d_0 = 1$ has overlap with both the bound states and the scattering states, resulting in an intermediate value of $0 < \mathcal{O}_1^M < 1$.

The variation of $\mathcal{O}_1^M$ discussed above will determine the time evolution of the initial state for various V_1 and L . We first fix the value of $L/a = 0.5$ and see the effect of increasing V_1 onto the dynamics. Fig. [5.8(a-d)] shows the scaled probability distribution for the parameters in Fig. [5.5(a-d)]. The corresponding points in the $\mathcal{O}_1^M$ are shown by white circles in Fig. [5.7(b)]. For $V_1 = 0$, we observe the anti-bunching dynamics as discussed in the non-interacting excitation section. This can be explained based on the absence of the bound states in the spectrum and the vanishing overlap $\mathcal{O}_1^M$. With the increase in $V_1/J = 0.2$, the bound state dynamics start to appear in the dynamics indicated by non-zero values along the diagonal in Fig. [5.8b]. Since the bound state band is not fully separated from the scattering state and $\mathcal{O}_1^M < 1$, we observe the co-existence of anti-bunching and bound state dynamics. This onset of bound state dynamics is due to finite $\mathcal{O}_1^M$ in Fig. [5.7b], resulting from a partially separated zeroth-order bound state band in Fig. [5.5b]. Further increase in the value of V_1 increases the $\mathcal{O}_1^M$, which suppresses the anti-bunching dynamics and enhances the bound state dynamics. For $V_1/J = 0.5$ there is complete bound state dynamics due $\mathcal{O}_1^M \approx 1$ due to completely separated bound state band. Further increase in V_1 monotonously increases both the separation of the bound state band from the scattering states and the overlap $\mathcal{O}_1^M = 1$ resulting in complete bound state dynamics. Notice for $V_1/J = 1$ the dynamics is slower than that of $V_1/J = 0.5$. This is attributed to the decreased curvature of the bound state band for $V_1/J = 1$ Fig. [5.5d].

On the other hand for a fixed value of V_1 increase in L has the opposite effect. For $V_1/J = 0.5$ there is a completely separated bound state band for $L/a = 0.4$ Fig [5.5a]. The overlap function $\mathcal{O}_1^M \approx 1$ Fig. [5.7b][white triangle]. This explains the dominant bound state dynamics observed Fig. [5.9a]. An increase in $L/a = 0.65$ modifies the spectrum in a such way that the bound state band gets partially merged

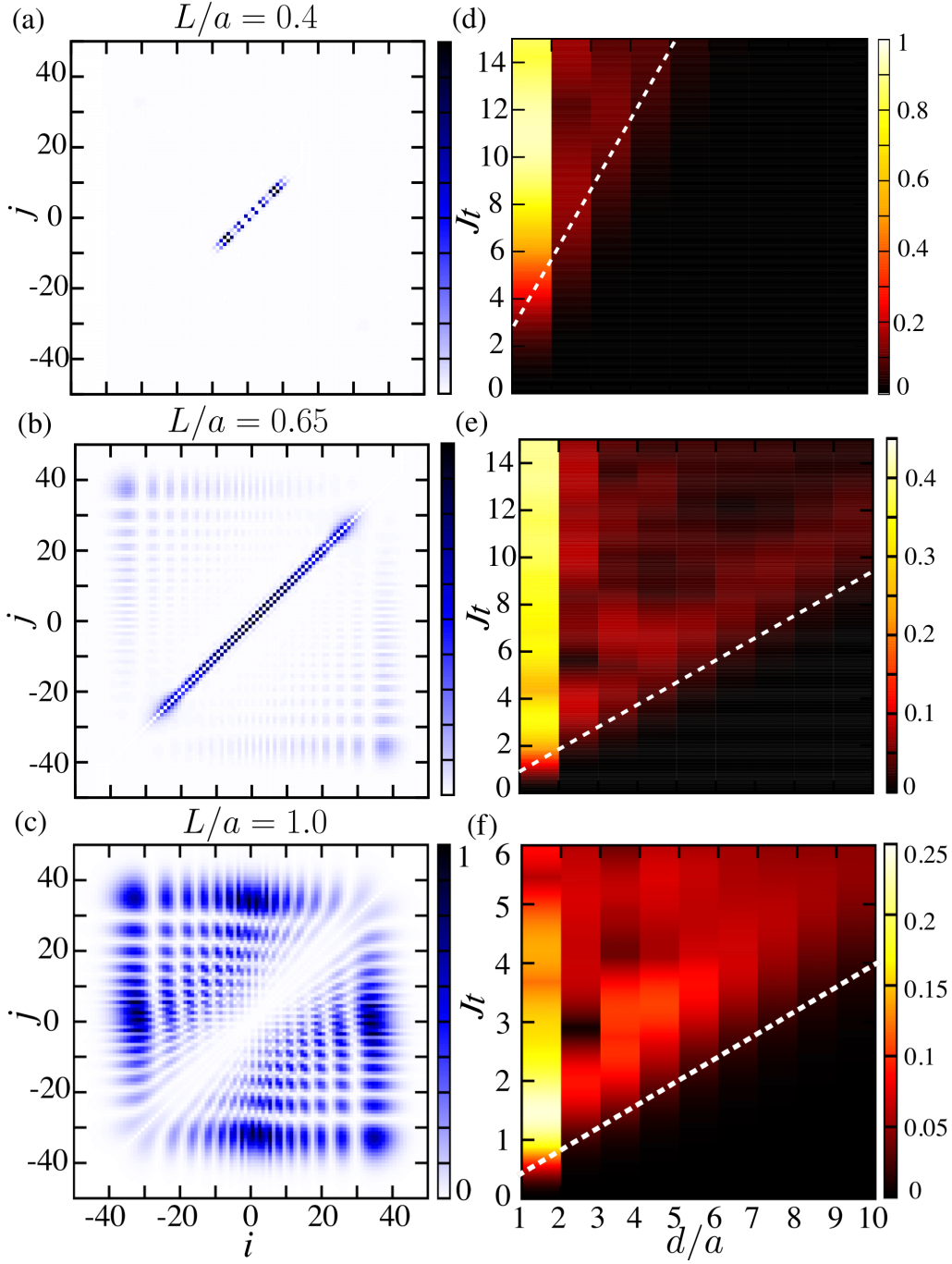


Figure 5.9: (a)-(c) show the two-excitation dynamics $[\Gamma_{ij}(t)]$ for the initial state in which the two excitations are localized in the nearest neighbor sites ($d_0 = 1$) at the center of the lattice. The interaction parameters are given above each plot, and the excitation spectrum for the same parameters are shown in Fig. 5.6(a)-5.6(c). The plots (d)-(f) show the corresponding correlations $C(d, t)$ for the dynamics shown in (a)-(c), respectively. The dashed line in (d)-(f) shows the theoretical estimate from maximum group velocity. The times at which each of the snapshots are taken (a) $Jt = 150$, (b) $Jt = 150$, and (c) $Jt = 30$.

with the scattering states resulting in the decrease in $\mathcal{O}_1^M$. This alters the dynamics from purely bound state to coexisting bound state and anti-bunching dynamics. Fig [5.9b]. Further increase in L completely merges the bound state band into the scattering states resulting in $\mathcal{O}_1^M \approx 0$ leading to completely delocalized dynamics for $L/a = 1$ as shown in Fig. [5.9c]. Hence both L and V_1 can be used to control the nature of the dynamics observed in the system.

To characterize the correlations building up in the system during the time evolution we look at the two-point correlations in the excitation dynamics given by,

$$C(d, t) = \sum_i (\langle \hat{\sigma}_{ee}^i \hat{\sigma}_{ee}^{i+d} \rangle - \langle \hat{\sigma}_{ee}^i \rangle \langle \hat{\sigma}_{ee}^{i+d} \rangle) \quad (5.10)$$

where $\langle \dots \rangle \equiv \langle \psi(t) | \dots | \psi(t) \rangle$. For all the parameters mentioned above, we show the corresponding correlation dynamics plots alongside the scaled distribution plots Fig. [5.8(e-h)] and Fig. [5.9(d-f)]. The parameter values for which there is either a partially or completely separated bound state band and have non-zero overlap function $\mathcal{O}_1^M$ we observe the spreading of correlations across the system as excitations get delocalized. This spreading of correlations results in the light cone-like behavior [see Fig. [5.8(e,g)]. The light cone boundaries can be obtained from the maximum group velocity as $da/(2v_g^{max})$. Beyond these light-cone boundaries, the correlation function decays exponentially. This type of Lieb-Robinson upper bound is known to be a feature of short-range [129] or weakly long-range interacting quantum systems [130]. Light cone behavior persists even for large values of exchange couplings $L/a = 1$. However for larger values of L the slope of the light cone boundary decreases due to an increase in v_g^{max} , indicating a faster propagation of correlations. For large V_1 values which result in complete bound state dynamics, we see no propagation of correlations. The formation of the bound state with excitation separated by a lattice site results in a constant correlation at $d = a$ at all the time during the time evolution Fig. [5.8(g-h)].

Effect of the initial separation between excitations.— So far we studied the initial state for which excitations were kept in the adjacent lattice sites ($d_0 = 1$). In this section, we show how the initial separation can drastically alter the dynamics and can lead to a counter-intuitive phenomenon. We focus on the case of $d_0 = 2$. To explain the complex dynamics observed in this case we need to look at both $\mathcal{O}_2^M$ and $\mathcal{O}_2^{M-1}$ which represent the overlap of the initial state with the zeroth order and the first order bound state bands respectively. The non-monotonous behavior of $\mathcal{O}_2^M$ [see Fig. 5.10a] leads to interesting dynamics.

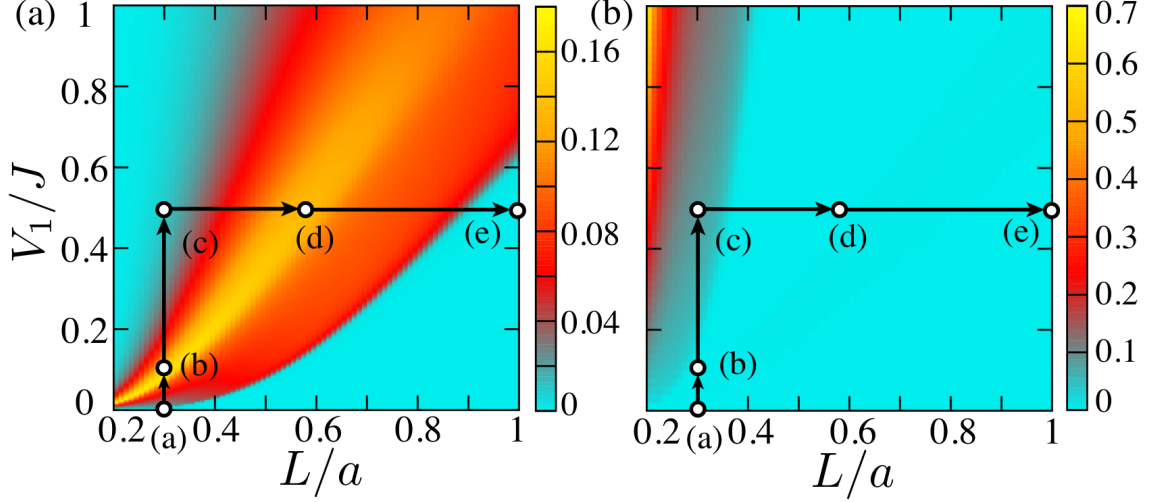


Figure 5.10: The initial state overlaps (a) $\mathcal{O}_2^M$ and (b) $\mathcal{O}_2^{M-1}$ for $d_0 = 2$. For the points marked as a, b, c, d, and e, the dynamics and correlations are shown in Fig. [5.11].

The excitation and two-point correlation dynamics as a function of V_1 and L for $d_0 = 2$ are shown in Fig. [5.11]. For $d_0 = 1$, we have seen that the presence of bound states in the dynamics monotonously increases with V_1 while keeping L constant or decreases with L for a fixed V_1 . On the contrary, for $d_0 = 2$ (see Fig. [5.11]), the two excitation dynamics shows a non-monotonous behavior as a function of both L and V_1 . For $V_1/J = 0$, we observe the delocalization behavior which is completely different than anti-bunching behavior observed for $d_0 = 1$ case (see Fig. [5.11a]). With an increase in $V_1/J = 0.1$ we observe the onset of bound state dynamics Fig. [5.11b] which is due to an increase in the value of both $\mathcal{O}_2^M$ and $\mathcal{O}_2^{M-1}$ see Fig. [5.10]. Surprisingly, further increase in $V_1/J = 0.5$ reduces the bound state dynamics resulting in anti-bunching dynamics Fig. [5.11c]. In contrast to $d_0 = 1$ case where an increase in V_1 favored the bound state, for $d_0 = 2$, increase in V_1 favors the anti-bunching dynamics! This can be explained by looking at $\mathcal{O}_2^M$ in 5.10(a), where increase in V_1 leads to the region in which we have $\mathcal{O}_2^M \approx 0$ and $\mathcal{O}_2^{M-1} \approx 0$. This implies that for a certain value of $V_1 \neq 0$ the initial state $d_0 = 2$ will have zero overlap with the bound state bands and complete overlap with the scattering states resulting in dominant anti-bunching even at large V_1 . Similarly, for a fixed value of $V_1/J = 0.5$ increase in $L/a = 0.58$ enhances the bound state dynamics in contrast to $d_0 = 1$ case, where an increase in L reduced the bound state dynamics. This is because at $V_1/J = 0.5$, increase in L/a from 0.3 to 0.58 changes the overlap such that the initial state has finite overlap with $\mathcal{O}_2^M$ Fig. [5.10a] which results in the onset of bound state dynamics. However further increment of L eliminates this

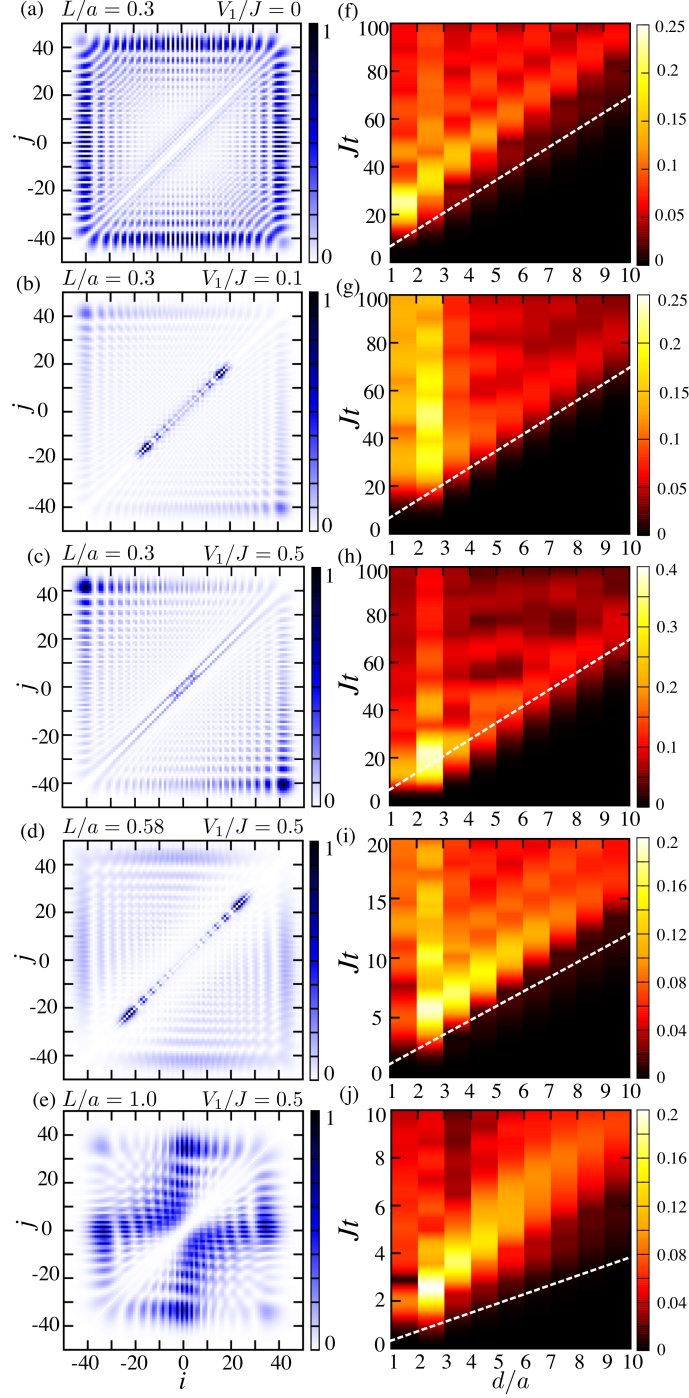


Figure 5.11: (a)-(e) show the dynamics with $d_0 = 2$ for the points (a)-(e) marked in Fig. [5.10]. The corresponding dynamics of the correlations $C(d, t)$ are shown in (f)-(j), respectively. The dashed line shows the theoretical estimate of maximum group velocity from the single excitation spectrum. In (g) and (i), the bound state character is revealed by the prominent peak along $d = 2$. In all these cases, we see a light-cone like structure in the correlation dynamics. The times at which each of the snapshots are taken (a)-(c) $Jt = 600$, (d) $Jt = 110$, and (e) $Jt = 30$.

bound state dynamics as seen in Fig. [5.11e] for $L/a = 1$. For all these cases, we see a light-cone like structure in the propagation of two-point correlations, as shown in Fig.[5.11(f-j)], due to presence of scattering states.

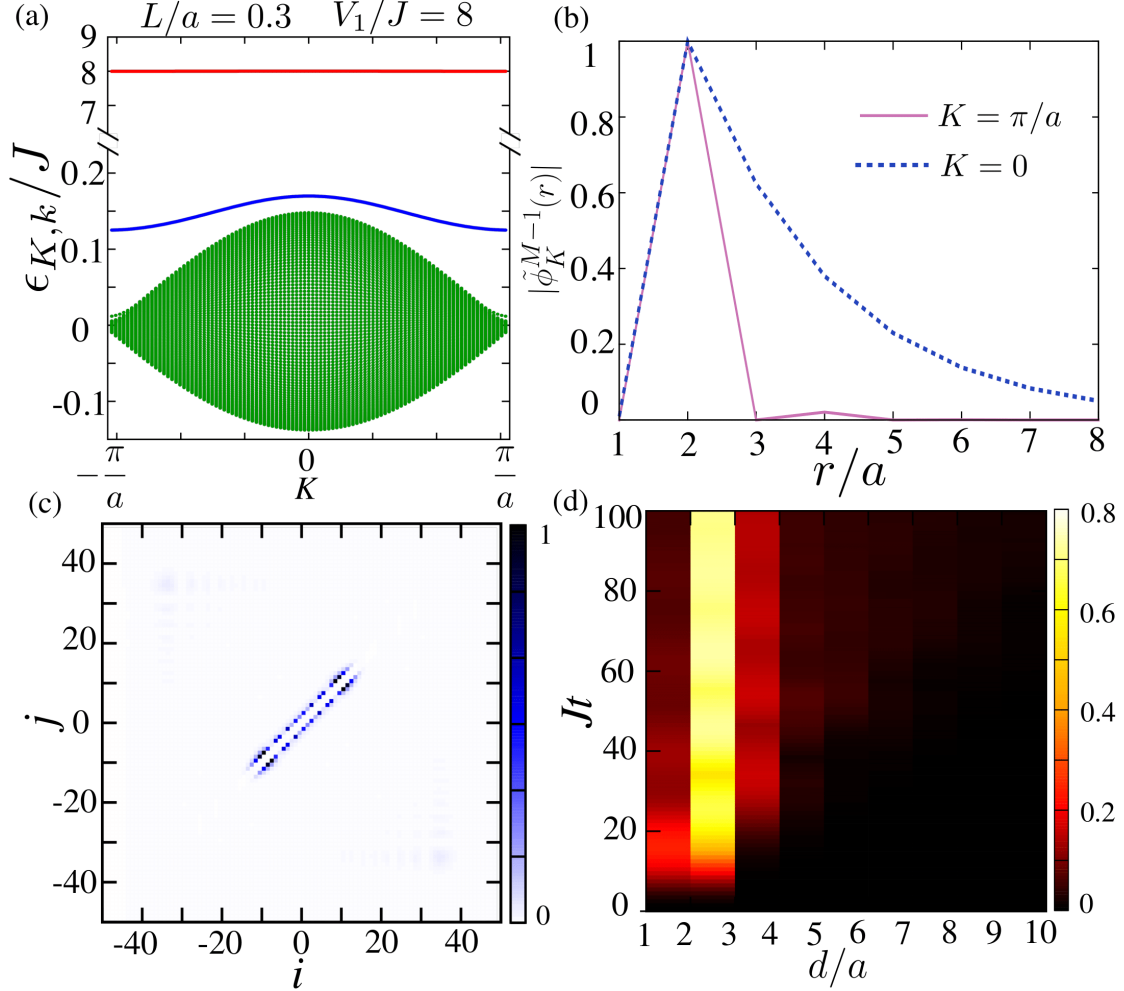


Figure 5.12: (a) The quasi-particle spectrum with two bands of bound states. The top most one we term it as the zeroth order bound states, with radial functions $\{\phi_K^M(r)\}$ having a peak at $r = a$. The second highest band of bound states are represented by $\{\phi_K^{M-1}(r)\}$ having a peak at $r = 2a$ as shown in (b) $K = 0$ (dashed line) and $K = \pi/a$ (solid line). (c) The scaled probability distribution for the initial state with $d_0 = 2$ and interaction parameters as (a) shown at $Jt = 500$. (d) The two point correlation function for the parameters in (a)

Strongly interacting case.— For $V_1 \gg V_{cr}^2$, bands of higher-order bound states emerge in the spectrum. Depending upon the value of V_1 , there will exist partially or fully separated bound state bands in the spectrum. The existence of these higher-order bound state bands will affect the excitation dynamics depending upon the initial conditions. As shown in Fig. [5.12a], for $V_1/J = 8$ and $L/a = 0.3$ there exist

two fully separated bound state bands corresponding to zeroth order (red line) and first-order (blue line) bound states. The wavefunctions for the first order bound state are peaked at $r = 2a$. Fig. [5.12b] shows the corresponding wavefunctions at $K = 0$ and $K = \pm\pi$. Now for the initial state with $d_0 = 2$ and interaction parameters mentioned above, we observe the formation of a first-order bound state. The excitations are separated by two lattice sites during the time evolution as shown in Fig. [5.12c]. Accordingly, the two-point correlation function has peaked at $d/a = 2$

To conclude this section, we studied the dynamics for $d_0 = 2$ for different values of V_1 and L . For specific values of parameters, we observed an increase in V_1 favoring the delocalization while an increase in L favored the formation of bound states. This unusual behavior was explained using the overlap of the initial state onto the eigenstates of the Hamiltonian. In the next section, we study the effect of RRI on entanglement dynamics.

5.3.3 Entanglement entropy

In this section, we extend the analysis of $\mathcal{S}_A(t)$, to include the effect of RRIs. In particular, we look at the impact of interaction-induced bound states on the growth of bipartite entanglement. Again, we assume that the two excitations are initially localized in the subsystem B , as shown in Fig. [5.4d], and use the basis states having zero, one, and two excitations, as discussed in Sec. 5.2.2. We see that RRIs do not affect the growth of $\mathcal{S}_A(t)$ qualitatively but only quantitatively. To show this, we fix $L/a = 0.5$ (for which $V_{cr}^1/J \sim 0.073$ and $V_{cr}^2/J \sim 0.303$) and vary V_1 . We consider different values of V_1 from three different regions: R3 ($V_1 < V_{cr}^1$), R2 ($V_{cr}^1 < V_1 < V_{cr}^2$), and R1 ($V_1 > V_{cr}^2$) as in Fig. [5.7a]. In the region R3, $0 < V_1/J < 0.07$, RRI has a small influence on the eigenstates. The eigenstates of the hamiltonian just start to become localized in the region R3. This is reflected in the probability distribution where the probability to find the excitations closer to each other increases for $V_1/J = 0.07$ Fig. 5.14(b). This decreases the flow of the probability across the boundary of the sub-system which eventually reduces the value of both $\mathcal{S}_A$ and $\bar{\mathcal{S}}_A$ Fig. [5.13]. With an increase in V_1 , in region R2, we have the presence of both anti-bunching and bound state dynamics Fig. [5.14c]. The simultaneous existence of anti-bunching and bound state enhances the probability distribution crossing the sub-system boundary which leads to an increase in the $\bar{\mathcal{S}}_A$

in the region R2. Further increase in V_1 suppresses the probability flow due to anti-bunching and favors only the bound state dynamics. This results in a decrease of $\mathcal{S}_A$ and $\bar{\mathcal{S}}_A$ for larger V_1 . The change in the oscillation frequency of $\mathcal{S}_A$ can be explained based on the underlying dynamics responsible for the entanglement generation. In region R1, it's due to single excitation hopping, which has a higher hopping rate hence the higher frequency. Since the region R2 consists of both single excitation hopping and bound state hopping, there is no well-defined oscillation frequency of $\mathcal{S}_A$. For R3, the bound state has a smaller hopping rate due to the second-order nature of the hopping. This results in a smaller oscillation frequency of $\mathcal{S}_A$ Fig. [5.13a].

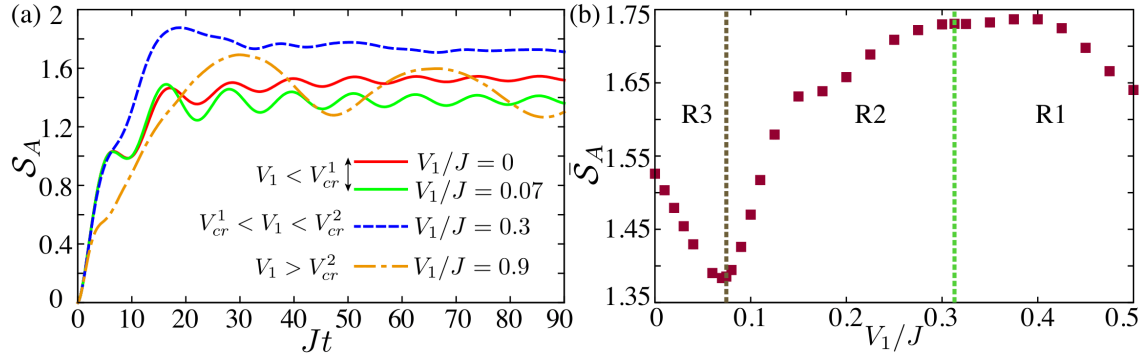


Figure 5.13: The dynamics of $\mathcal{S}_A(t)$ for $d_0 = 1$ and $L/a = 0.5$ with different values of V_1 . The values of V_1 covers three different regions (R1, R2, and R3) based on the nature of excitation spectrum. In R3, we have $V_1 < V_{cr}^1$, and the excitation spectrum possesses no bound states, and the effect of interaction is to reduce the effective exchange couplings. In R2 ($V_{cr}^1 < V_1 < V_{cr}^2$), excitation spectrum has a partially separated band of bound states and, in R1 ($V_1 > V_{cr}^2$) the spectrum possesses an isolated band of bound states. Deep in R1, the initial state becomes a source of bound state quasi-particles. (b) shows the behavior of $\bar{\mathcal{S}}_A$ in three different regions, and dashed vertical lines show V_{cr}^1 (left) and V_{cr}^2 (right).

5.4 Dissipative Dynamics

Similar to the case of single excitation, we study the effect of spontaneous emission on two excitations dynamics. We show that all the features observed above are present in the case of dissipation. In particular, we show the anti-bunching dynamics for $V_1 = 0$ Fig. [5.15a], the presence of both bound states and anti-bunching Fig. [5.15b], and the quantum walk of a bound pair of excitations as we increase V_1 .

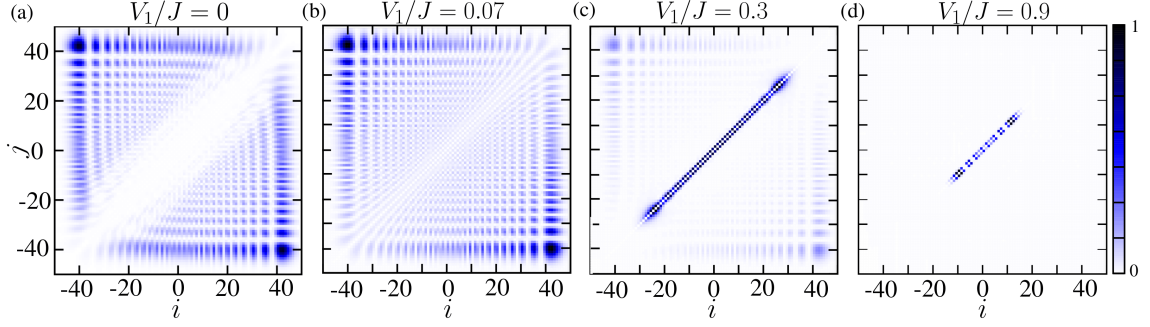


Figure 5.14: The scaled probability distribution for the initial state with $d_0 = 1$ and exchange coupling $L/a = 0.5$ (a)-(d) $V_1/J = 0, 0.07, 0.3$ and 0.9 shown at $Jt = 150$

Fig. [5.15(c-d)] depicts the dynamics of zeroth and first-order bound states in Fig. [5.15(c-d)], respectively. In these simulations we have taken $\gamma = 0.01J$, and also verified that the features are survived up to a decay rate of $\gamma = 0.05J$. Note that, for the single excitation case, we could afford to have a larger decay rate compared to that for two excitations in order to see all the characteristic features.

5.5 Experimental Parameters

Finally, we propose a realistic set of parameters for an experiment with Rubidium atoms coupled to a PCW. The hopping strength J and the range L of the exchange interactions can be tuned by either varying the properties of PCW (e.g. band curvature α) or of the excited atomic state $|e\rangle$. In particular, the strength of the hopping ($J \propto d_{eg}^2$) and of the RRIIs $C_6 \propto d_{eg}^4$ can be made significantly large (of several MHz) by choosing a highly excited Rydberg state $|e\rangle$ with a large dipole moment d_{eg} . For instance, if we take a Rydberg $45S_{1/2}$ state of a Rubidium atom, the lifetime is approximately $101 \mu s$ [131] or equivalently $\gamma/J = 0.0099$ ($\sim 1\%$ of J) if $J = 1 \text{ MHz}$. Therefore, by choosing a significantly high $nS_{1/2}$ Rydberg state, with $n > 30$, we strongly reduce the effect of the spontaneous emission. Note that, in order to use Rubidium $nS_{1/2}$ Rydberg states, one has to rely on either three-level ladder [113] or a lambda scheme [95], which in turn can be used to modify exchange interaction strength J beyond the values set by the PCW structure. Alternatively, one could prepare a $nP_{3/2}$ Rydberg excited state, for which the C_6 coefficient exhibits an additional angular dependence $C_6 \propto \sin^4 \theta$, where θ is the angle between the quantization axis and radial vector between the two Rydberg excitations. In this way, we can externally control the Rydberg-Rydberg interactions from zero (non-interacting

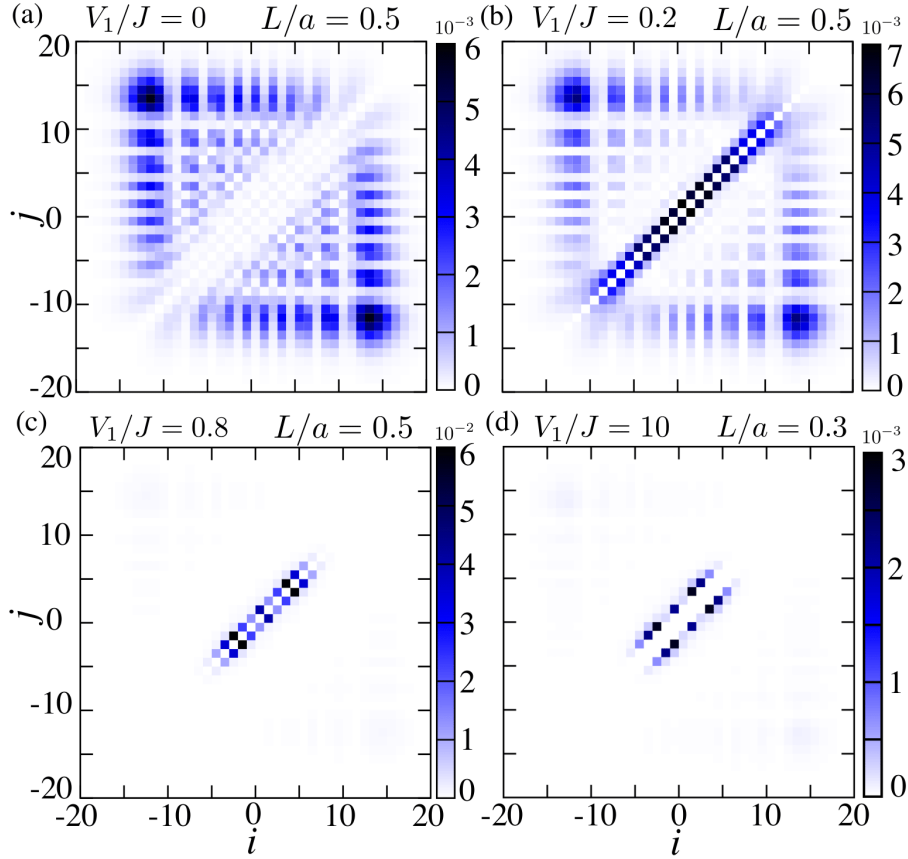


Figure 5.15: Two-excitation dissipative dynamics for $L/a = 0.5$ and (a) $V_1 = 0$, $V_1/J = 0.2$, and $V_1/J = 0.8$ with $\gamma/J = 0.01$. (a) shows the anti-bunching dynamics, (b) exhibits both anti-bunching and bound state dynamics, and (c)-(d) shows the quantum walk of a bound pair of two excitations. (c) and (d) shows the zeroth and first order bound states, respectively. For (d) $L/a = 0.3$ and $V_1/J = 10$. The times at which each of the snapshots are taken (a)-(c) $Jt = 50$, and (d) $Jt = 200$.

case) to a maximum value by changing the angle θ for a fixed n [63, 132].

In the following, we comment on how to read out the excitation dynamics in our setup. Since the atomic resonant frequency lies at the bandgap, we cannot map the atomic excitation into the photons of the waveguide modes. One way would be to optically transfer the atomic excitation into the lowest atomic state so that the information can be mapped into guided photons. Another way, which is currently being employed in atomic lattices with Rydberg excitations [133], is to first remove the traps for all atoms, and then use dipole traps to recapture the ground-state atoms. The presence of ground-state atoms can be detected using fluorescence imaging. Once the ground state population is estimated, the same for the Rydberg excitations can be calculated by simple subtraction. In this way, a significantly long

coherent exchange dynamics of Rydberg excitations via Förster resonance, up to $4\mu\text{s}$ has been demonstrated in [133].

Currently, there is intense effort to improve nano-photonic device fabrication, and eventually to realize one-dimensional (1D) and two-dimensional (2D) lattices of atoms near the PC waveguides using an array of optical tweezers [134]. In particular, it has been demonstrated a lattice with 17 tweezer sites with $10\mu\text{m}$ separation between the adjacent sites and a distance of $1\mu\text{m}$ to $10\mu\text{m}$ away from the PCW. The separation between the PCW and atom lattice is sufficiently large compared to the radius of $nS_{1/2}$ Rydberg state with $n = 40 - 100$, which ranges from 108 nm to 740 nm. Thus, one can adjust the separation between atoms and PCW to suppress unwanted effects from stray fields or PCW surfaces [112, 113].

5.6 Summary

In the case of two Rydberg excitations, the RRIs enter into play, and there exists a competition between the scattering and bound states that emerge in the dynamics. The latter leads to non-trivial dynamics for both excitations and the resulting correlations. We observe anti-bunching, co-existence of anti-bunching and bound-state dynamics, and a CTQW of a bound pair of two excitations. We extended the analysis of bipartite entanglement entropy in the presence of two excitations. In contrast to the single excitation case, the entanglement entropy for two excitations is not globally bounded as it depends on the system parameters. Moreover, we analyzed the two-point correlation function for two excitations, which reveals a light-cone behavior even for sufficiently long-range exchange couplings.

We also discussed the dissipative dynamics, including imperfections due to the spontaneous emission from the Rydberg state into photons outside the waveguide. We showed that the features of the coherent dynamics for one and two Rydberg excitations are intact up to reasonable decay rates of 5% of the hopping rate. The complex dynamics of the Rydberg excitations and their quantum correlations when propagating through the waveguide could be measured via photo-detection or multi-photon homodyne measurement techniques at the photonic outputs of the waveguide [135–139].

The excitation transport has been previously studied in Rydberg gases but mediated by dipole-dipole interactions involving multiple Rydberg states (via Förster resonances) [133, 140–142] and the environment also played a crucial role in the

transport properties. Therefore, one new direction would be to probe the role of the environment in the quantum diffusion of Rydberg excitations in a PC setup. Besides, if multiple Rydberg states are involved, the competition between dipole-dipole and cavity-mediated exchange interactions may lead to non-trivial scenarios. Further, if we allowed overlapping the Rydberg orbitals of two excitations, the strong Coulomb interactions between the delocalized electrons may lead to novel correlated phases, assuming the Penning ionization rates can be significantly suppressed [143]. Our analysis on bound states of two excitations can shed new light on the mechanisms for stabilizing bound states by repulsive interactions, using a completely different setup compared to the traditional Hubbard models. In addition, our approach can be extended to three or more excitations, where the emergence of three-body bound states would be very relevant in the context of Efimov physics [144].

This work is a part of following publication: Dynamics of Rydberg excitations and quantum correlations in an atomic array coupled to a photonic crystal waveguide [111]

5.7 Appendix

5.7.1 Two excitation dispersion

Generalized two excitation state can be written as,

$$|\psi\rangle = \sum_{l_2 > l_1}^N c_{l_1, l_2} |l_1 l_2\rangle \quad (5.11)$$

Solving for

$$\hat{H}_t |\psi\rangle = \epsilon |\psi\rangle$$

$$J \sum_{l_2 > l_1}^N \sum_{j, l}^N C_{l_1, l_2} e^{-|j-l|a/L} \sigma_{eg}^j \sigma_{ge}^l |l_1 l_2\rangle + \sum_{l_2 > l_1}^N \sum_{j, l} C_{l_1, l_2} \frac{V_0}{(|j-l|a)^6} \sigma_{ee}^j \sigma_{ee}^l |l_1 l_2\rangle = \sum_{l_1, l_2} \epsilon C_{l_1, l_2} |l_1 l_2\rangle \quad (5.12)$$

The first term on the LHS becomes,

$$J \sum_{l_2 > l_1} \sum_{j, l} C_{l_1, l_2} e^{-|j-l|a/L} (\delta_{l_1, l} |j l_2\rangle + \delta_{l_2, l} |l_1 j\rangle)$$

$$J \sum_{l_2 > l_1}^N C_{l_1, l_2} \left(\sum_{j < l_1} e^{-|j-l_1|a/L} |jl_2\rangle + \sum_{j > l_1} e^{-|j-l_1|a/L} |jl_2\rangle + \sum_{j < l_2} e^{-|j-l_2|a/L} |l_1j\rangle + \sum_{j > l_2} e^{-|j-l_2|a/L} |l_1j\rangle \right)$$

Let $d = j - l_1$ or $d' = j - l_2$

$$J \sum_{l_2 > l_1}^N C_{l_1, l_2} \left(\sum_{d=1}^{l_1-1} e^{-da/L} |l_1 - d, l_2\rangle + \sum_{d=1}^{N-l_2} e^{-da/L} |l_1, l_2 + d\rangle + \sum_{1 < d < l_2 - l_1} e^{-da/L} |l_1 + d, l_2\rangle + \sum_{1 < d' < l_2 - l_1} e^{-d'a/L} |l_1, l_2 - d'\rangle + \sum_{l_2 - l_1 < d' < N - l_1} e^{-d'a/L} |l_1 + d', l_2\rangle + \sum_{l_2 - l_1 < d' < l_2} e^{-d'a/L} |l_1, l_2 - d'\rangle \right)$$

In the last two terms of the Hamiltonian, the states are changed such that the first index is larger than the second one, Hence we exchange the indices of the Ket to satisfy the condition $l_2 > l_1$.

$$J \sum_{l_2 > l_1}^N C_{l_1, l_2} \left(\sum_{d=1}^{l_1-1} e^{-da/L} |l_1 - d, l_2\rangle + \sum_{d=1}^{N-l_2} e^{-da/L} |l_1, l_2 + d\rangle + \sum_{1 < d < l_2 - l_1} e^{-da/L} |l_1 + d, l_2\rangle + \sum_{1 < d < l_2 - l_1} e^{-da/L} |l_1, l_2 - d\rangle + \sum_{l_2 - l_1 < d < N - l_1} e^{-da/L} |l_2, l_1 + d\rangle + \sum_{l_2 - l_1 < d < l_2} e^{-da/L} |l_2 - d, l_1\rangle \right)$$

Taking projection on to the state $\langle l'_1 l'_2 |$, we get,

$$J \sum_{l'_1, l'_2} \sum_{l_2 > l_1}^N C_{l'_1, l'_2}^* C_{l_1, l_2} \left(\sum_{d=1}^{l_1-1} e^{-da/L} \langle l'_1 l'_2 | l_1 - d, l_2\rangle + \sum_{d=1}^{N-l_2} e^{-da/L} \langle l'_1 l'_2 | l_1, l_2 + d\rangle + \sum_{1 < d < l_2 - l_1} e^{-da/L} \langle l'_1 l'_2 | l_1 + d, l_2\rangle + \sum_{1 < d < l_2 - l_1} e^{-da/L} \langle l'_1 l'_2 | l_1, l_2 - d\rangle + \sum_{l_2 - l_1 < d < N - l_1} e^{-da/L} \langle l'_1 l'_2 | l_2, l_1 + d\rangle + \sum_{l_2 - l_1 < d < l_2} e^{-da/L} \langle l'_1 l'_2 | l_2 - d, l_1\rangle \right) \quad (5.13)$$

Similarly, for other terms we get as

$$\sum_{l'_1, l'_2}^N \sum_{l_2 > l_1} \sum_{j, l} C_{l'_1, l'_2}^* C_{l_1, l_2} \frac{V_0}{(|l_2 - l_1|a)^6} \langle l_1^* l_2^* | l_1 l_2 \rangle \quad (5.14)$$

Define $J_d = J e^{-da/L}$ and using $\langle pq | rs \rangle = \delta_{p,r} \delta_{q,s}$ we get,

$$\begin{aligned} & \sum_{l_2 > l_1}^N \left(\sum_{d=1}^{l_1-1} J_d C_{l_1-d, l_2} + \sum_{d=1}^{N-l_2} J_d C_{l_1, l_2+d} + \sum_{1 < d < l_2-l_1} J_d C_{l_1+d, l_2} + \right. \\ & \left. \sum_{1 < d < l_2-l_1} J_d C_{l_1, l_2-d} + \sum_{l_2-l_1 < d < N-l_1} J_d C_{l_2, l_1+d} + \sum_{l_2-l_1 < d < l_2} J_d C_{l_2-d, l_1} \right) + \\ & \sum_{l_2 > l_1}^N C_{l_1, l_2} \frac{V_0}{(|l_2 - l_1|a)^6} = \sum_{l_1 l_2} \epsilon C_{l_1 l_2} \end{aligned}$$

Let $R = (i + j)a/2$ and $r = (j - i)a$. And taking the ansatz as $c_{ij} = \exp(iKR)\phi_K(r)$ with $\phi_K(r) = \phi_K(-r)$ and $\phi_K(0) = 0$ (hard-core constraint), we get

$$\begin{aligned} & \sum_{l_2 > l_1}^N \left(\sum_{d=1}^{l_1-1} J_d e^{-iKd/2} \phi_K(r+d) + \sum_{d=1}^{N-l_2} J_d e^{+iKd/2} \phi_K(r+d) + \sum_{1 < d < r} J_d (e^{iKd/2} + e^{-iKd/2}) \phi_K(r-d) + \right. \\ & \left. \sum_{r < d < N-l_1} J_d e^{+iKd/2} \phi_K(d-r) + \sum_{r < d < l_2} J_d e^{-iKd/2} \phi_K(d-r) \right) + \frac{V_0}{r^6} \phi_K(r) = \sum_{l_2 > l_1}^N \epsilon_{K,k} \phi_K(r) \end{aligned}$$

Taking the limit $N \rightarrow \infty$ can combining the terms to form cos we get,

$$\begin{aligned} & \sum_{d>1}^{N-1} 2J_d \cos(Kd/2) \phi_K(r+d) + \sum_{d<r} 2J_d \cos(Kd/2) \phi_K(r-d) + \\ & \sum_{d>r}^{N-1} 2J_d \cos(Kd/2) \phi_K(d-r) + \frac{V_0}{r^6} \phi_K(r) = \epsilon_{K,k} \phi_K(r) \end{aligned} \quad (5.15)$$

Which is the Eqn 5.2 of the main text

Chapter 6

Conclusion

The focus of this work has been to integrate Rydberg atoms with various systems in order to achieve control over various aspects of the system. The exaggerated properties of Rydberg atoms were used along with the system-specific properties in order to demonstrate the control over the interactions, correlations, and entanglement in a one-dimensional array of Rydberg atoms.

In particular, in the first chapter, we studied the extended Bose-Hubbard model with Rydberg-dressed interaction for atoms in the two lowest vibrational bands. We calculated the Wannier functions for particles in the two lowest bands. Using those Wannier functions, we calculated the Hubbard parameters for the Rydberg dressed interaction. The by controlling the range of the Rydberg dressed interaction, we showed that the nearest neighbor and the next nearest neighbor interaction strengths can be made to be of equal strengths. Moreover, the strength of the Hubbard parameters was shown to saturate to its maximum value at a large interaction range and at large lattice depths. This is in sharp contrast to the standard Bose-Hubbard model for which Hubbard parameters decayed exponentially with increasing spatial separation and depth of the lattice. Also, we identified the dominant density assisted tunneling processes for the Rydberg dressed interaction and studied their behavior as a function of lattice depth and range of the Rydberg dressed interaction. The amplitude of these density-assisted tunneling processes was shown to depend on the relative separation between the particles and the range of Rydberg dressed interaction.

The processes similar to the density-assisted tunneling in the extended Hubbard model were studied for the periodically driven chain of Rydberg atoms. The process called correlated Rabi oscillations was identified as a consequence of the long-range

nature of vdW interaction between two Rydberg atoms. It was shown that the Rydberg blockade can be explained using correlated Rabi oscillations. By introducing periodic driving to the system, the behavior of these processes was studied with the help of effective Hamiltonians and correlation functions. The correlated Rabi oscillations showed interesting behavior for various driving parameters.

In the hybrid system consisting of a photonic crystal waveguide coupled to a one-dimensional chain of atoms, the dynamics of a single atomic excitation was studied as a function of the range of the exchange interaction. The exchange interaction arose due to the photonic part of the system, whose range was controllable by external parameters. For a small range of exchange interaction, excitation probability was similar to that of a continuous-time quantum walk whereas for a large range we observed quasi localization of excitation. We quantified this change in the dynamics using various parameters such as kurtosis, IPR, Shannon entropy, edge-center population imbalance. We also studied the entanglement dynamics of the system and showed that the entanglement entropy is bounded by the maximum value of one, reflecting the effective two-level picture of the system.

In the final chapter, we studied the effect of the addition of one more excitation to the system. We observed different probability distributions for different initial separations between excitations. We observed the anti-bunching of excitations as well as quasi localization of excitations for different values of exchange interaction range. For the case of Rydberg excitations, the strong vdW interaction leads to the formation of bound states of the excitations. The competition between Rydberg interaction and exchange interaction was studied with the help of various parameters. For different initial separations between two excitations, the dynamics showed non-monotonous behavior as a function of vdW interaction strength and exchange interaction range. The dynamics was explained by calculating the two excitation spectrums and the overlap of the initial state onto the eigenstate of the Hamiltonian.

In conclusion, Rydberg atoms provide us with a plethora of exciting physics when combined with different systems. With the tremendous experimental progress happening in the area of atom trapping and manipulation we hope to observe the phenomena shown in this work in the near future.

Bibliography

- [1] M. H. Anderson et al. “Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor”. In: *Science* 269.5221 (1995), pp. 198–201. ISSN: 0036-8075. DOI: [10.1126/science.269.5221.198](https://doi.org/10.1126/science.269.5221.198). eprint: <https://science.sciencemag.org/content/269/5221/198.full.pdf>. URL: <https://science.sciencemag.org/content/269/5221/198>.
- [2] A. Ashkin. “Acceleration and Trapping of Particles by Radiation Pressure”. In: *Phys. Rev. Lett.* 24 (4 Jan. 1970), pp. 156–159. DOI: [10.1103/PhysRevLett.24.156](https://doi.org/10.1103/PhysRevLett.24.156). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.24.156>.
- [3] A. Ashkin. “Trapping of Atoms by Resonance Radiation Pressure”. In: *Phys. Rev. Lett.* 40 (12 Mar. 1978), pp. 729–732. DOI: [10.1103/PhysRevLett.40.729](https://doi.org/10.1103/PhysRevLett.40.729). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.40.729>.
- [4] Steven Chu et al. “Experimental Observation of Optically Trapped Atoms”. In: *Phys. Rev. Lett.* 57 (3 July 1986), pp. 314–317. DOI: [10.1103/PhysRevLett.57.314](https://doi.org/10.1103/PhysRevLett.57.314). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.57.314>.
- [5] J. D. Miller, R. A. Cline, and D. J. Heinzen. “Far-off-resonance optical trapping of atoms”. In: *Phys. Rev. A* 47 (6 June 1993), R4567–R4570. DOI: [10.1103/PhysRevA.47.R4567](https://doi.org/10.1103/PhysRevA.47.R4567). URL: <https://link.aps.org/doi/10.1103/PhysRevA.47.R4567>.
- [6] Rudolf Grimm, Matthias Weidemüller, and Yurii B. Ovchinnikov. “Optical Dipole Traps for Neutral Atoms”. In: ed. by Benjamin Bederson and Herbert Walther. Vol. 42. *Advances In Atomic, Molecular, and Optical Physics*. Academic Press, 2000, pp. 95–170. DOI: [https://doi.org/10.1016/S1049-250X\(08\)60186-X](https://doi.org/10.1016/S1049-250X(08)60186-X). URL: <https://www.sciencedirect.com/science/article/pii/S1049250X0860186X>.

-
- [7] Henning Moritz et al. “Exciting Collective Oscillations in a Trapped 1D Gas”. In: *Phys. Rev. Lett.* 91 (25 Dec. 2003), p. 250402. DOI: [10.1103/PhysRevLett.91.250402](https://doi.org/10.1103/PhysRevLett.91.250402). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.91.250402>.
- [8] Markus Greiner et al. “Exploring Phase Coherence in a 2D Lattice of Bose-Einstein Condensates”. In: *Phys. Rev. Lett.* 87 (16 Oct. 2001), p. 160405. DOI: [10.1103/PhysRevLett.87.160405](https://doi.org/10.1103/PhysRevLett.87.160405). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.87.160405>.
- [9] S. -P. Yu et al. “Nanowire photonic crystal waveguides for single-atom trapping and strong light-matter interactions”. In: *App. Phys. Lett.* 104.11 (2017/09/19 2014), p. 111103. DOI: [10.1063/1.4868975](https://doi.org/10.1063/1.4868975). URL: <http://dx.doi.org/10.1063/1.4868975>.
- [10] C-L Hung et al. “Trapped atoms in one-dimensional photonic crystals”. In: *New J. Phys.* 15.8 (2013), p. 083026. URL: <http://stacks.iop.org/1367-2630/15/i=8/a=083026>.
- [11] Mingyang Guo et al. “The low-energy Goldstone mode in a trapped dipolar supersolid”. In: *Nature* 574.7778 (Oct. 2019), pp. 386–389. ISSN: 1476-4687. DOI: [10.1038/s41586-019-1569-5](https://doi.org/10.1038/s41586-019-1569-5). URL: <https://doi.org/10.1038/s41586-019-1569-5>.
- [12] B. DeMarco and D. S. Jin. “Onset of Fermi Degeneracy in a Trapped Atomic Gas”. In: *Science* 285.5434 (1999), pp. 1703–1706. ISSN: 0036-8075. DOI: [10.1126/science.285.5434.1703](https://doi.org/10.1126/science.285.5434.1703). eprint: <https://science.sciencemag.org/content/285/5434/1703.full.pdf>. URL: <https://science.sciencemag.org/content/285/5434/1703>.
- [13] Andrew G. Truscott et al. “Observation of Fermi Pressure in a Gas of Trapped Atoms”. In: *Science* 291.5513 (2001), pp. 2570–2572. ISSN: 0036-8075. DOI: [10.1126/science.1059318](https://doi.org/10.1126/science.1059318). eprint: <https://science.sciencemag.org/content/291/5513/2570.full.pdf>. URL: <https://science.sciencemag.org/content/291/5513/2570>.
- [14] Zoran Hadzibabic et al. “Berezinskii–Kosterlitz–Thouless crossover in a trapped atomic gas”. In: *Nature* 441.7097 (June 2006), pp. 1118–1121. ISSN: 1476-4687. DOI: [10.1038/nature04851](https://doi.org/10.1038/nature04851). URL: <https://doi.org/10.1038/nature04851>.

-
- [15] P. A. Murthy et al. “Observation of the Berezinskii-Kosterlitz-Thouless Phase Transition in an Ultracold Fermi Gas”. In: *Phys. Rev. Lett.* 115 (1 June 2015), p. 010401. DOI: [10.1103/PhysRevLett.115.010401](https://doi.org/10.1103/PhysRevLett.115.010401). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.115.010401>.
- [16] Markus Greiner et al. “Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms”. In: *Nature* 415.6867 (Jan. 2002), pp. 39–44. ISSN: 1476-4687. DOI: [10.1038/415039a](https://doi.org/10.1038/415039a). URL: <https://doi.org/10.1038/415039a>.
- [17] Sepehr Ebadi et al. *Quantum Phases of Matter on a 256-Atom Programmable Quantum Simulator*. 2020. arXiv: [2012.12281](https://arxiv.org/abs/2012.12281) [quant-ph].
- [18] Jonathon A. Sedlacek et al. “Microwave electrometry with Rydberg atoms in a vapour cell using bright atomic resonances”. In: *Nature Physics* 8.11 (Nov. 2012), pp. 819–824. ISSN: 1745-2481. DOI: [10.1038/nphys2423](https://doi.org/10.1038/nphys2423). URL: <https://doi.org/10.1038/nphys2423>.
- [19] Haoquan Fan et al. “Atom based RF electric field sensing”. In: *Journal of Physics B: Atomic, Molecular and Optical Physics* 48.20 (Sept. 2015), p. 202001. DOI: [10.1088/0953-4075/48/20/202001](https://doi.org/10.1088/0953-4075/48/20/202001). URL: <https://doi.org/10.1088/0953-4075/48/20/202001>.
- [20] D. Jaksch et al. “Fast Quantum Gates for Neutral Atoms”. In: *Phys. Rev. Lett.* 85 (10 Sept. 2000), pp. 2208–2211. DOI: [10.1103/PhysRevLett.85.2208](https://doi.org/10.1103/PhysRevLett.85.2208). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.85.2208>.
- [21] E. Urban et al. “Observation of Rydberg blockade between two atoms”. In: *Nature Physics* 5.2 (Feb. 2009), pp. 110–114. ISSN: 1745-2481. DOI: [10.1038/nphys1178](https://doi.org/10.1038/nphys1178). URL: <https://doi.org/10.1038/nphys1178>.
- [22] L. Isenhower et al. “Demonstration of a Neutral Atom Controlled-NOT Quantum Gate”. In: *Phys. Rev. Lett.* 104 (1 Jan. 2010), p. 010503. DOI: [10.1103/PhysRevLett.104.010503](https://doi.org/10.1103/PhysRevLett.104.010503). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.104.010503>.
- [23] T. Wilk et al. “Entanglement of Two Individual Neutral Atoms Using Rydberg Blockade”. In: *Phys. Rev. Lett.* 104 (1 Jan. 2010), p. 010502. DOI: [10.1103/PhysRevLett.104.010502](https://doi.org/10.1103/PhysRevLett.104.010502). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.104.010502>.

-
- [24] Peter Schauss. “Quantum simulation of transverse Ising models with Rydberg atoms”. In: *Quantum Science and Technology* 3.2 (Jan. 2018), p. 023001. DOI: [10.1088/2058-9565/aa9c59](https://doi.org/10.1088/2058-9565/aa9c59). URL: <https://doi.org/10.1088/2058-9565/aa9c59>.
- [25] Antoine Browaeys and Thierry Lahaye. “Many-body physics with individually controlled Rydberg atoms”. In: *Nature Physics* 16.2 (Feb. 2020), pp. 132–142. ISSN: 1745-2481. DOI: [10.1038/s41567-019-0733-z](https://doi.org/10.1038/s41567-019-0733-z). URL: <https://doi.org/10.1038/s41567-019-0733-z>.
- [26] Peter Schauß et al. “Observation of spatially ordered structures in a two-dimensional Rydberg gas”. In: *Nature* 491.7422 (Nov. 2012), pp. 87–91. ISSN: 1476-4687. DOI: [10.1038/nature11596](https://doi.org/10.1038/nature11596). URL: <https://doi.org/10.1038/nature11596>.
- [27] P. Schauß et al. “Crystallization in Ising quantum magnets”. In: *Science* 347.6229 (2015), pp. 1455–1458. ISSN: 0036-8075. DOI: [10.1126/science.1258351](https://doi.org/10.1126/science.1258351). eprint: <https://science.sciencemag.org/content/347/6229/1455.full.pdf>. URL: <https://science.sciencemag.org/content/347/6229/1455>.
- [28] Henning Labuhn et al. “Tunable two-dimensional arrays of single Rydberg atoms for realizing quantum Ising models”. In: *Nature* 534.7609 (June 2016), pp. 667–670. ISSN: 1476-4687. DOI: [10.1038/nature18274](https://doi.org/10.1038/nature18274). URL: <https://doi.org/10.1038/nature18274>.
- [29] D. Bluvstein et al. “Controlling quantum many-body dynamics in driven Rydberg atom arrays”. In: *Science* 371.6536 (2021), pp. 1355–1359. ISSN: 0036-8075. DOI: [10.1126/science.abg2530](https://doi.org/10.1126/science.abg2530). eprint: <https://science.sciencemag.org/content/371/6536/1355.full.pdf>. URL: <https://science.sciencemag.org/content/371/6536/1355>.
- [30] Robert Löw et al. “An experimental and theoretical guide to strongly interacting Rydberg gases”. In: *Journal of Physics B: Atomic, Molecular and Optical Physics* 45.11 (May 2012), p. 113001. DOI: [10.1088/0953-4075/45/11/113001](https://doi.org/10.1088/0953-4075/45/11/113001). URL: <https://doi.org/10.1088/0953-4075/45/11/113001>.
- [31] Kilian Singer et al. “Long-range interactions between alkali Rydberg atom pairs correlated to thens–ns,np–np andnd–nd asymptotes”. In: *Journal of Physics B: Atomic, Molecular and Optical Physics* 38.2 (Jan. 2005), S295–

-
- S307. DOI: [10.1088/0953-4075/38/2/021](https://doi.org/10.1088/0953-4075/38/2/021). URL: <https://doi.org/10.1088/0953-4075/38/2/021>.
- [32] J. Hubbard and Brian Hilton Flowers. “Electron correlations in narrow energy bands”. In: *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* 276.1365 (1963), pp. 238–257. DOI: [10.1098/rspa.1963.0204](https://royalsocietypublishing.org/doi/pdf/10.1098/rspa.1963.0204). eprint: <https://royalsocietypublishing.org/doi/pdf/10.1098/rspa.1963.0204>. URL: <https://royalsocietypublishing.org/doi/abs/10.1098/rspa.1963.0204>.
- [33] Matthew P. A. Fisher et al. “Boson localization and the superfluid-insulator transition”. In: *Phys. Rev. B* 40 (1 July 1989), pp. 546–570. DOI: [10.1103/PhysRevB.40.546](https://link.aps.org/doi/10.1103/PhysRevB.40.546). URL: <https://link.aps.org/doi/10.1103/PhysRevB.40.546>.
- [34] Omjyoti Dutta et al. “Non-standard Hubbard models in optical lattices: a review”. In: *Reports on Progress in Physics* 78.6 (May 2015), p. 066001. DOI: [10.1088/0034-4885/78/6/066001](https://doi.org/10.1088/0034-4885/78/6/066001). URL: <https://doi.org/10.1088/0034-4885/78/6/066001>.
- [35] Korbinian Kottmann et al. *Supersolid-Superfluid phase separation in the extended Bose-Hubbard model*. 2021. arXiv: [2106.05893](https://arxiv.org/abs/2106.05893) [[cond-mat.quant-gas](https://arxiv.org/abs/2106.05893)].
- [36] M. Iskin. “Route to supersolidity for the extended Bose-Hubbard model”. In: *Phys. Rev. A* 83 (5 May 2011), p. 051606. DOI: [10.1103/PhysRevA.83.051606](https://link.aps.org/doi/10.1103/PhysRevA.83.051606). URL: <https://link.aps.org/doi/10.1103/PhysRevA.83.051606>.
- [37] S. Baier et al. “Extended Bose-Hubbard models with ultracold magnetic atoms”. In: *Science* 352.6282 (2016), pp. 201–205. ISSN: 0036-8075. DOI: [10.1126/science.aac9812](https://science.sciencemag.org/content/352/6282/201.full.pdf). eprint: <https://science.sciencemag.org/content/352/6282/201.full.pdf>. URL: <https://science.sciencemag.org/content/352/6282/201>.
- [38] Thomas Jennewein et al. “Quantum Cryptography with Entangled Photons”. In: *Phys. Rev. Lett.* 84 (20 May 2000), pp. 4729–4732. DOI: [10.1103/PhysRevLett.84.4729](https://link.aps.org/doi/10.1103/PhysRevLett.84.4729). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.84.4729>.
- [39] D. S. Naik et al. “Entangled State Quantum Cryptography: Eavesdropping on the Ekert Protocol”. In: *Phys. Rev. Lett.* 84 (20 May 2000), pp. 4733–4736.

-
- DOI: [10.1103/PhysRevLett.84.4733](https://doi.org/10.1103/PhysRevLett.84.4733). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.84.4733>.
- [40] D. Boschi et al. “Experimental Realization of Teleporting an Unknown Pure Quantum State via Dual Classical and Einstein-Podolsky-Rosen Channels”. In: *Phys. Rev. Lett.* 80 (6 Feb. 1998), pp. 1121–1125. DOI: [10.1103/PhysRevLett.80.1121](https://doi.org/10.1103/PhysRevLett.80.1121). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.80.1121>.
- [41] Michael Levin and Xiao-Gang Wen. “Detecting Topological Order in a Ground State Wave Function”. In: *Phys. Rev. Lett.* 96 (11 Mar. 2006), p. 110405. DOI: [10.1103/PhysRevLett.96.110405](https://doi.org/10.1103/PhysRevLett.96.110405). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.96.110405>.
- [42] Hong-Chen Jiang, Zhenghan Wang, and Leon Balents. “Identifying topological order by entanglement entropy”. In: *Nature Physics* 8.12 (Dec. 2012), pp. 902–905. ISSN: 1745-2481. DOI: [10.1038/nphys2465](https://doi.org/10.1038/nphys2465). URL: <https://doi.org/10.1038/nphys2465>.
- [43] Jens Eisert and Tobias J. Osborne. “General Entanglement Scaling Laws from Time Evolution”. In: *Phys. Rev. Lett.* 97 (15 Oct. 2006), p. 150404. DOI: [10.1103/PhysRevLett.97.150404](https://doi.org/10.1103/PhysRevLett.97.150404). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.97.150404>.
- [44] Tobias J. Osborne and Michael A. Nielsen. “Entanglement in a simple quantum phase transition”. In: *Phys. Rev. A* 66 (3 Sept. 2002), p. 032110. DOI: [10.1103/PhysRevA.66.032110](https://doi.org/10.1103/PhysRevA.66.032110). URL: <https://link.aps.org/doi/10.1103/PhysRevA.66.032110>.
- [45] Alioscia Hamma, Radu Ionicioiu, and Paolo Zanardi. “Bipartite entanglement and entropic boundary law in lattice spin systems”. In: *Phys. Rev. A* 71 (2 Feb. 2005), p. 022315. DOI: [10.1103/PhysRevA.71.022315](https://doi.org/10.1103/PhysRevA.71.022315). URL: <https://link.aps.org/doi/10.1103/PhysRevA.71.022315>.
- [46] Ingo Peschel. “On the entanglement entropy for an XY spin chain”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2004.12 (Dec. 2004), P12005. DOI: [10.1088/1742-5468/2004/12/p12005](https://doi.org/10.1088/1742-5468/2004/12/p12005). URL: <https://doi.org/10.1088/1742-5468/2004/12/p12005>.

-
- [47] J. Eisert and M. Cramer. “Single-copy entanglement in critical quantum spin chains”. In: *Phys. Rev. A* 72 (4 Oct. 2005), p. 042112. DOI: [10.1103/PhysRevA.72.042112](https://doi.org/10.1103/PhysRevA.72.042112). URL: <https://link.aps.org/doi/10.1103/PhysRevA.72.042112>.
- [48] Philip Richerme et al. “Non-local propagation of correlations in quantum systems with long-range interactions”. In: *Nature* 511.7508 (July 2014), pp. 198–201. ISSN: 1476-4687. DOI: [10.1038/nature13450](https://doi.org/10.1038/nature13450). URL: <https://doi.org/10.1038/nature13450>.
- [49] Marc Cheneau et al. “Light-cone-like spreading of correlations in a quantum many-body system”. In: *Nature* 481.7382 (Jan. 2012), pp. 484–487. ISSN: 1476-4687. DOI: [10.1038/nature10748](https://doi.org/10.1038/nature10748). URL: <https://doi.org/10.1038/nature10748>.
- [50] Bruno Nachtergaele, Yoshiko Ogata, and Robert Sims. “Propagation of Correlations in Quantum Lattice Systems”. In: *Journal of Statistical Physics* 124.1 (July 2006), pp. 1–13. ISSN: 1572-9613. DOI: [10.1007/s10955-006-9143-6](https://doi.org/10.1007/s10955-006-9143-6). URL: <https://doi.org/10.1007/s10955-006-9143-6>.
- [51] P. L. Kapitza. In: *Sov. Phys. JETP* 588 (1951).
- [52] F. Grossmann et al. “Coherent destruction of tunneling”. In: *Phys. Rev. Lett.* 67 (4 July 1991), pp. 516–519. DOI: [10.1103/PhysRevLett.67.516](https://doi.org/10.1103/PhysRevLett.67.516). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.67.516>.
- [53] Y.-Y. Jau et al. “Entangling atomic spins with a Rydberg-dressed spin-flip blockade”. In: *Nature Physics* 12.1 (Jan. 2016), pp. 71–74. ISSN: 1745-2481. DOI: [10.1038/nphys3487](https://doi.org/10.1038/nphys3487). URL: <https://doi.org/10.1038/nphys3487>.
- [54] Johannes Zeiher et al. “Many-body interferometry of a Rydberg-dressed spin lattice”. In: *Nature Physics* 12.12 (Dec. 2016), pp. 1095–1099. ISSN: 1745-2481. DOI: [10.1038/nphys3835](https://doi.org/10.1038/nphys3835). URL: <https://doi.org/10.1038/nphys3835>.
- [55] N. Henkel, R. Nath, and T. Pohl. “Three-Dimensional Roton Excitations and Supersolid Formation in Rydberg-Excited Bose-Einstein Condensates”. In: *Phys. Rev. Lett.* 104 (19 May 2010), p. 195302. DOI: [10.1103/PhysRevLett.104.195302](https://doi.org/10.1103/PhysRevLett.104.195302). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.104.195302>.

-
- [56] C.-H. Hsueh et al. “Quantum crystals in a trapped Rydberg-dressed Bose-Einstein condensate”. In: *Phys. Rev. A* 86 (1 July 2012), p. 013619. DOI: [10.1103/PhysRevA.86.013619](https://doi.org/10.1103/PhysRevA.86.013619). URL: <https://link.aps.org/doi/10.1103/PhysRevA.86.013619>.
- [57] F. Cinti et al. “Supersolid Droplet Crystal in a Dipole-Blockaded Gas”. In: *Phys. Rev. Lett.* 105 (13 Sept. 2010), p. 135301. DOI: [10.1103/PhysRevLett.105.135301](https://doi.org/10.1103/PhysRevLett.105.135301). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.105.135301>.
- [58] Andreas Geißler, Ivana Vasić, and Walter Hofstetter. “Condensation versus long-range interaction: Competing quantum phases in bosonic optical lattice systems at near-resonant Rydberg dressing”. In: *Phys. Rev. A* 95 (6 June 2017), p. 063608. DOI: [10.1103/PhysRevA.95.063608](https://doi.org/10.1103/PhysRevA.95.063608). URL: <https://link.aps.org/doi/10.1103/PhysRevA.95.063608>.
- [59] F. Maucher et al. “Rydberg-Induced Solitons: Three-Dimensional Self-Trapping of Matter Waves”. In: *Phys. Rev. Lett.* 106 (17 Apr. 2011), p. 170401. DOI: [10.1103/PhysRevLett.106.170401](https://doi.org/10.1103/PhysRevLett.106.170401). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.106.170401>.
- [60] Rick Mukherjee, Thomas C. Killian, and Kaden R. A. Hazzard. “Accessing Rydberg-dressed interactions using many-body Ramsey dynamics”. In: *Phys. Rev. A* 94 (5 Nov. 2016), p. 053422. DOI: [10.1103/PhysRevA.94.053422](https://doi.org/10.1103/PhysRevA.94.053422). URL: <https://link.aps.org/doi/10.1103/PhysRevA.94.053422>.
- [61] A. Dauphin, M. Müller, and M. A. Martin-Delgado. “Rydberg-atom quantum simulation and Chern-number characterization of a topological Mott insulator”. In: *Phys. Rev. A* 86 (5 Nov. 2012), p. 053618. DOI: [10.1103/PhysRevA.86.053618](https://doi.org/10.1103/PhysRevA.86.053618). URL: <https://link.aps.org/doi/10.1103/PhysRevA.86.053618>.
- [62] Xiaopeng Li and S. Das Sarma. “Exotic topological density waves in cold atomic Rydberg-dressed fermions”. In: *Nature Communications* 6.1 (May 2015), p. 7137. ISSN: 2041-1723. DOI: [10.1038/ncomms8137](https://doi.org/10.1038/ncomms8137). URL: <https://doi.org/10.1038/ncomms8137>.
- [63] A. W. Glaetzle et al. “Quantum Spin-Ice and Dimer Models with Rydberg Atoms”. In: *Phys. Rev. X* 4 (4 Nov. 2014), p. 041037. DOI: [10.1103/PhysRevX.4.041037](https://doi.org/10.1103/PhysRevX.4.041037).

-
- PhysRevX.4.041037. URL: <https://link.aps.org/doi/10.1103/PhysRevX.4.041037>.
- [64] Alexander W. Glaetzle et al. “Designing Frustrated Quantum Magnets with Laser-Dressed Rydberg Atoms”. In: *Phys. Rev. Lett.* 114 (17 Apr. 2015), p. 173002. DOI: [10.1103/PhysRevLett.114.173002](https://link.aps.org/doi/10.1103/PhysRevLett.114.173002). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.114.173002>.
- [65] Tyler Keating et al. “Robust quantum logic in neutral atoms via adiabatic Rydberg dressing”. In: *Phys. Rev. A* 91 (1 Jan. 2015), p. 012337. DOI: [10.1103/PhysRevA.91.012337](https://link.aps.org/doi/10.1103/PhysRevA.91.012337). URL: <https://link.aps.org/doi/10.1103/PhysRevA.91.012337>.
- [66] Tyler Keating et al. “Adiabatic quantum computation with Rydberg-dressed atoms”. In: *Phys. Rev. A* 87 (5 May 2013), p. 052314. DOI: [10.1103/PhysRevA.87.052314](https://link.aps.org/doi/10.1103/PhysRevA.87.052314). URL: <https://link.aps.org/doi/10.1103/PhysRevA.87.052314>.
- [67] Marco Mattioli et al. “Cluster Luttinger Liquids of Rydberg-Dressed Atoms in Optical Lattices”. In: *Phys. Rev. Lett.* 111 (16 Oct. 2013), p. 165302. DOI: [10.1103/PhysRevLett.111.165302](https://link.aps.org/doi/10.1103/PhysRevLett.111.165302). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.111.165302>.
- [68] M. S. Safronova, Carl J. Williams, and Charles W. Clark. “Optimizing the fast Rydberg quantum gate”. In: *Phys. Rev. A* 67 (4 Apr. 2003), p. 040303. DOI: [10.1103/PhysRevA.67.040303](https://link.aps.org/doi/10.1103/PhysRevA.67.040303). URL: <https://link.aps.org/doi/10.1103/PhysRevA.67.040303>.
- [69] M. Saffman and T. G. Walker. “Analysis of a quantum logic device based on dipole-dipole interactions of optically trapped Rydberg atoms”. In: *Phys. Rev. A* 72 (2 Aug. 2005), p. 022347. DOI: [10.1103/PhysRevA.72.022347](https://link.aps.org/doi/10.1103/PhysRevA.72.022347). URL: <https://link.aps.org/doi/10.1103/PhysRevA.72.022347>.
- [70] R Mukherjee et al. “Many-body physics with alkaline-earth Rydberg lattices”. In: *Journal of Physics B: Atomic, Molecular and Optical Physics* 44.18 (Sept. 2011), p. 184010. DOI: [10.1088/0953-4075/44/18/184010](https://doi.org/10.1088/0953-4075/44/18/184010). URL: <https://doi.org/10.1088/0953-4075/44/18/184010>.
- [71] E. A. Goldschmidt et al. “Magic wavelengths for the 5s–18s transition in rubidium”. In: *Phys. Rev. A* 91 (3 Mar. 2015), p. 032518. DOI: [10.1103/PhysRevA.91.032518](https://link.aps.org/doi/10.1103/PhysRevA.91.032518).

-
- PhysRevA . 91 . 032518. URL: <https://link.aps.org/doi/10.1103/PhysRevA.91.032518>.
- [72] Turker Topcu and Andrei Derevianko. “Intensity landscape and the possibility of magic trapping of alkali-metal Rydberg atoms in infrared optical lattices”. In: *Phys. Rev. A* 88 (4 Oct. 2013), p. 043407. DOI: [10.1103/PhysRevA.88.043407](https://link.aps.org/doi/10.1103/PhysRevA.88.043407). URL: <https://link.aps.org/doi/10.1103/PhysRevA.88.043407>.
 - [73] W. Li, C. Ates, and I. Lesanovsky. “Nonadiabatic Motional Effects and Dissipative Blockade for Rydberg Atoms Excited from Optical Lattices or Microtraps”. In: *Phys. Rev. Lett.* 110 (21 May 2013), p. 213005. DOI: [10.1103/PhysRevLett.110.213005](https://link.aps.org/doi/10.1103/PhysRevLett.110.213005). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.110.213005>.
 - [74] T. Macrì and T. Pohl. “Rydberg dressing of atoms in optical lattices”. In: *Phys. Rev. A* 89 (1 Jan. 2014), p. 011402. DOI: [10.1103/PhysRevA.89.011402](https://link.aps.org/doi/10.1103/PhysRevA.89.011402). URL: <https://link.aps.org/doi/10.1103/PhysRevA.89.011402>.
 - [75] Karl D. Nelson, Xiao Li, and David S. Weiss. “Imaging single atoms in a three-dimensional array”. In: *Nature Physics* 3.8 (Aug. 2007), pp. 556–560. ISSN: 1745-2481. DOI: [10.1038/nphys645](https://doi.org/10.1038/nphys645). URL: <https://doi.org/10.1038/nphys645>.
 - [76] Yashwant Chougale and Rejish Nath. “Ab initio calculation of Hubbard parameters for Rydberg-dressed atoms in a one-dimensional optical lattice”. In: *Journal of Physics B: Atomic, Molecular and Optical Physics* 49.14 (June 2016), p. 144005. DOI: [10.1088/0953-4075/49/14/144005](https://doi.org/10.1088/0953-4075/49/14/144005). URL: <https://doi.org/10.1088/0953-4075/49/14/144005>.
 - [77] Ole Jürgensen et al. “Observation of Density-Induced Tunneling”. In: *Phys. Rev. Lett.* 113 (19 Nov. 2014), p. 193003. DOI: [10.1103/PhysRevLett.113.193003](https://link.aps.org/doi/10.1103/PhysRevLett.113.193003). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.113.193003>.
 - [78] F. Meinert et al. “Quantum Quench in an Atomic One-Dimensional Ising Chain”. In: *Phys. Rev. Lett.* 111 (5 July 2013), p. 053003. DOI: [10.1103/PhysRevLett.111.053003](https://link.aps.org/doi/10.1103/PhysRevLett.111.053003). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.111.053003>.

-
- [79] Luca D'Alessio and Marcos Rigol. “Long-time Behavior of Isolated Periodically Driven Interacting Lattice Systems”. In: *Phys. Rev. X* 4 (4 Dec. 2014), p. 041048. DOI: [10.1103/PhysRevX.4.041048](https://doi.org/10.1103/PhysRevX.4.041048). URL: <https://link.aps.org/doi/10.1103/PhysRevX.4.041048>.
- [80] Nicola Marzari et al. “Maximally localized Wannier functions: Theory and applications”. In: *Rev. Mod. Phys.* 84 (4 Oct. 2012), pp. 1419–1475. DOI: [10.1103/RevModPhys.84.1419](https://doi.org/10.1103/RevModPhys.84.1419). URL: <https://link.aps.org/doi/10.1103/RevModPhys.84.1419>.
- [81] M. Endres et al. “Observation of Correlated Particle-Hole Pairs and String Order in Low-Dimensional Mott Insulators”. In: *Science* 334.6053 (2011), pp. 200–203. ISSN: 0036-8075. DOI: [10.1126/science.1209284](https://doi.org/10.1126/science.1209284). eprint: <https://science.sciencemag.org/content/334/6053/200.full.pdf>. URL: <https://science.sciencemag.org/content/334/6053/200>.
- [82] Sagarika Basak, Yashwant Chougale, and Rejish Nath. “Periodically Driven Array of Single Rydberg Atoms”. In: *Phys. Rev. Lett.* 120 (12 Mar. 2018), p. 123204. DOI: [10.1103/PhysRevLett.120.123204](https://doi.org/10.1103/PhysRevLett.120.123204). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.120.123204>.
- [83] Fam Le Kien et al. “Nanofiber-mediated radiative transfer between two distant atoms”. In: *Phys. Rev. A* 72 (6 Dec. 2005), p. 063815. DOI: [10.1103/PhysRevA.72.063815](https://doi.org/10.1103/PhysRevA.72.063815). URL: <https://link.aps.org/doi/10.1103/PhysRevA.72.063815>.
- [84] David Dzsotjan, Anders S. Sørensen, and Michael Fleischhauer. “Quantum emitters coupled to surface plasmons of a nanowire: A Green’s function approach”. In: *Phys. Rev. B* 82 (7 Aug. 2010), p. 075427. DOI: [10.1103/PhysRevB.82.075427](https://doi.org/10.1103/PhysRevB.82.075427). URL: <https://link.aps.org/doi/10.1103/PhysRevB.82.075427>.
- [85] Fam Le Kien and K. Hakuta. “Cooperative enhancement of channeling of emission from atoms into a nanofiber”. In: *Phys. Rev. A* 77 (1 Jan. 2008), p. 013801. DOI: [10.1103/PhysRevA.77.013801](https://doi.org/10.1103/PhysRevA.77.013801). URL: <https://link.aps.org/doi/10.1103/PhysRevA.77.013801>.
- [86] Darrick E. Chang et al. “A single-photon transistor using nanoscale surface plasmons”. In: *Nat. Phys.* 3.11 (Nov. 2007), pp. 807–812. URL: <http://dx.doi.org/10.1038/nphys708>.

-
- [87] Ephraim Shahmoon and Gershon Kurizki. “Nonradiative interaction and entanglement between distant atoms”. In: *Phys. Rev. A* 87 (3 Mar. 2013), p. 033831. DOI: [10.1103/PhysRevA.87.033831](https://doi.org/10.1103/PhysRevA.87.033831). URL: <https://link.aps.org/doi/10.1103/PhysRevA.87.033831>.
 - [88] M Akbari, S N Andrianov, and A A Kalachev. “Quantum logic gates based on off-resonant cavity-assisted interaction between three-level atoms and single photons”. In: *Laser Physics* 27.7 (June 2017), p. 075202. DOI: [10.1088/1555-6611/aa7547](https://doi.org/10.1088/1555-6611/aa7547). URL: <https://doi.org/10.1088/1555-6611/aa7547>.
 - [89] Michael J. Hartmann, Fernando G. S. L. Brandao, and Martin B. Plenio. “Strongly interacting polaritons in coupled arrays of cavities”. In: *Nat. Phys.* 2.12 (Dec. 2006), pp. 849–855. URL: <http://dx.doi.org/10.1038/nphys462>.
 - [90] Andrew D. Greentree et al. “Quantum phase transitions of light”. In: *Nat. Phys.* 2.12 (Dec. 2006), pp. 856–861. URL: <http://dx.doi.org/10.1038/nphys466>.
 - [91] Dimitris G. Angelakis, Marcelo Franca Santos, and Sougato Bose. “Photon-blockade-induced Mott transitions and XY spin models in coupled cavity arrays”. In: *Phys. Rev. A* 76 (3 Sept. 2007), p. 031805. DOI: [10.1103/PhysRevA.76.031805](https://link.aps.org/doi/10.1103/PhysRevA.76.031805). URL: <https://link.aps.org/doi/10.1103/PhysRevA.76.031805>.
 - [92] Kristian Baumann et al. “Dicke quantum phase transition with a superfluid gas in an optical cavity”. In: *Nature* 464.7293 (Apr. 2010), pp. 1301–1306. URL: <http://dx.doi.org/10.1038/nature09009>.
 - [93] C. -L. Hung et al. “Quantum spin dynamics with pairwise-tunable, long-range interactions”. In: *Proc. Nat. Aca. Sci.* 113.34 (Aug. 2016), E4946–E4955. URL: [http://www.pnas.org/content/113/34/E4946.abstract%20N2%20-%20We%20present%20a%20platform%20for%20the%20simulation%20of%20quantum%20magnetism%20with%20full%20control%20of%20interactions%20between%20pairs%20of%20spins%20at%20arbitrary%20distances%20in%201D%20and%202D%20lattices.%20In%20our%20scheme,%20two%20internal%20atomic%20states%20represent%20a%20pseudospin%20for%20atoms%20trapped%20within%20a%20photonic%20crystal%20waveguide%20\(PCW\).%20With%20the%20atomic%20transition%20frequency%20aligned%](http://www.pnas.org/content/113/34/E4946.abstract%20N2%20-%20We%20present%20a%20platform%20for%20the%20simulation%20of%20quantum%20magnetism%20with%20full%20control%20of%20interactions%20between%20pairs%20of%20spins%20at%20arbitrary%20distances%20in%201D%20and%202D%20lattices.%20In%20our%20scheme,%20two%20internal%20atomic%20states%20represent%20a%20pseudospin%20for%20atoms%20trapped%20within%20a%20photonic%20crystal%20waveguide%20(PCW).%20With%20the%20atomic%20transition%20frequency%20aligned%20)

inside a band gap of the PCW, virtual photons mediate coherent spin² interactions between lattice sites. To obtain full control of interaction coefficients at arbitrary atom² separations, ground-state energy shifts are introduced as a function of distance across the PCW. In conjunction with auxiliary pump fields, spin-exchange versus atom² separation can be engineered with arbitrary magnitude and phase, and arranged to introduce nontrivial Berry phases in the spin lattice, thus opening new avenues for realizing topological spin models. We illustrate the broad applicability of our scheme by explicit construction for several well-known spin models.

- [94] Marco T. Manzoni, Ludwig Mathey, and Darrick E. Chang. “Designing exotic many-body states of atomic spin and motion in photonic crystals”. In: *Nat. Comm.* 8 (Mar. 2017), 14696 EP -. URL: <http://dx.doi.org/10.1038/ncomms14696>.
- [95] J. S. Douglas et al. “Quantum many-body models with cold atoms coupled to photonic crystals”. In: *Nat. Phot.* 9.5 (May 2015), pp. 326–331. URL: <http://dx.doi.org/10.1038/nphoton.2015.57>.
- [96] Edward Farhi and Sam Gutmann. “Quantum computation and decision trees”. In: *Phys. Rev. A* 58 (2 Aug. 1998), pp. 915–928. DOI: [10.1103/PhysRevA.58.915](https://link.aps.org/doi/10.1103/PhysRevA.58.915). URL: <https://link.aps.org/doi/10.1103/PhysRevA.58.915>.
- [97] Apoorva Patel, K. S. Raghunathan, and Pranaw Rungta. “Quantum random walks do not need a coin toss”. In: *Phys. Rev. A* 71 (3 Mar. 2005), p. 032347. DOI: [10.1103/PhysRevA.71.032347](https://link.aps.org/doi/10.1103/PhysRevA.71.032347). URL: <https://link.aps.org/doi/10.1103/PhysRevA.71.032347>.
- [98] K Manouchehri and J B Wang. “Continuous-time quantum random walks require discrete space”. In: *J. Phys. A: Math. Theor.* 40.45 (2007), p. 13773. URL: <http://stacks.iop.org/1751-8121/40/i=45/a=016>.
- [99] Hagai B. Perets et al. “Realization of Quantum Walks with Negligible Decoherence in Waveguide Lattices”. In: *Phys. Rev. Lett.* 100 (17 May 2008),

-
- p. 170506. DOI: [10.1103/PhysRevLett.100.170506](https://doi.org/10.1103/PhysRevLett.100.170506). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.100.170506>.
- [100] Oliver Mülken and Alexander Blumen. “Continuous-time quantum walks: Models for coherent transport on complex networks”. In: *Phys. Rep.* 502.2 (2011), pp. 37–87. ISSN: 0370-1573. DOI: <https://doi.org/10.1016/j.physrep.2011.01.002>. URL: <http://www.sciencedirect.com/science/article/pii/S0370157311000184>.
- [101] Salvador Elias Venegas-Andraca. “Quantum walks: a comprehensive review”. In: *Quantum Inf. Processing* 11.5 (2012), pp. 1015–1106. DOI: [10.1007/s11128-012-0432-5](https://doi.org/10.1007/s11128-012-0432-5). URL: <https://doi.org/10.1007/s11128-012-0432-5>.
- [102] Renato Portugal, Stefan Boettcher, and Stefan Falkner. “One-dimensional coinless quantum walks”. In: *Phys. Rev. A* 91 (5 May 2015), p. 052319. DOI: [10.1103/PhysRevA.91.052319](https://doi.org/10.1103/PhysRevA.91.052319). URL: <https://link.aps.org/doi/10.1103/PhysRevA.91.052319>.
- [103] Analia Zwick and Omar Osenda. “Quantum state transfer in aXXchain with impurities”. In: *J. Phys. A: Math. Theor.* 44.10 (2011), p. 105302. DOI: [10.1088/1751-8113/44/10/105302](https://doi.org/10.1088/1751-8113/44/10/105302). URL: <http://dx.doi.org/10.1088/1751-8113/44/10/105302>.
- [104] Guo-Zhu Song et al. “Photon transport mediated by an atomic chain trapped along a photonic crystal waveguide”. In: *Phys. Rev. A* 98 (2 Aug. 2018), p. 023814. DOI: [10.1103/PhysRevA.98.023814](https://doi.org/10.1103/PhysRevA.98.023814). URL: <https://link.aps.org/doi/10.1103/PhysRevA.98.023814>.
- [105] Guo-Zhu Song et al. “Microwave transmission through an artificial atomic chain coupled to a superconducting photonic crystal”. In: *Phys. Rev. A* 99 (4 Apr. 2019), p. 043830. DOI: [10.1103/PhysRevA.99.043830](https://doi.org/10.1103/PhysRevA.99.043830). URL: <https://link.aps.org/doi/10.1103/PhysRevA.99.043830>.
- [106] James S. Douglas, Tommaso Caneva, and Darrick E. Chang. “Photon Molecules in Atomic Gases Trapped Near Photonic Crystal Waveguides”. In: *Phys. Rev. X* 6 (3 Aug. 2016), p. 031017. DOI: [10.1103/PhysRevX.6.031017](https://doi.org/10.1103/PhysRevX.6.031017). URL: <https://link.aps.org/doi/10.1103/PhysRevX.6.031017>.

-
- [107] Alejandro J Martinez and Mario I Molina. “Diffusion in infinite and semi-infinite lattices with long-range coupling”. In: *J. Phys. A: Math. Theor.* 45.27 (2012), p. 275204. URL: <http://stacks.iop.org/1751-8121/45/i=27/a=275204>.
- [108] Stefano Iubini et al. “Transport of quantum excitations coupled to spatially extended nonlinear many-body systems”. In: *New J. Phys.* 17.11 (2015), p. 113030. URL: <http://stacks.iop.org/1367-2630/17/i=11/a=113030>.
- [109] Pasquale Calabrese and John Cardy. “Evolution of entanglement entropy in one-dimensional systems”. In: *J. Stat. Mech.: Theor. Exp.* 04 (2005), P04010. DOI: [10.1088/1742-5468/2005/04/p04010](https://doi.org/10.1088/1742-5468/2005/04/p04010). URL: <http://dx.doi.org/10.1088/1742-5468/2005/04/P04010>.
- [110] J. Schachenmayer et al. “Entanglement Growth in Quench Dynamics with Variable Range Interactions”. In: *Phys. Rev. X* 3 (3 Sept. 2013), p. 031015. DOI: [10.1103/PhysRevX.3.031015](https://doi.org/10.1103/PhysRevX.3.031015). URL: <https://link.aps.org/doi/10.1103/PhysRevX.3.031015>.
- [111] Yashwant Chougale et al. “Dynamics of Rydberg excitations and quantum correlations in an atomic array coupled to a photonic crystal waveguide”. In: *Phys. Rev. A* 102 (2 Aug. 2020), p. 022816. DOI: [10.1103/PhysRevA.102.022816](https://doi.org/10.1103/PhysRevA.102.022816). URL: <https://link.aps.org/doi/10.1103/PhysRevA.102.022816>.
- [112] G. Epple et al. “Rydberg atoms in hollow-core photonic crystal fibres”. In: *Nat. Comm.* 5.1 (2014), p. 4132. DOI: [10.1038/ncomms5132](https://doi.org/10.1038/ncomms5132). URL: <https://doi.org/10.1038/ncomms5132>.
- [113] Maria Langbecker et al. “Rydberg excitation of cold atoms inside a hollow-core fiber”. In: *Phys. Rev. A* 96 (4 Oct. 2017), p. 041402. DOI: [10.1103/PhysRevA.96.041402](https://doi.org/10.1103/PhysRevA.96.041402). URL: <https://link.aps.org/doi/10.1103/PhysRevA.96.041402>.
- [114] Krishnapriya Subramonian Rajasree et al. “Generation of cold Rydberg atoms at submicron distances from an optical nanofiber”. In: *Phys. Rev. Research* 2 (1 Feb. 2020), p. 012038. DOI: [10.1103/PhysRevResearch.2.012038](https://doi.org/10.1103/PhysRevResearch.2.012038). URL: <https://link.aps.org/doi/10.1103/PhysRevResearch.2.012038>.

-
- [115] Xizhou Qin et al. “Statistics-dependent quantum co-walking of two particles in one-dimensional lattices with nearest-neighbor interactions”. In: *Phys. Rev. A* 90 (6 Dec. 2014), p. 062301. DOI: [10.1103/PhysRevA.90.062301](https://doi.org/10.1103/PhysRevA.90.062301). URL: <https://link.aps.org/doi/10.1103/PhysRevA.90.062301>.
- [116] Andrea Beggi et al. “Probing the sign of the Hubbard interaction by two-particle quantum walks”. In: *Phys. Rev. A* 97 (1 Jan. 2018), p. 013610. DOI: [10.1103/PhysRevA.97.013610](https://doi.org/10.1103/PhysRevA.97.013610). URL: <https://link.aps.org/doi/10.1103/PhysRevA.97.013610>.
- [117] Yoav Lahini et al. “Quantum walk of two interacting bosons”. In: *Phys. Rev. A* 86 (1 July 2012), p. 011603. DOI: [10.1103/PhysRevA.86.011603](https://doi.org/10.1103/PhysRevA.86.011603). URL: <https://link.aps.org/doi/10.1103/PhysRevA.86.011603>.
- [118] Takeshi Fukuhara et al. “Microscopic observation of magnon bound states and their dynamics”. In: *Nature* 502 (Sept. 2013), 76 EP -. URL: <https://doi.org/10.1038/nature12541>.
- [119] Philipp M. Preiss et al. “Strongly correlated quantum walks in optical lattices”. In: *Science* 347.6227 (Mar. 2015), p. 1229. DOI: [10.1126/science.1260364](https://doi.org/10.1126/science.1260364). URL: <http://science.sciencemag.org/content/347/6227/1229.abstract>.
- [120] Claudia Benedetti, Fabrizio Buscemi, and Paolo Bordone. “Quantum correlations in continuous-time quantum walks of two indistinguishable particles”. In: *Phys. Rev. A* 85 (4 Apr. 2012), p. 042314. DOI: [10.1103/PhysRevA.85.042314](https://doi.org/10.1103/PhysRevA.85.042314). URL: <https://link.aps.org/doi/10.1103/PhysRevA.85.042314>.
- [121] T. Chattaraj and R. V. Krems. “Effects of long-range hopping and interactions on quantum walks in ordered and disordered lattices”. In: *Phys. Rev. A* 94 (2 Aug. 2016), p. 023601. DOI: [10.1103/PhysRevA.94.023601](https://doi.org/10.1103/PhysRevA.94.023601). URL: <https://link.aps.org/doi/10.1103/PhysRevA.94.023601>.
- [122] M Valiente and D Petrosyan. “Two-particle states in the Hubbard model”. In: *J. Phys. B: Atm. Mol. Opt. Phys.* 41.16 (2008), p. 161002. DOI: [10.1088/0953-4075/41/16/161002](https://doi.org/10.1088/0953-4075/41/16/161002). URL: <http://dx.doi.org/10.1088/0953-4075/41/16/161002>.
- [123] K. Winkler et al. “Repulsively bound atom pairs in an optical lattice”. In: *Nature* 441.7095 (2006), pp. 853–856. DOI: [10.1038/nature04918](https://doi.org/10.1038/nature04918). URL: <https://doi.org/10.1038/nature04918>.

-
- [124] Rune Piil and Klaus Mølmer. “Tunneling couplings in discrete lattices, single-particle band structure, and eigenstates of interacting atom pairs”. In: *Phys. Rev. A* 76 (2 Aug. 2007), p. 023607. DOI: [10.1103/PhysRevA.76.023607](https://doi.org/10.1103/PhysRevA.76.023607). URL: <https://link.aps.org/doi/10.1103/PhysRevA.76.023607>.
- [125] David Petrosyan et al. “Quantum liquid of repulsively bound pairs of particles in a lattice”. In: *Phys. Rev. A* 76 (3 Sept. 2007), p. 033606. DOI: [10.1103/PhysRevA.76.033606](https://doi.org/10.1103/PhysRevA.76.033606). URL: <https://link.aps.org/doi/10.1103/PhysRevA.76.033606>.
- [126] M Valiente and D Petrosyan. “Scattering resonances and two-particle bound states of the extended Hubbard model”. In: *J. Phys. B: Atm. Mol. Opt. Phys.* 42.12 (2009), p. 121001. DOI: [10.1088/0953-4075/42/12/121001](https://doi.org/10.1088/0953-4075/42/12/121001). URL: <http://dx.doi.org/10.1088/0953-4075/42/12/121001>.
- [127] Fabian Letscher and David Petrosyan. “Mobile bound states of Rydberg excitations in a lattice”. In: *Phys. Rev. A* 97 (4 Apr. 2018), p. 043415. DOI: [10.1103/PhysRevA.97.043415](https://doi.org/10.1103/PhysRevA.97.043415). URL: <https://link.aps.org/doi/10.1103/PhysRevA.97.043415>.
- [128] Limin Wang, Li Wang, and Yunbo Zhang. “Quantum walks of two interacting anyons in one-dimensional optical lattices”. In: *Phys. Rev. A* 90 (6 Dec. 2014), p. 063618. DOI: [10.1103/PhysRevA.90.063618](https://doi.org/10.1103/PhysRevA.90.063618). URL: <https://link.aps.org/doi/10.1103/PhysRevA.90.063618>.
- [129] Elliott H. Lieb and Derek W. Robinson. “The finite group velocity of quantum spin systems”. In: *Commun. Math. Phys.* 28.3 (1972), pp. 251–257. DOI: [10.1007/BF01645779](https://doi.org/10.1007/BF01645779). URL: <https://doi.org/10.1007/BF01645779>.
- [130] P. Hauke and L. Tagliacozzo. “Spread of Correlations in Long-Range Interacting Quantum Systems”. In: *Phys. Rev. Lett.* 111 (20 Nov. 2013), p. 207202. DOI: [10.1103/PhysRevLett.111.207202](https://doi.org/10.1103/PhysRevLett.111.207202). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.111.207202>.
- [131] I. I. Beterov et al. “Quasiclassical calculations of blackbody-radiation-induced depopulation rates and effective lifetimes of Rydberg nS , nP , and nD alkali-metal atoms with $n \leq 80$ ”. In: *Phys. Rev. A* 79 (5 May 2009), p. 052504. DOI: [10.1103/PhysRevA.79.052504](https://doi.org/10.1103/PhysRevA.79.052504). URL: <https://link.aps.org/doi/10.1103/PhysRevA.79.052504>.

-
- [132] A. Reinhard et al. “Level shifts of rubidium Rydberg states due to binary interactions”. In: *Phys. Rev. A* 75 (3 Mar. 2007), p. 032712. DOI: [10.1103/PhysRevA.75.032712](https://doi.org/10.1103/PhysRevA.75.032712). URL: <https://link.aps.org/doi/10.1103/PhysRevA.75.032712>.
- [133] Daniel Barredo et al. “Coherent Excitation Transfer in a Spin Chain of Three Rydberg Atoms”. In: *Phys. Rev. Lett.* 114 (11 Mar. 2015), p. 113002. DOI: [10.1103/PhysRevLett.114.113002](https://doi.org/10.1103/PhysRevLett.114.113002). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.114.113002>.
- [134] Xingsheng Luan et al. “The Integration of Photonic Crystal Waveguides with Atom Arrays in Optical Tweezers”. In: *Advanced Quantum Technologies* n/a.n/a (2020/06/12 2020), p. 2000008. DOI: [10.1002/qute.202000008](https://doi.org/10.1002/qute.202000008). URL: <https://doi.org/10.1002/qute.202000008>.
- [135] T. Legero et al. “Time-resolved two-photon quantum interference”. In: *App. Phys. B* 77.8 (2003), pp. 797–802. DOI: [10.1007/s00340-003-1337-x](https://doi.org/10.1007/s00340-003-1337-x). URL: <https://doi.org/10.1007/s00340-003-1337-x>.
- [136] Marcus P. da Silva et al. “Schemes for the observation of photon correlation functions in circuit QED with linear detectors”. In: *Phys. Rev. A* 82 (4 Oct. 2010), p. 043804. DOI: [10.1103/PhysRevA.82.043804](https://doi.org/10.1103/PhysRevA.82.043804). URL: <https://link.aps.org/doi/10.1103/PhysRevA.82.043804>.
- [137] R Di Candia et al. “Dual-path methods for propagating quantum microwaves”. In: *New J. Phys.* 16.1 (2014), p. 015001. DOI: [10.1088/1367-2630/16/1/015001](https://doi.org/10.1088/1367-2630/16/1/015001). URL: <http://dx.doi.org/10.1088/1367-2630/16/1/015001>.
- [138] Tomás Ramos and Juan José Garcia-Ripoll. “Multiphoton Scattering Tomography with Coherent States”. In: *Phys. Rev. Lett.* 119 (15 Oct. 2017), p. 153601. DOI: [10.1103/PhysRevLett.119.153601](https://doi.org/10.1103/PhysRevLett.119.153601). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.119.153601>.
- [139] Pierre Türschmann et al. “Coherent nonlinear optics of quantum emitters in nanophotonic waveguides”. In: *Nanophotonics* 8.10 (2019), pp. 1641–1657. DOI: <https://doi.org/10.1515/nanoph-2019-0126>. URL: <https://www.degruyter.com/view/journals/nanoph/8/10/article-p1641.xml>.
- [140] G. Günter et al. “Observing the Dynamics of Dipole-Mediated Energy Transport by Interaction-Enhanced Imaging”. In: *Science* 342.6161 (Nov. 2013),

-
- p. 954. DOI: [10.1126/science.1244843](https://doi.org/10.1126/science.1244843). URL: <http://science.sciencemag.org/content/342/6161/954.abstract>.
- [141] D. W. Schönleber et al. “Quantum Simulation of Energy Transport with Embedded Rydberg Aggregates”. In: *Phys. Rev. Lett.* 114 (12 Mar. 2015), p. 123005. DOI: [10.1103/PhysRevLett.114.123005](https://doi.org/10.1103/PhysRevLett.114.123005). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.114.123005>.
- [142] H. Schempp et al. “Correlated Exciton Transport in Rydberg-Dressed-Atom Spin Chains”. In: *Phys. Rev. Lett.* 115 (9 Aug. 2015), p. 093002. DOI: [10.1103/PhysRevLett.115.093002](https://doi.org/10.1103/PhysRevLett.115.093002). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.115.093002>.
- [143] M. Mizoguchi et al. “Ultrafast creation of overlapping Rydberg electrons in an atomic BEC and Mott-insulator lattice”. In: *arXiv:1910.05292* (2019).
- [144] Pascal Naidon and Shimpei Endo. “Efimov physics: a review”. In: *Rep. Prog. Phys.* 80.5 (2017), p. 056001. DOI: [10.1088/1361-6633/aa50e8](https://doi.org/10.1088/1361-6633/aa50e8). URL: <http://dx.doi.org/10.1088/1361-6633/aa50e8>.