

The University of Nottingham



DOCTORAL THESIS

Ultracold gases of Rydberg-dressed atoms in multi-well traps

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Abstract

Rydberg-dressed ground state atoms are atoms with an electron off-resonantly excited to a very high energy state, i.e., a state of high principal quantum number $n \gg 1$. This thesis investigates the quantum dynamics of interacting Rydberg-dressed ground state atoms trapped in several multi-well potential traps. Rydberg atoms are atoms with exaggerated properties. One of their most interesting properties is that they exhibit a strong and long-ranged interaction that can be tuned leading to a variety of different quantum behaviours. My work focuses on studying the effects of these interacting atoms when loaded in multi-well potential traps. Generally, multi-well systems are considered as the simplest example of a finite optical lattice structure. For this reason, this thesis covers three research topics that examine the effects of long-range interaction on Rydberg-dressed atoms trapped in several potential confinements.

I begin, in the introduction, by discussing the theoretical background of relevance to this work. It starts with presenting the physics of Bose-Einstein condensate. Then, the fundamentals of the interaction between two-level atom and light are analytically studied. This study has the purpose of understanding both; the dressed interacting atoms and optical lattices. The definition, characteristics, and the nature of the interaction between Rydberg atoms are analysed afterwards.

The second chapter examines the dynamics of an ensemble of interacting Rydberg-dressed atoms trapped in static, i.e., time-independent, multi-well potentials using

a mean-field theoretical approach. I choose one-dimensional double- and triple-well in addition to a two-dimensional quadruple-well potentials. The time-dependent non-linear Gross-Pitaevskii equation is used to numerically explore the ensemble's quantum dynamics. Solving the dynamical differential equations along with tuning the strength of the applied long-range interaction shows that the behaviour of non-interacting Rydberg-dressed atoms does not differ conceptually according to the geometry of the trapping potential. However, this changes when the interactions are switched on where the shape of the confinement leads to interesting outcomes especially in the non-linear interacting limit, such as macroscopic quantum self trapping.

After investigating an ensemble of interacting Rydberg-dressed atoms in static multi-well potential traps, the second research topic examines the dynamical evolution of these atoms when loaded in a finite optical lattice using the extended Bose-Hubbard model. In this chapter, the atoms ensemble is assumed to be in a superfluid state where I investigate both, the order parameter when the Rydberg excitation laser is applied and the interference pattern of the condensates in different dimensions. The study shows the emerging long-range interactions lead to a rapid collapse of the superfluid order parameter and in general allow only for partial revivals. In addition, the interference experiments can directly reveal the interaction between Rydberg-dressed atoms.

In the fourth chapter, the dynamics of Rydberg-dressed atoms trapped in a dynamical, i.e., time-dependent, potential confinement is presented. The dynamical trap is constructed such that it begins as a harmonic oscillator and ends as a double-well potential. The analysis investigates an ensemble of contact-interacting atoms via the time-dependent non-linear GP equation.

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CHAPTER 1

Introduction and theoretical background

In this work we aspire a thorough investigation and exploration of the quantum dynamics of interacting Rydberg-dressed ground state atoms trapped in multi-well potential traps. The presented study covers not only static, i.e., time-independent, traps, but also an adiabatic dynamical, i.e., time-dependent, potential confinement is taken into consideration. The idea to load a quantum gas into several potential wells has existed for quite some time and was first realised only two years after the achievement of the first Bose-Einstein condensate [5]. Since optical lattices consist of large periodic arrays of lattice sites, the multi-well system is suited to focus on a few single wells and to study properties such as tunnelling and interaction, short- or long-ranged, between neighbouring ones.

This thesis comprises four chapters. It begins with an introduction that covers only the common theoretical background related to the subsequent three topics, each of which presents a detailed analysis of trapped Rydberg-dressed atoms in different types of confinement:

- Chapter 2 studies via mean-field theory, using the time-dependent non-linear Gross-Pitaevskii equation, the quantum dynamics of N Rydberg-dressed atoms trapped in static one-dimensional double- and triple-well potentials, in addition to two-dimensional quadruple-well potential traps. The dynamical differential equations are solved numerically in order to describe the behaviour of the atoms whether they are non- or strongly interacting atoms.
- In chapter 3 we extend the study of N trapped Rydberg-dressed atoms from a multi-well system to an optical lattice potential. The analysis in this chapter depends on the model of extended Bose-Hubbard model that enables us to investigate interesting properties of the system. The order parameter and the interference pattern of the Bose-Einstein condensates are analysed in one-, two- and three-dimensional optical lattice potential trap.
- Chapter 4 moves forward with the study to cover a dynamical potential trap. The method being used to numerically study the dynamics of interacting atoms is the adiabatic evolution. This chapter investigate the behaviour of N contact-interacting atoms trapped in a time-dependent potential via mean-field description using the time-dependent non-linear Gross-Pitaevskii equation.

In this introduction, three main sections are presented where firstly the physics of the Bose-Einstein condensate (BEC) is discussed. Afterwards, the interaction of a two-level atom and light is analysed. The last section studies the main characteristics of Rydberg atoms and their interaction.

1.1. Bose-Einstein condensation

Bose-Einstein condensation is a many-body quantum phenomenon that takes place in dilute gases of bosonic particles when their temperature is reduced below a critical temperature, which is typically of the order of tens to hundreds of nanoKelvin. Below this temperature the de Broglie wavelength of individual atoms becomes comparable to the mean inter-particle spacing and their wave functions start to overlap, giving rise to quantum coherence phenomena in the gas. The resulting many-particle state, the Bose-Einstein condensate (BEC), is characterized by the macroscopic occupation of a single-particle state [6]. The experimental realisation in 1995 of Bose-Einstein condensation (BEC) in dilute atomic gases marked the beginning of a very rapid development in the study of quantum gases [7]. Trapped Bose-Einstein condensate atomic gases are remarkable because, in spite of the fact that these are very dilute systems, they exhibit a coherent dynamical behaviour when perturbed [8]. The dilute quantum gases differ from ordinary gases, liquids and solids, in a number of ways. The particle density at the centre of Bose-Einstein condensed atomic cloud is typically $10^{13} - 10^{15} \text{cm}^{-3}$, whereas in liquids and solids the density of atoms is of order 10^{22}cm^{-3} . To observe quantum phenomena in such low-density systems, the temperature must be of order 10^{-5} K or less [7].

The realisation of Bose-Einstein condensation requires techniques to cool gases to sub-microkelvin temperatures and atom traps to confine them at high densities and to keep them away from the hot walls of the vacuum chamber [9]. Laser cooling of atoms and ions has become a routine tool for atomic physics and quantum optics in the past two decades. It provides the basis for many of the modern experiments such as, e.g., quantum information processing using atoms and ions for the quantum memory [10]. The development of cooling methods for neutral atoms has proceeded at breathtaking speed during the last decade, and numerous excellent reviews have

been written illuminating these developments (Foot, 1991; Arimondo et al., 1992; Metcalf and van der Straten, 1994; Sengstock and Ertmer, 1995; Ketterle and van Druten, 1996; Adams and Riis, 1997; Chu, 1998; CohenTannoudji, 1998; Phillips, 1998). Different cooling methods have been improved, for instance, Doppler cooling [11, 12], Polarisation-gradient cooling [11, 13, 14], Raman cooling [11, 15], Resolved-sideband Raman cooling [11, 16], Evaporative cooling [11, 17, 18] and Adiabatic expansion [11, 19].

Storing such ultracold quantum gases in artificial periodic potentials of light has opened innovative manipulation and control possibilities, in many cases creating structures far beyond those currently achievable in typical condensed-matter physics systems [20]. Optical confinement of Bose-Einstein condensates was demonstrated for the first time in a pioneering MIT experiment in Cambridge by Stamper-Kurn *et al.*, (1998a). A periodic potential is formed simply by overlapping two counter-propagating laser beams. The interference between the two laser beams forms an optical standing wave, which can trap the atoms. By interfering more laser beams, one can obtain one-, two- and three-dimensional periodic potentials. One important advantage of using optical fields to create a periodic trapping potential is that the geometry and depth of the potential are under the complete control of the experimentalist.

1.1.1. Non-interacting Bose gas

A many-particle system of identical bosons follows two important quantum statistical rules. First of all, bosons do not obey the Pauli exclusion principle and are thus allowed to accumulate in a single state of the system. Therefore, at zero temperature $T = 0$, a non-interacting Bose gas is fully Bose condensed and all N particles are described by identical single-particle wave functions [21], which means that adding atoms to the condensate does not increase its volume, just like the increase of atoms [22]. The many body wave function is therefore given by the product over these identical single-particle wave functions $\psi(\vec{r})$ [21]

$$\Psi_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i=1}^N \psi(\vec{r}_i).$$

In addition, the many-body wave function of the system is symmetric under interchange of the coordinates of any two bosons

$$\Psi_N(\dots \vec{r}_i \dots \vec{r}_j \dots) = \Psi_N(\dots \vec{r}_j \dots \vec{r}_i \dots).$$

For non-interacting bosons in the thermodynamic equilibrium, the mean occupation number of the single-particle state i is given by the Bose-Einstein distribution function,

$$f(E_i, T) = \left[\exp\left(\frac{E_i - \mu}{k_B T}\right) - 1 \right]^{-1}, \quad (1.1)$$

where k_B is the Boltzman constant, E_i is the energy of the i -th single-particle eigenstate, T is the temperature and μ is the chemical potential which can be uniquely determined by the normalization condition where the total number of particles is equal to the sum of the occupancies of the individual levels.

At high temperatures the chemical potential lies well below E_0 , the energy of the lowest single-particle state, since in this limit the mean occupation number of any state is much less than unity, and therefore, in particular, $\exp\left(\frac{E_i - \mu}{k_B T}\right) \gg 1$. As the temperature lowered, the chemical potential rises. However, the chemical potential cannot exceed E_0 , otherwise the Bose distribution function in Eq.(1.1) evaluated for the lowest single-particle state would be negative, and hence unphysical. Consequently, the mean occupation number of any excited single-particle state cannot exceed the value $1/\left[\exp\left(\frac{E_i - E_0}{k_B T}\right) - 1\right]$ [7].

The ideal gas of bosons with mass m in equilibrium at a temperature T is characterised by a thermal *de Broglie* wavelength

$$\lambda_{DB} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}},$$

which quantifies the average spatial extent of the atomic wave packets [23]. At high temperatures, the Heisenberg uncertainty principle dictates that the particles are well localised. As the temperature is reduced, the position uncertainty increases and the wave nature of the particles becomes more apparent. At sufficiently low temperatures (especially below the critical temperature $T_C < T$), the de Broglie wavelength is long enough (comparable with or larger than the mean inter-particle

distance $n_0^{-1/3}$, where n_0 is the atomic density) that the individual atomic wave functions overlap and the lowest quantum state (i.e. the ground state) is populated with more than one particle, and a condensate forms.

We consider neutral atoms trapped in an external three-dimensional harmonic potential

$$V_{\text{trap}}(x, y, z) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (1.2)$$

where m is the atomic mass and ω_i the trap oscillation frequencies in the three spacial directions $i = x, y, z$. Assuming an ideal (non-interacting) gas, the many-body Hamiltonian is expressed as the sum of single-particle Hamiltonians with the well known eigenenergies:

$$\epsilon_{n_x, n_y, n_z} = \sum_{i=x, y, z} \left(n_i + \frac{1}{2} \right) \hbar \omega_i = \left(n_x + \frac{1}{2} \right) \hbar \omega_x + \left(n_y + \frac{1}{2} \right) \hbar \omega_y + \left(n_z + \frac{1}{2} \right) \hbar \omega_z, \quad (1.3)$$

with $\{n_x, n_y, n_z\}$ non negative integers. The N particle ground state of non-interacting bosons in a harmonic potential is obtained by putting all the particles in the lowest single-particle state ($n_x = n_y = n_z = 0$), namely $\phi_0(\vec{r}_1, \dots, \vec{r}_N) = \prod_i \phi_0(\vec{r}_i)$ of the single particle ground states

$$\phi_0(\vec{r}) = \left(\frac{m\omega_{\text{ho}}}{\pi\hbar} \right)^{\frac{3}{4}} \exp \left[-\frac{m}{2\hbar} \left(\sum_{i=x, y, z} \omega_i i^2 \right) \right], \quad (1.4)$$

where $\omega_{\text{ho}} = (\omega_x \omega_y \omega_z)^{\frac{1}{3}}$ is the geometric average of the oscillator frequencies. The density distribution then becomes $n(\vec{r}) = N |\phi_0(\vec{r})|^2$ and its value grows with N . The size of the cloud is instead independent of N and is fixed by the harmonic oscillator length

$$\xi = \left(\frac{\hbar}{m\omega_{\text{ho}}} \right)^{\frac{1}{2}}, \quad (1.5)$$

which corresponds to the average width of the Gaussian distribution in Eq.(1.4) and considered as an important length scale of the system. At finite temperature only part of the atoms occupy the lowest state, the others being thermally distributed in the excited states at higher energy.

1.1.2. Critical temperature and condensate fraction

In the grand-canonical ensemble, the total number of particles at a given temperature is

$$N = \sum_{n_x, n_y, n_z} \{\exp[\beta(\epsilon_{n_x, n_y, n_z} - \mu)] - 1\}^{-1}, \quad (1.6)$$

where $\beta = 1/(k_B T)$ is the temperature parameter. The corresponding total energy is given by

$$E = \sum_{n_x, n_y, n_z} \epsilon_{n_x, n_y, n_z} \{\exp[\beta(\epsilon_{n_x, n_y, n_z} - \mu)] - 1\}^{-1}. \quad (1.7)$$

Below a given temperature the population of the lowest state becomes macroscopic and this corresponds to the onset of Bose-Einstein condensation. As in the case of a uniform Bose gas, it is convenient to separate out the lowest eigenvalue ϵ_{000} from the sum in Eq.(1.6) and call N_0 the number of particles in this state. This number can be macroscopic, i.e., of the order of N , when the chemical potential becomes equal to the energy of the lowest state,

$$\mu \longrightarrow \mu_c = \frac{3}{2}\hbar\bar{\omega},$$

where $\bar{\omega} = (\omega_x + \omega_y + \omega_z)/3$ is the arithmetic average of the trapping frequencies. Inserting this value in the rest of Eq.(1.6), one writes

$$N - N_0 = \sum_{n_x, n_y, n_z \neq 0} \frac{1}{\exp[\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)] - 1}. \quad (1.8)$$

In order to evaluate this sum explicitly, one usually assumes that the level spacing becomes smaller and smaller when $N \longrightarrow \infty$, so that the sum can be replaced by an integral¹

$$N - N_0 = \int_0^\infty \frac{dn_x dn_y dn_z}{\exp[\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)] - 1}. \quad (1.9)$$

This assumption corresponds to a semiclassical description of the excited states. Its validity implies that the relevant excitation energies, contributing to the sum in

¹Replacing the sum by an integral is usually a good choice if the density of states is high.

Eq.(1.8), are much larger than the level spacing fixed by the oscillator frequencies. The accuracy of the semiclassical approximation in Eq.(1.9) is expected to be good if the number of trapped atoms is large and $k_B T \gg \hbar \omega_{\text{ho}}$. The integral expressed in Eq.(1.9) can be easily calculated by changing variables ($\beta \hbar \omega_x n_x = \tilde{n}_x$, etc.) and one finds

$$N - N_0 = \zeta(3) \left(\frac{k_B T}{\hbar \omega_{\text{ho}}} \right)^3, \quad (1.10)$$

where $\zeta(n)$ is the Riemann zeta function. By imposing $N_0 \rightarrow 0$, we can find the critical temperature for Bose-Einstein condensation:

$$T_C = \frac{\hbar \omega_{\text{ho}}}{k_B} \left(\frac{N}{\zeta(3)} \right)^{\frac{1}{3}}. \quad (1.11)$$

For this kind of system, the adequate thermodynamic limit $N \rightarrow \infty$, $\omega_{\text{ho}} \rightarrow 0$ with $N \omega_{\text{ho}}^3$ constant, well defining the above critical temperature. Inserting the above expression for T_C into Eq.(1.10) one gets the condensate fraction in the thermodynamic limit

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_C} \right)^3. \quad (1.12)$$

The above analysis points out the existence of two relevant scales of energy for the ideal gas: the transition temperature $k_B T_C$ and the average level spacing $\hbar \omega_{\text{ho}}$ [24].

1.1.3. Dilute gas of interacting bosons

Although quantum gases are very dilute systems, most of their properties are governed by the interaction between particles [25]. As Bose-Einstein condensation is a quantum many-body effect that appears in a gas of bosons at a very low temperature, it can be described by the Hamiltonian [6]

$$\hat{H} = \sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i=1}^N V_{\text{ext}}(\vec{r}_i) + \sum_{i < j} V_{\text{int}}(\vec{r}_i, \vec{r}_j), \quad (1.13)$$

where N is the number of particles, $\hbar$ is the reduced Planck constant, m is the mass of the particle, V_{ext} is the trapping potential and V_{int} is the two-body interaction potential.

The atom-atom interaction in a cold dilute gas of bosonic atoms is dominated by elastic binary collisions and can be treated in the framework of scattering theory [21]. Usually, in the ultracold regime characteristic of quantum gases, only s -wave scattering between particles can occur [25]. This means that the only relevant two-body collisions taking place are those where the relative angular momentum between the atoms is zero $l = 0$ [6]. This allows one to replace the real interatomic potential (which at long distances is the usual van der Waals interaction) by a pseudo-potential, which is short-ranged, isotropic, and characterized by a single parameter, the s -wave scattering length a , which is known as the pseudo-potential description [26]. This interaction is called contact-interaction and it reads [25]

$$V_{\text{int}}(\vec{r} - \vec{r}') \approx V_{\text{sw}}(\vec{r} - \vec{r}') = g\delta(\vec{r} - \vec{r}'), \quad (1.14)$$

where the coupling constant g is related to the s -wave scattering length a through

$$g = \frac{4\pi\hbar^2 a}{m}. \quad (1.15)$$

The s -wave scattering length represents the interparticle interactions and should be much smaller than the other length scales in order to ensure a valid dilute gas description. Typical values for a usually lie in the range of a few nm, but much larger values are possible close to interaction resonances [27]. This length can either have positive or negative values. In the former case, which is the case of the majority of condensed atomic species, two-body interactions are repulsive and the ground state is always stable. When the scattering length is negative, contact-interactions are attractive and the condensate becomes unstable if a critical number of particles, N_{cr} , is exceeded² [6]. This approximation is valid in the case that the scattering length is much smaller than the inter-particle distance [21].

1.1.4. Gross-Pitaevskii equation

From a theoretical standpoint, and for a wide range of experimentally relevant conditions, the dynamics of a BEC can be described by means of an effective mean-field

²For $N < N_{\text{cr}}$ the condensate is in a meta-stable state, provided by a local minimum of energy. For $N = N_{\text{cr}}$ this local minimum disappears and the system is brought to the global minimum, where it collapses.

theory. This approach is much simpler than treating the full many-body Schrödinger equation and can describe quite accurately the static and dynamical properties of BECs [28]. The basic idea for a mean-field description of a dilute Bose gas was formulated by Bogoliubov (1947) [24]. To derive the mean-field equations for a BEC, a possible approach is to address the many-body problem in second quantization formalism [6] where the many-body Hamiltonian for N interacting bosons of mass m confined by an external potential $V_{\text{trap}}(\vec{r})$ is given by

$$\begin{aligned} \hat{H} = & \int d\vec{r} \hat{\Psi}^\dagger(\vec{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\vec{r}) \right] \hat{\Psi}(\vec{r}) \\ & + \frac{1}{2} \int d\vec{r} d\vec{r}' \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}(\vec{r}') V_{\text{int}}(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}') \hat{\Psi}(\vec{r}), \end{aligned} \quad (1.16)$$

where $\hat{\Psi}^\dagger$ and $\hat{\Psi}$ are the boson field operators, that create and annihilate a particle at the position $\vec{r}$, respectively, and satisfy the commutation relations

$$[\hat{\Psi}(\vec{r}), \hat{\Psi}^\dagger(\vec{r}')] = \delta(\vec{r} - \vec{r}') \quad [\hat{\Psi}(\vec{r}), \hat{\Psi}(\vec{r}')] = [\hat{\Psi}^\dagger(\vec{r}), \hat{\Psi}^\dagger(\vec{r}')] = 0.$$

Since the field operator is indeed an operator, its time evolution is given by the Heisenberg equation

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\vec{r}, t) = [\hat{\Psi}(\vec{r}, t), \hat{H}], \quad (1.17)$$

which leads to the time-evolution equation for the field operator³

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\vec{r}, t) = & \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\vec{r}) \right. \\ & \left. + \int d\vec{r}' \hat{\Psi}^\dagger(\vec{r}', t) V_{\text{int}}(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}', t) \right] \hat{\Psi}(\vec{r}, t). \end{aligned} \quad (1.18)$$

Since the condensate state involves the macroscopic occupation of a single state when $N_0 \gg 1$, where N_0 is the number of particles in the ground state, the crucial idea due to Bogoliubov (1947) and later generalised by Beliaev is to decompose the

³Full derivation is found in Appendix A

Bose field operator into two terms

$$\hat{\Psi}(\vec{r}, t) = \langle \hat{\Psi}(\vec{r}, t) \rangle + \hat{\psi}'(\vec{r}, t), \quad (1.19)$$

where

- i. The first term $\langle \hat{\Psi}(\vec{r}, t) \rangle \equiv \psi(\vec{r}, t)$ has a macroscopic ensemble average which is defined as the expectation value of the field operator⁴ identified as the Bose condensate wave function. This quantity plays the role of the order parameter for the superfluid phase transition

$$\begin{aligned} \psi(\vec{r}, t) &= 0, & T > T_C, \\ \psi(\vec{r}, t) &\neq 0, & T < T_C. \end{aligned} \quad (1.20)$$

and acts like a classical field. Another interpretation of the macroscopic wave function comes from statistical mechanics. In a continuous phase transition typically a symmetry of the system is spontaneously broken. Any quantity that appears in a continuous phase transition and characterises the breaking of the symmetry may be called an order parameter. The macroscopic wave function can be viewed as the order parameter associated with the spontaneous breaking of the global phase or “gauge” symmetry of quantum mechanics [29].

- ii. The second term $\hat{\psi}'(\vec{r}, t)$ is the fluctuation term which takes care of the non-condensate fraction. We assume the limit of a zero temperature, such that the thermal component of the system is non-existent. Furthermore, due to the weakly interacting nature of the condensate (i.e., $a \ll n_0^{-1/3}$), quantum depletion at zero temperature is expected to be minimal. It is then reasonable to neglect the non-condensed atoms $\hat{\psi}'(\vec{r}, t) \rightarrow 0$ and consider only the classical field $\hat{\Psi}(\vec{r}, t) \rightarrow \psi(\vec{r}, t)$ [30].

Thus, one obtains the time-evolution equation

⁴Its modulus fixes the condensate density through $n_0(\vec{r}, t) = |\psi(\vec{r}, t)|^2$

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\vec{r}) + \int d\vec{r}' \psi^*(\vec{r}', t) V_{\text{int}}(\vec{r} - \vec{r}') \psi(\vec{r}', t) \right] \psi(\vec{r}, t). \quad (1.21)$$

Inserting Eqs.(1.14,1.15) in Eq.(1.21) we get

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\vec{r}) + g|\psi(\vec{r}, t)|^2 \right] \psi(\vec{r}, t). \quad (1.22)$$

This equation, known as the time-dependent Gross-Pitaevskii equation (GPE) or the non-linear time-dependent Schrödinger equation, was derived independently by Gross (1961 – 1963) and Pitaevskii (1961) [24]. Its non-linearity comes from the mean-field term, which is proportional to the particle density $n(\vec{r}) = |\psi(\vec{r}, t)|^2$ [31]. This equation allows to describe, both qualitatively and quantitatively, the macroscopic behaviour of a Bose-Einstein condensate on a length scale larger than the mean interatomic distance [21]. In the absence of interaction, i.e., $g = 0$, this equation reduces to the usual time-dependent Schrödinger equation for the single-particle Hamiltonian [24].

As a result, For Eq.(1.22) to be applicable, the most important conditions that have to be fulfilled are summarized here [6]

1. Even if $T = 0$ in a real system interactions prevent all the particles to be in the same single-particle state. There is always a fraction of particles occupying excited states known as quantum depletion. To derive GP equation, quantum depletion is neglected, which is a good approximation only for large N . To treat properly the condensate plus the higher occupied states one should work with the density matrix. This is the so-called first Born approximation.
2. The GP equation is valid to describe a dilute condensate. This means that the inter-particle separation must be larger than the characteristic length of collisions a , and this is usually referred to as the second Born approximation.

To obtain the the ground state of this approximation, we write

$$\psi(\vec{r}, t) = \phi(\vec{r}) \exp(-i\mu t/\hbar),$$

where $\phi(\vec{r})$ being real and normalized to the total particle number $\int |\phi(\vec{r})|^2 d\vec{r} = N_0 = N$, and μ is the chemical potential which characterizes the ground state energy of the condensate. By this one obtains the time-independent Gross-Pitaevskii equation [31]

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\vec{r}) + g|\phi(\vec{r})|^2 \right] \phi(\vec{r}) = \mu \phi(\vec{r}). \quad (1.23)$$

1.1.5. Thomas-Fermi approximation

The form of the full GPE can be difficult to probe analytically. It is therefore instructive to consider approximations that simplify the GPE, whilst still providing useful observations. Perhaps the most useful of these approximations is the Thomas-Fermi approximation [32]. For pure contact repulsive interaction $a > 0$, when the atom number increasing $N \gg 1$, the condensate size increases and the zero-point kinetic energy becomes smaller and smaller [33] and thus the condensate wave function is essentially dominated by the interaction energy, i.e., $E_{\text{int}} \gg E_{\text{kin}}$. The Thomas-Fermi approximation consists in neglecting the kinetic energy term in the time-dependent GPE in Eq.(1.22), where in one-dimensional case we get

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} \stackrel{\text{TF}}{\approx} [V_{\text{trap}}(x) + g_{1D}|\psi(x, t)|^2] \psi(x, t). \quad (1.24)$$

with g_{1D} is the one-dimensional coupling constant. It is worth mentioning that this of course is never true for a condensate with an attractive contact-interaction, i.e., $a < 0$, since the kinetic energy is the stabilizing factor in preventing the collapse of the condensate to a more dense phase [34, 35]. The time-independent version in Eq.(1.23) is, therefore, written as

$$\mu \phi(x) \stackrel{\text{TF}}{\approx} [V_{\text{trap}}(x) + g_{1D}|\phi(x)|^2] \phi(x), \quad (1.25)$$

$\phi(x)$ can be chosen to be a real function with $N = \int dx |\phi(x)|^2$ and thus related to the particle density as $|\phi(x)|^2 = n(x)$. This leads to what is known in literature as the Thomas-Fermi solution of the Gross-Pitaevskii equation,

$$n(x) = |\phi(x)|^2 = \begin{cases} \frac{\mu - V_{\text{trap}}(x)}{g_{1\text{D}}} & \mu > V_{\text{trap}}(x), \\ 0 & \mu \leq V_{\text{trap}}(x). \end{cases} \quad (1.26)$$

It is clear that this solution holds in the region where the right hand side is positive, i.e., $V_{\text{trap}}(x) > \mu$, while $|\phi(x)| = 0$ otherwise. However, near the boundary region where $V_{\text{trap}}(x) \sim \mu$, the kinetic energy term cannot be longer ignored and the Thomas-Fermi approximation is inadequate. Our purpose now is to find a relation between the coupling constant $g_{1\text{D}}$ and the parabolic density parameters in case of a harmonic oscillator potential.

Consider $N \gg 1$ atoms trapped in an one-dimensional harmonic oscillator potential $V_{\text{trap}}(x) = V_{\text{ho}}(x) = \frac{1}{2}m\omega^2 x^2$, we write the time-independent GPE in Eq.(1.25) as:

$$\mu \phi_{\text{ho}}(x) \stackrel{\text{TF}}{\approx} \left[\frac{1}{2}m\omega^2 x^2 + g_{1\text{D}} |\phi_{\text{ho}}(x)|^2 \right] \phi_{\text{ho}}(x),$$

therefore, the non-vanishing Thomas-Fermi solution is written as

$$n_{\text{ho}}(x) = |\phi_{\text{ho}}(x)|^2 = \frac{\mu - V_{\text{ho}}(x)}{g_{1\text{D}}} = \frac{\mu}{g_{1\text{D}}} - \frac{m\omega^2 x^2}{2g_{1\text{D}}}.$$

For a harmonic trap, this approximation gives a density distribution of the shape of an inverted parabola. To find the height of the parabola, we evaluate $n_{\text{ho}}(x) = |\phi_{\text{ho}}(x)|^2$ at the minimum of the harmonic trap, i.e., $x_{\text{min}} = 0$, then we find:

$$n_{\text{ho}}(x_{\text{min}}) = |\phi_{\text{ho}}(x_{\text{min}})|^2 = \frac{\mu}{g_{1\text{D}}} - \frac{m\omega^2 (x_{\text{min}} = 0)^2}{2g_{1\text{D}}} = \frac{\mu}{g_{1\text{D}}}. \quad (1.27)$$

It is clearly shows that the height of the parabolic density is proportional to $\propto \frac{1}{g_{1\text{D}}}$, so by increasing $g_{1\text{D}}$ the height gets smaller. To find both boundaries of the parabola, we put $n_{\text{ho}}(x) = |\phi_{\text{ho}}(x)|^2 = 0$ and get the corresponding x_{ho} as following:

$$n_{\text{ho}}(x) = |\phi_{\text{ho}}(x)|^2 = \frac{\mu}{g_{1\text{D}}} - \frac{m\omega^2 x^2}{2g_{1\text{D}}} = 0 \implies x_{\text{ho}} = \pm \sqrt{\frac{2\mu}{m\omega^2}}. \quad (1.28)$$

Here x_{ho} describes the size of the condensate and it is usually known as the Thomas-Fermi radius. To find a relation between the coupling constant $g_{1\text{D}}$ and Thomas-Fermi radius x_{ho} we start from the normalization relation:

$$N = \int dx |\phi_{\text{ho}}(x)|^2 = \int dx \left(\frac{\mu}{g_{1\text{D}}} - \frac{m\omega^2 x^2}{2g_{1\text{D}}} \right) = \frac{2\mu}{3g_{1\text{D}}} \sqrt{\frac{2\mu}{m\omega^2}}, \quad (1.29)$$

solve this equation for μ we get:

$$\mu = \frac{(3Ng_{1\text{D}})^{\frac{2}{3}}}{2} (m\omega^2)^{\frac{1}{3}}. \quad (1.30)$$

Substituting Eq.(1.30) in Eq.(1.28) gives:

$$x_{\text{ho}} = \pm \left(\frac{3Ng_{1\text{D}}}{m\omega^2} \right)^{\frac{1}{3}}, \quad (1.31)$$

which obviously shows that $x_{\text{ho}} \propto g_{1\text{D}}^{\frac{1}{3}}$.

1.2. Interaction of a two-level atom with an electromagnetic field

Methods for storage and trapping of charged and neutral particles have very often served as the experimental key to great scientific advances, covering physics in the vast energy range from elementary particles to ultracold atomic quantum matter. Traps for neutral atoms can be realised on the basis of three different mechanisms; radiation-pressure traps, magnetic traps and optical dipole traps, each class having specific properties and offering particular advantages [11]. The optical dipole traps rely on the interaction between atoms and an electromagnetic field which is governed primarily by the electric field inducing an atomic dipole moment which subsequently interacts with the inducing field [36]. For example, three orthogonal, independent standing laser fields with wave vector $k = 2\pi/\lambda$ can produce a three-dimensional optical lattice periodic trapping potential

$$V(x, y, z) = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz), \quad (1.32)$$

with a tunable amplitude V_0 [26], where the idea and the creation of an optical lattice trap will be thoroughly discussed in sub section (1.2.1). In order to understand this interaction, we consider a single atom that has only two internal levels $|g\rangle$ and $|e\rangle$, as shown in Fig(1.1), interacting classically with an electromagnetic field such as a

laser field $\vec{E}(\vec{r}, t)$. The total Hamiltonian for this system is the sum of two terms

$$\hat{H} = \hat{H}_{\text{atom}} + \hat{H}_{\text{int}}, \quad (1.33)$$

where $\hat{H}_{\text{atom}}$ is the Hamiltonian which describes the two-level atom, and $\hat{H}_{\text{int}}$ is the Hamiltonian describing the atom-light interaction. The Hamiltonian of the two-level atom is written as

$$\hat{H}_{\text{atom}} = E_g |g\rangle\langle g| + E_e |e\rangle\langle e|. \quad (1.34)$$

The basis states are eigenstates of $\hat{H}_{\text{atom}}$, e.g. $\hat{H}_{\text{atom}}|g\rangle = E_g|g\rangle$. Without losing the generality, one can set the electronic ground state energy to be zero, i.e. $E_g = 0$ for simplicity. A non-zero E_g can be thought as an overall energy shift to the system [37]. Therefore, the energy of $|e\rangle$ corresponds to the gap between the two levels $\hbar\omega_a$ [38] which represents the transition energy between $|g\rangle$ and $|e\rangle$. Thus, one gets

$$\hat{H}_{\text{atom}} = \hbar\omega_a |e\rangle\langle e|. \quad (1.35)$$

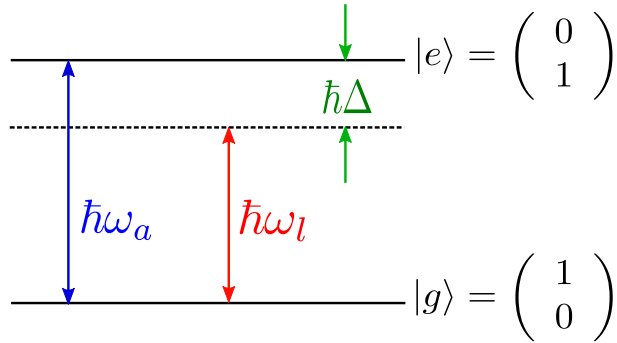


Figure 1.1.: Energy level diagram for a two-level atom acting with an electromagnetic driving field of frequency ω_l . The resonant frequency between the two atomic levels is ω_a and the detuning $\Delta = \omega_a - \omega_l$.

We introduce now the laser field as a plane wave with a momentum $k = 2\pi/\lambda$ and frequency ω_l as

$$\vec{E}(\vec{r}, t) = \hat{e} E_0(\vec{r}) \cos(\omega_l t - k \vec{r}), \quad (1.36)$$

where $E_0(\vec{r})$ is the light field amplitude, $\hat{e}$ is the unit polarization vector. We

work here within the electric dipole approximation, i.e., the wave length λ of the of electromagnetic radiation which induces transitions between different atomic energy levels is much larger than the typical size of the atom $ka_B \ll 1$, and hence is legitimate to neglect the spatial variations of the electromagnetic field over the size of the system [39]. In this case, one can write the interaction Hamiltonian between the laser field and the two-level atom as

$$\hat{H}_{\text{int}} = \sum_{i,j} \langle i | \hat{d} | j \rangle \cdot \vec{E}(\vec{r}, t) \cdot |i\rangle \langle j| = \sum_{i,j} \langle i | e \hat{r} | j \rangle \cdot \hat{e} E_0(\vec{r}) \cos(\omega_L t) \cdot |i\rangle \langle j|, \quad (1.37)$$

where $i, j = |g\rangle, |e\rangle$ and $\hat{d} = e\hat{r}$ is the dipole moment operator of the atom. The interaction Hamiltonian can be written as a matrix

$$\hat{H}_{\text{int}} = e\hat{e}E_0 \cos(\omega_L t) \begin{pmatrix} \langle g | \hat{r} | g \rangle & \langle g | \hat{r} | e \rangle \\ \langle e | \hat{r} | g \rangle & \langle e | \hat{r} | e \rangle \end{pmatrix}, \quad (1.38)$$

where the matrix elements are calculated using

$$\langle i | \hat{r} | j \rangle = \int_{-\infty}^{+\infty} \Psi_i^* \hat{r} \Psi_j d^3 \vec{r}.$$

The diagonal matrix elements become zero when $i = j$ since $\hat{r}$ is an odd parity operator and both states have the same parity which makes the integrand odd and hence the dipole transition matrix elements equal to zero. The dipole matrix element can therefore only connect states of opposite parity, in order for parity to be conserved overall. For $i \neq j$ the off-diagonal matrix elements are absorbed in the so-called Rabi frequency

$$\Omega_0 = \frac{e\hat{e}E_0}{\hbar} \langle g | \hat{r} | e \rangle \quad \Omega_0^* = \frac{e\hat{e}E_0}{\hbar} \langle e | \hat{r} | g \rangle. \quad (1.39)$$

On the assumption that Rabi frequency represents a real-valued quantity, i.e., $\Omega_0 \in \mathbb{R}$, which implies $\Omega_0 = \Omega_0^*$, therefore, the interaction Hamiltonian in Eq.(1.38) becomes

$$\hat{H}_{\text{int}} = \hbar \Omega_0 \cos(\omega_L t) (|g\rangle \langle e| + |e\rangle \langle g|) \quad (1.40)$$

Summing both Eq.(1.35) and Eq.(1.40) we get the total Hamiltonian

$$\hat{H} = \hat{H}_{\text{atom}} + \hat{H}_{\text{int}} = \hbar [\Omega_0 \cos(\omega_l t) (|g\rangle\langle e| + |e\rangle\langle g|) + \omega_a |e\rangle\langle e|]. \quad (1.41)$$

Clearly, this is a time-dependent Hamiltonian. To eliminate its time dependence, we go into a rotating frame by means of a unitary transformation

$$\hat{U} = |g\rangle\langle g| + e^{-i\omega_l t} |e\rangle\langle e|. \quad (1.42)$$

This operator transforms the time-dependent Schrödinger equation such that [38]

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi \quad \longrightarrow \quad i\hbar \frac{\partial}{\partial t} \tilde{\Psi} = \hat{\mathcal{H}} \tilde{\Psi},$$

with

$$\tilde{\Psi} = \hat{U}^\dagger \Psi \quad \hat{\mathcal{H}} = \hat{U}^\dagger \hat{H} \hat{U} - i\hbar \hat{U}^\dagger \frac{\partial}{\partial t} \hat{U}.$$

Therefore, we can write the new effective Hamiltonian as

$$\hat{\mathcal{H}} = \hbar \left[\frac{\Omega_0}{2} (1 + e^{-2i\omega_l t}) |g\rangle\langle e| + \frac{\Omega_0}{2} (1 + e^{+2i\omega_l t}) |e\rangle\langle g| + (\omega_a - \omega_l) |e\rangle\langle e| \right].$$

where the relation $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$ has been used. To make the two-level approximation, which limits us to only two coupling internal states, we assume that the laser is near resonance with a single atomic transition, i.e. $|\omega_a - \omega_l| \ll \omega_a$ [39]. Thus, the exponential terms $e^{\pm 2i\omega_l t}$ are quickly oscillating phases of the Rabi frequency compared to both the Rabi frequency itself and that associated with the detuning. Since an exponential is a composition of sine and cosine waves, these high frequency components will quickly average to zero. Therefore, on a time scale allowing us to observe the Rabi oscillations, these rapidly oscillating phases can be neglected [40]. This is the so-called *rotating wave approximation* (RWA). Applying this approximation the effective Hamiltonian will be reduced to,

$$\hat{\mathcal{H}} \approx \frac{\hbar}{2} \left[\Omega_0 (|g\rangle\langle e| + |e\rangle\langle g|) + 2\Delta |e\rangle\langle e| \right], \quad (1.43)$$

where $\hbar\Delta = \hbar\omega_a - \hbar\omega_l$ is the laser detuning which corresponds to the energy difference

between the atomic and laser photons.

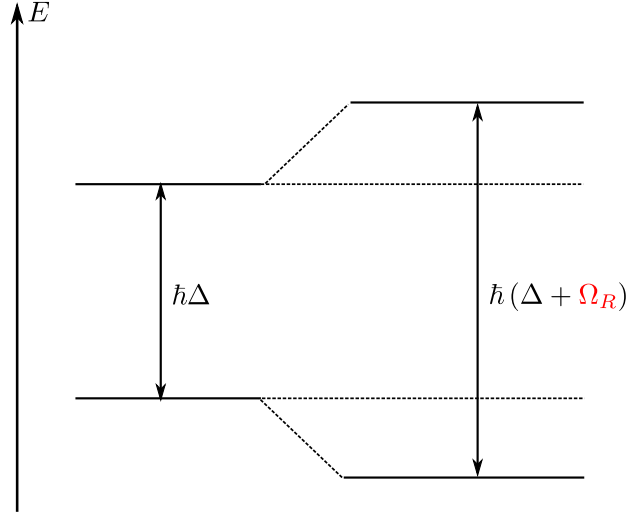


Figure 1.2.: Energy-level splitting due to the interaction of the atom with an electromagnetic field. The split levels on the right are the energy levels of the dressed states, with $\Omega_R = \sqrt{\Delta^2 + \Omega_0^2}$ being the effective Rabi frequency between the dressed states and Δ is the detuning.

Diagonalising the two-level effective Hamiltonian in Eq.(1.43) gives us the energy shift of both energy states, $|g\rangle$ and $|e\rangle$,

$$E = \frac{\hbar}{2} \left(\Delta \pm \sqrt{\Delta^2 + \Omega_0^2} \right). \quad (1.44)$$

This energy shift is called the light shift or AC, or dynamic, Stark shift, and the eigenstates corresponding to the new levels are called the dressed states of the atom, or as the Jaynes-Cummings doublets, and are thoroughly explained in Ref [22, 39]. As shown in Fig.(1.2), we see the energy of the excited state is increased and that of the ground state is lowered. It is a simple calculation to see that the spacing between the energy levels has been increased by the value $\hbar\sqrt{\Omega_0^2 + \Delta^2}$. In the limit where $\Omega_0 \ll |\Delta|$, the resulting energies are shifted by⁵

$$\Delta E \approx \pm \frac{\hbar\Omega_0^2}{4\Delta}. \quad (1.45)$$

In the limit $\Omega_0 \gg |\Delta|$, the solutions give

⁵It can be clearly noticed that in the resonant case, the energy shift $\Delta E_{|g\rangle,|e\rangle}$ is proportional to the electric field amplitude E_0 due to the relation of Rabi frequency Ω_0 in Eq.(1.39).

$$\Delta E \approx \pm \frac{\hbar \Omega_0}{2}. \quad (1.46)$$

If the system begins at $t = 0$ in the state $|g\rangle$ and the field is applied, then the probability for the two-level atom to be in the excited state $|e\rangle$ has the expression

$$P_e(t) = \frac{\Omega_0^2}{\Omega_R^2} \sin^2 \left(\frac{\Omega_R}{2} t \right), \quad (1.47)$$

where $\Omega_R^2 = \Omega_0^2 + \Delta^2$ is the effective Rabi frequency. It can be seen that the dynamic behaviour of the system is governed by only two parameters; the coupling strength Ω_0 (proportional to the electromagnetic field strength) and the detuning Δ which determines how far the field is away from resonance [41]. The time dependence of this probability is shown in Fig.(1.3, a) where it is clear that as the frequency of the laser becomes further detuned from that of the atomic transition, the population transfer is reduced whereas the frequency of the oscillations is increased [36]. At $t = \pi/\Omega_R$ the atom is in the upper level, whereas at $t = 2\pi/\Omega_R$ it is back in the lower level. The process then repeats itself with a period equal to $2\pi/\Omega_R$. The atom thus oscillates back and forth between the lower and upper levels at a frequency equal to $\Omega_R/2\pi$. This oscillatory behaviour in response to the field is called Rabi oscillation or Rabi flopping [42].

1.2.1. Optical lattice potential

We have shown so far that the interaction between two-level atom and a light field induces a dipole moment of the atom. This interaction causes a shift in the potential energy, called the AC-Stark shift. Principally, for large detunings of the light versus the atomic resonances, spontaneous emission processes can be neglected and the energy shift can be used to create a conservative trapping potential for neutral atoms [21]. The goal in this subsection is to have a regular array of potential trap. It begins with describing an optical dipole trap, then it takes a route through the basic physics of optical lattice potential.

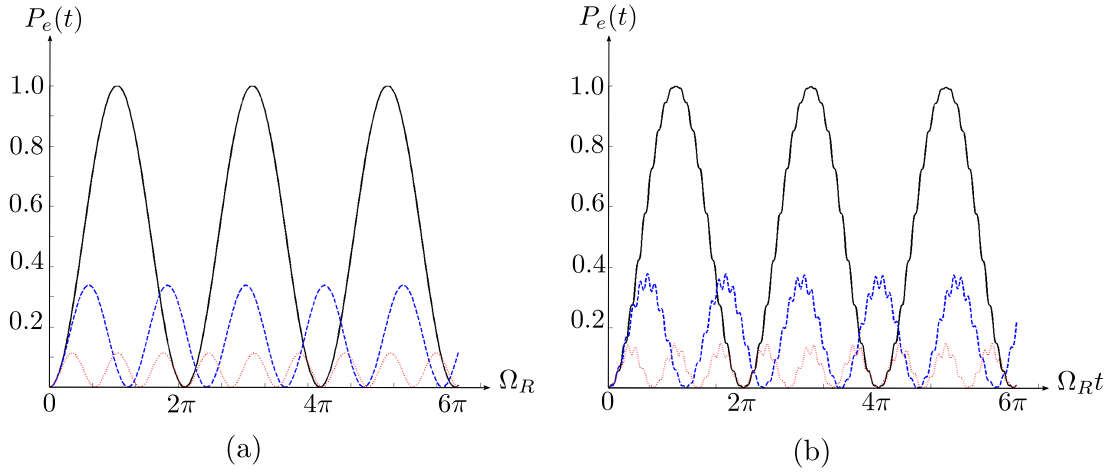


Figure 1.3.: Rabi oscillations: Probability of populating the excited state of a two-level atom is plotted for various values of detuning as a function of $\Omega_R t$. Plot (a) shows the probability of the atom to be in the excited state within the rotating wave approximation and it can be seen how the oscillation is smoothed out due to the application of this approximation. Plot (b) shows the same probability without the removal of the antiresonant terms via the rotating wave approximation. The black solid line is for $\Delta = 0$, the dashed blue line is for $\Delta = 2.8\Omega_0$ and the dotted red line is for $\Delta = 5.6\Omega_0$.

1.2.1.1. Optical dipole trap

Placing a two-level atom with an atomic transition of frequency ω_a into a laser field $\vec{E}(\vec{r}, t)$ and frequency ω_l of the electric field, will induce a dipole moment $\hat{d}$ in the atom as was discussed in Section (1.2) where the Hamiltonian describing this interaction in the rotating wave approximation is given by Eq.(1.43). If the detuning is large compared to the Rabi frequency, i.e., $|\Delta = \omega_a - \omega_l| \gg \Omega$, the effect of the interaction can be determined with the second order perturbation theory. For this case, we separate the Hamiltonian in Eq.(1.43) into two parts, unperturbed and perturbed,

$$\hat{\mathcal{H}} \approx \hat{H}_{\text{unperturbed}} + \hat{H}_{\text{perturbed}}$$

Therefore, if we assume that $\vec{\mathcal{E}}(\vec{r}) = \hat{e}\mathcal{E}_0 \cos(k\vec{r})$ is the electric field evaluated at the atomic position $\vec{r}$, then Rabi frequency acquires a spatial dependence, i.e.,

$$\Omega_0(\vec{r}) = \frac{\vec{\mathcal{E}}(\vec{r})}{\hbar} \langle e | \hat{d} | g \rangle,$$

then, inserting in Eq.(1.45) gives

$$\Delta E^{(2)} = V_{\text{dip}}(\vec{r}) = \frac{|\vec{\mathcal{E}}(\vec{r})|^2}{4\hbar\Delta} |\langle e|\hat{d}|g\rangle|^2. \quad (1.48)$$

In the limit of a far-detuned laser field which results a small excited state probability, the atom resides most of its time in the ground state and we can interpret the light-shifted ground state as the relevant potential for the motion of atoms [11]. It is clearly observed that the optical potential is proportional to the intensity of the light field $I \propto |\vec{\mathcal{E}}(\vec{r})|^2$ and the sign of the laser detuning Δ . For a red detuning $\Delta > 0$, the sign is positive resulting in an attractive potential, and the potential minima correspond to the points with zero light intensity. A blue detuning light field $\Delta < 0$ creates a repulsive potential with a negative sign, and the minima correspond to the places with maximum light intensity [43].

So far, the possibility for atoms to scatter a photon from the beam was neglected. Such an event destroys any coherence present in the system and thus has to have a low possibility during the experiment time [44]. For a large detuning, the scattering rate Γ_{scatt} is given by [11]

$$\hbar\Gamma_{\text{scatt}} = \frac{\Gamma_e}{\Delta} V_{\text{dip}}(\vec{r}) \propto \Gamma_e \frac{I}{\Delta^2}, \quad (1.49)$$

where

$$\Gamma_e = \frac{\omega_a^3}{3\pi\epsilon_0\hbar c^3} |\langle e|\hat{d}|g\rangle|^2, \quad (1.50)$$

is the spontaneous emission rate (damping rate) of the excited state $|e\rangle$, with ϵ_0 , c are the permittivity of free space and the speed of light, respectively. It obvious that the scattering rate is inversely proportional to the detuning squared, therefore, the laser detuning for a dipole trap should be chosen as large as possible within the available laser power in order to minimise inelastic scattering processes and create a conservative potential [21].

1.2.1.2. Optical lattice potential

Now, we will investigate the case where a dipole trap is not formed by a single laser beam but by the interference pattern of two counter propagating laser beams. This

changes the situation drastically, as it creates a periodic potential resembling the crystalline potential structure of an idealized, simple-cubic solid [45]. Consider the two laser beams to be monochromatic plane waves of frequency ω_l and propagating in the x direction; then the resulting electric field is given by

$$\begin{aligned}\vec{E}(x, t) &= \vec{E}_+(x, t) + \vec{E}_-(x, t) \\ &= E_+(x, t)\hat{\epsilon}_+e^{-i\omega_l t} + E_-(x, t)\hat{\epsilon}_-e^{-i\omega_l t},\end{aligned}\tag{1.51}$$

where: $E_{\pm}(x, t) = E_0e^{\pm ikx}$ with $k = 2\pi/\lambda$ is the wave number of the laser, and $\hat{\epsilon}_{\pm}$ are the polarisation vectors. The potential felt by the atoms is proportional to the intensity of both laser beams assuming that $\epsilon_+ = \epsilon_-$ is⁶

$$I = |\vec{E}(x, t)|^2 = |E_0e^{+ikx}\hat{\epsilon}_+e^{-i\omega_l t} + E_0e^{-ikx}\hat{\epsilon}_-e^{-i\omega_l t}|^2 = 4|E_0|^2 \cos^2(kx).\tag{1.52}$$

A more convenient parametrisation leads us to the potential

$$V_{\text{Latt}}(x) = V_0 \sin^2(kx) = V_0 \sin^2\left(\frac{\pi}{a}x\right),\tag{1.53}$$

where V_0 is the maximally achievable potential depth, and $a = \lambda/2$ is the periodicity of the lattice. This equation describes one-dimensional periodic potential, which is often referred to as a one-dimensional optical lattice. Along the propagation axis of the laser beams, we can therefore identify several periodically spaced potential minima that we will call from now on optical lattice sites [45]. This can be extended to higher dimensions by adding additional standing waves as for instance Eq.(1.32) represents a three-dimensional optical lattice.

The trapping frequency in the optical lattice at low energies is also obtained considering that the atoms are trapped at the minima of the optical lattice (at the lowest possible energy state) which represent local harmonic traps, as the pink dashed line illustrates in Fig(1.4), then we can expand Eq.(1.53) around $x_{\text{min}} = 0$ to find

⁶With using the trigonometric relation $\cos(2kx) = 2\cos^2(kx) - 1$

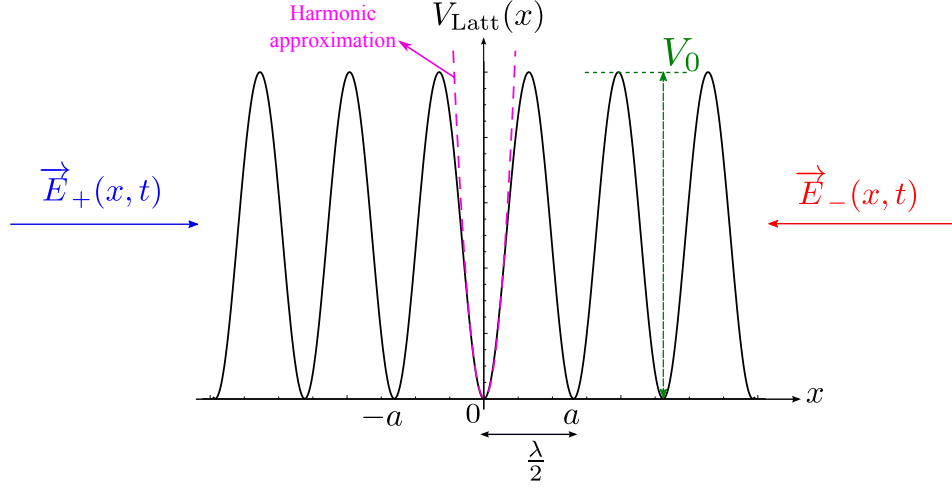


Figure 1.4.: One-dimensional optical lattice potential along x axis.

$$\frac{1}{2!} \left(\frac{d^2 V_{\text{Latt}}(x)}{dx^2} \right)_{x=x_{\min}} (x - x_{\min})^2 = \frac{1}{2} m \omega_{\text{trap}}^2 (x - x_{\min})^2.$$

$$\implies \omega_{\text{trap}} = \sqrt{\frac{2V_0 k^2}{m}},$$

where m is the mass of a single atom.

Optical lattices have several advantages with respect to solid systems. They can be made to be largely free from defects. Such defects, for example, prevent the observation of Bloch oscillations in crystalline solids. Optical lattices can also be controlled very easily by changing the laser field properties. For instance, the lattice depth can be changed by modifying the laser intensity, the lattice can be moved by changing the polarisation of the light or chirping the laser frequency and the lattice geometry can be modified by changing the laser configuration. Moreover, in contrast to solids, where the lattice spacings are generally of order of Angström units, the lattice constants in optical lattices are typically three order of magnitude larger [43].

1.3. Rydberg atoms

A Rydberg atom is an atom with an electron excited to a very high energy state, i.e. a state of high principal quantum number $n \gg 1$. The high n leads to exaggerated atomic properties, including a strong interaction between two nearby Rydberg

atoms [46]. The name "Rydberg atom" is in honor of the Swedish physicist Johannes Rydberg, who introduced the Rydberg formula and the Rydberg constant as an empirical way to determine the energy of the spectral lines in hydrogen [47]. Rydberg atoms are like hydrogen in their essential properties and they are usually studied in the context of alkali atoms, which have a single valence electron and hence relatively simple level diagrams [46]. The main difference between hydrogen atoms and alkali atoms is that the core electrons have an influence on the valence electron [48] where the simple $1/r$ Coloumb potential is not applicable anymore. Consider, as an example, rubidium ^{87}Rb , which is the most commonly used species for ultracold boson experiments [49], that has a single valence electron and a core, which consists of 36 electrons in filled electronic shells and 37 protons. When the valence electron is far from the core, the core appears as a point charge of +1. Thus, if the electron's orbit stays far from the core, the energy levels are the same as in hydrogen. On the other hand, when the electron is near the core, it sees how the charge is distributed in space. For instance, when the electron is inside the core, it sees the +37 charge of the nucleus, which increases the binding energy and decreases the total energy. In addition, the electron polarised the core, which also decreases the energy. Thus, when the electron's orbit is close to the core, the energy levels differ significantly from those of hydrogen [46]. There are two transition components for ^{87}Rb : D_1 and D_2 , where the D_1 line appears in the transition ($5^2S_{\frac{1}{2}} \rightarrow 5^2P_{\frac{1}{2}}$), and D_2 line appears in the transition ($5^2S_{\frac{1}{2}} \rightarrow 5^2P_{\frac{3}{2}}$). The D_2 transition is of much more relevance to current quantum and atom optics experiments, because it has a cycling transition that is perfectly suited for laser cooling applications [1]. The D_1 transition does not possess a closed transition and is therefore not taken into consideration. The overall physical properties of ^{87}Rb are given in Table (1.1).

1.3.1. Hydrogen atom

The structure of alkali atoms is similar to hydrogen, thus they are well described by the time-independent Schrödinger equation for hydrogen with an electron moving in the Coulomb field of the nucleus⁷

⁷Full derivation can be found in Ref[2]

Atomic Numbers	Z	37
Total Nucleons	$Z + N$	87
Relative Natural Abundance	$\eta(^{87}\text{Rb})$	27.83(2)%
Nuclear Lifetime	τ_n	4.88×10^{10} yr
Atomic Mass	m	86.909180520(15) u $1.44316060(11) \times 10^{-25}$ kg
Density at 25°C	ρ_m	1.53g/cm ³
Melting Point	T_M	39.31°C
Boiling Point	T_B	688°C
Specific Heat Capacity	c_p	0.363J/g.K
Molar Heat Capacity	C_p	31.060J/mol.k
Nuclear Spin	I	3/2
Ionization Limit	E_I	33690.8048(2)cm ⁻¹ 4.1771270(2)eV

Table 1.1.: Physical properties of ^{87}Rb taken from [1].

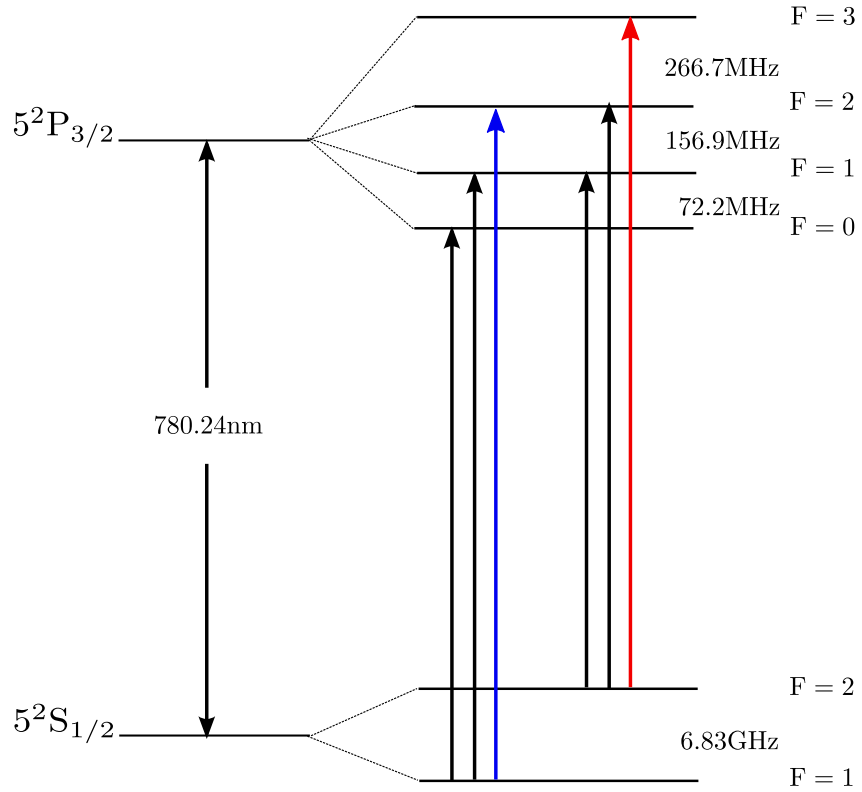


Figure 1.5.: Rubidium ^{87}Rb D₂ transition hyperfine structure, with frequency splitting between the hyperfine energy levels. Allowed transitions are shown between the ground state $5^2S_{1/2}$ and the excited $5^2P_{3/2}$ states. The cycling "cooling" transition which cools and traps the atoms is shown in red. the recycling "repump" transition which prevents the atoms from accumulating in the $F=1$ ground state is shown in blue. Stated values are taken from [1].

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V(r) \right] \psi_e = E_e \psi_e, \quad (1.54)$$

where r is the distance of the electron from the centre of nucleus, assumed to be infinitely massive, and E_e is its energy. This problem is simplified using the spherical coordinates. Expanding ∇^2 in the spherical coordinates (r, θ, ϕ)

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}, \quad (1.55)$$

where θ and ϕ are the polar and the azimuthal angles, respectively. Substituting in Eq.(1.54) we find

$$\left\{ -\frac{\hbar^2}{2m_e} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi_e(r, \theta, \phi)}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi_e(r, \theta, \phi)}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi_e(r, \theta, \phi)}{\partial \phi^2} \right] \right\} + V(r) \psi_e(r, \theta, \phi) - E_e \psi_e(r, \theta, \phi) = 0. \quad (1.56)$$

the total wave function $\psi_e(r, \theta, \phi)$ can be accordingly separated into a radial part and an angular part, i.e.,

$$\psi_e(r, \theta, \phi) = Y(\theta, \phi) R(r). \quad (1.57)$$

Inserting in Eq.(1.56) we obtain after multiplying with $r^2/R(r)Y(\theta, \phi)$

$$\begin{aligned} & \frac{1}{R(r)} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2m_e r^2}{\hbar^2} (E - V(r)) R(r) \right] \\ & + \frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right] = 0. \end{aligned} \quad (1.58)$$

It can be clearly noticed that both terms depend only on $R(r)$ and $Y(\theta, \phi)$, respectively, so they can be solved independently.

The solution for the angular part is the so-called normalised spherical harmonics,

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(l-m)!}{(l+m)!} \frac{2l+1}{4\pi}} P_l^m(\cos \theta) e^{im\phi}, \quad (1.59)$$

where l and m are the orbital angular momentum and the magnetic quantum number which takes integral values from l to $-l$ repressively. $P_l^m(x)$ are the associated Legendre functions, themselves obtainable from the Legendre polynomials $P_l(x)$ [50]

$$P_l^m(x) = (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx} \right)^m P_l(x).$$

$P_l(x)$ is itself generated by

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l.$$

In case of a hydrogen atom, the potential is expressed as the usual Coulomb potential,

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r},$$

and the radial solution for the radial equation can be solved analytically for a bound electron satisfying the appropriate boundary conditions where the wave function vanishes at $r \rightarrow \infty$ and remains finite at $r \rightarrow 0$ is

$$R_{n,l}(r) = -\sqrt{\left[\frac{(n-l-1)!}{2n[(n+l)!]^3} \left(\frac{2Z}{na_0} \right)^{l+\frac{3}{2}} \right]} r^l e^{-\frac{Zr}{na_0}} L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right), \quad (1.60)$$

where $L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right)$ are the associated Laguerre polynomials which can be expressed explicitly [51]

$$L_{n+l}^{2l+1}(x) = \sum_{k=0}^{n-l-1} (-1)^{k+1} \frac{\{(n+l)!\}^2}{(n-l-1-k)!(2l+1+k)!k!} \cdot x^k.$$

Therefore, we can write the mathematical form of the total wave function of the hydrogen atom as,

$$\begin{aligned} \psi_{n,l,m}(r, \theta, \phi) = & \sqrt{\frac{(l-m)!}{(l+m)!} \frac{2l+1}{4\pi}} P_l^m(\cos \theta) e^{im\phi} \\ & \cdot \left\{ -\sqrt{\left[\frac{(n-l-1)!}{2n[(n+l)!]^3} \left(\frac{2Z}{na_0} \right)^{l+\frac{3}{2}} \right]} r^l e^{-\frac{Zr}{na_0}} L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right) \right\}. \end{aligned} \quad (1.61)$$

Looking at the ground state i.e., $n = 1, l = 0, m = 0$, the total wave function becomes

$$\left. \begin{aligned} Y_0^0(\theta, \phi) &= \frac{1}{\sqrt{4\pi}} \\ R_{10}(r) &= 2 \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}} \end{aligned} \right\} \implies \psi_{100}(r, \theta, \phi) = \sqrt{\frac{Z^3}{a_0^3 \pi}} e^{-\frac{Zr}{a_0}}. \quad (1.62)$$

1.3.2. Alkali atoms

For alkali Rydberg atoms, an effective potential must be employed for $V(r)$ in Eq.(1.54) where this potential is perturbed compared to the Coulomb potential by the core polarisation, the screening of the nucleus with $Z \neq 1$ and the spin-orbit interaction of the electron [52]. Taking into account the new effective potential the equation of the radial part in (1.58) cannot be solved analytically anymore to obtain $R_{nl}(r)$, it has to be integrated numerically from the classically forbidden range at large r to 0 by, for example, using Numerov method [53].

The binding energy of a Rydberg state is given by the Rydberg formula [2]

$$E_{nl} = -\frac{R_y}{(n - \delta_{nlj})^2}, \quad (1.63)$$

where R_y is the Rydberg constant and it is defined by

$$R_y = \frac{Z^2 e^4 m_e}{32 \pi^2 \epsilon_0^2 \hbar^2} = 13.6 Z^2 \text{eV}, \quad (1.64)$$

where Z is the charge of the nucleus, e is the charge of the electron, m_e the mass of the electron and ϵ_0 is the permittivity of free space. The quantum defect δ_{nlj} which accounts for the deviations due to the finite core size, depends on the principle quantum number n , the angular momentum quantum number l and the total angular momentum quantum number j . It is calculated from the Rydberg-Ritz formula [54]

$$\delta_{nlj} = \delta_0 + \frac{\delta_2}{(n - \delta_0)^2} + \frac{\delta_4}{(n - \delta_0)^4} + \frac{\delta_6}{(n - \delta_0)^6} + \dots, \quad (1.65)$$

where higher order terms are usually omitted as they contribute only insignificantly, where the values of δ_0 can be found in Table (1.2). For hydrogen atoms, the quantum defect is zero [55], therefore, the energy levels are independent of l , which means that electronic states of the same n with different l are degenerate. For high angular momentum states $l \geq 4$, the basic properties are the same as hydrogen atom since the

valence electron in this kind of orbit does not “see” the inner structure of the core. When l takes low values, as in the case of the s,p or d states, the valence electron penetrates the inner core [38] and the quantum defect breaks the degeneracy and hence making the electronic states l -dependent. It is customary to define an effective principle quantum number

$$n^* = n - \delta_{nlj} \quad \Longrightarrow \quad E_{nl} = -\frac{R_y}{(n^*)^2}, \quad (1.66)$$

to take account for the modification by the quantum defect [55]. As a consequence, the properties of Rydberg atoms will depend on the magnitude of quantum defect, and hence, its angular momentum. In the following, we will denote n instead of n^* .

State	δ_0
$ns_{1/2}$	3.13109(2)
$np_{1/2}$	2.65456(15)
$np_{3/2}$	2.64145(20)
$nd_{3/2,5/2}$	1.347157(80)
$nf_{5/2,7/2}$	0.016312

Table 1.2.: Quantum defects parameters (first order Rydberg-Rietz coefficients) for ^{85}Rb expressed in Eq.(1.65) [2].

Rydberg atoms are remarkably long-lived. The long lifetimes of Rydberg states can be explained in terms of the overlapping of wave functions. The wave function of an excited Rydberg electron has a very little overlap with the wave functions of the inner electrons and hence remains relatively unperturbed. Gounard computed and calculated the radiative lifetimes for several alkali atoms and expressed the lifetimes τ of a series of states n with the general expression [3]

$$\tau = \tau_0 n^\alpha, \quad (1.67)$$

where τ_0 and α are parameters obtained from a numerical fit of the τ values. It can be seen from the theoretical and the experimental values of α in Table (1.3) for rubidium which are extracted from Ref. [3, 4] respectively, that all the α values are close to ≈ 3 , which means that the lifetime of the Rydberg atom is proportional to $\tau \propto n^3$, meaning that these highly excited states are longer lived as the level of excitation increases [36].

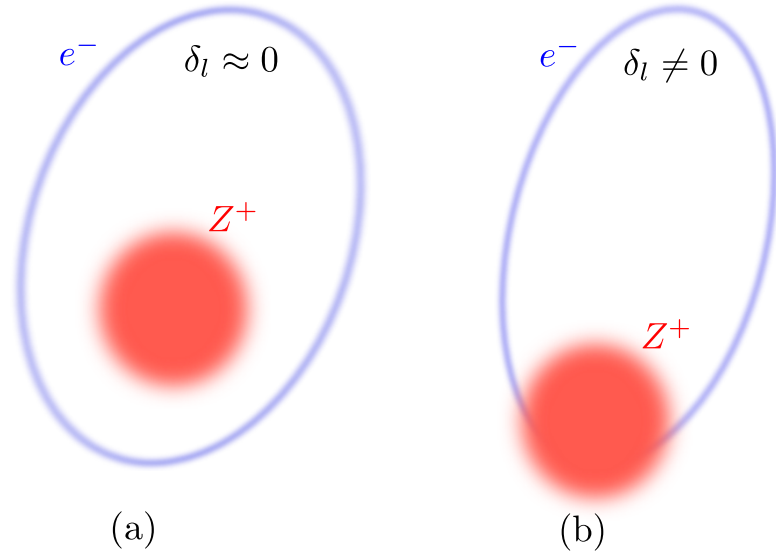


Figure 1.6.: An illustration of a hydrogen-like atom. (a) the electron e^- is far away from the core that has a positive charge Z^+ which can be considered as a point-like charge and as a result the quantum defect is negligible. (b) the electron e^- "dives" into the cloud of the inner electrons and the quantum defect cannot be neglected, thus the effective principle quantum number has to be used to calculate the atom properties.

States	$\tau_0(\text{Theo})(\text{nsec})$	$\alpha(\text{Theo})$	$\tau_0(\text{Exp})(\text{nsec})$	$\alpha(\text{Exp})$
S	1.43	2.94	1.45 ± 0.03	3.02 ± 0.02
P	2.76	3.02	2.80 ± 0.03	3.01 ± 0.03
D	2.09	2.85	2.10 ± 0.02	2.89 ± 0.02

Table 1.3.: α and τ_0 parameters for rubidium atom obtained theoretically from Ref[3] and experimentally from Ref[4].

Another interesting feature of Rydberg atoms is their large polarisability which is a measure of the extent to which the electric field can displace the electric charge from its equilibrium position [56]. Since a Rydberg electron ranges far from its nucleus, the atom is highly polarisable and relatively small electric fields, on the order of $10 - 100 \text{ mVcm}^{-1}$, can lead to significant perturbations [57]. The polarisability is defined by [58]

$$\alpha_{\text{polar}} = \sum_{nl \neq n'l'} \frac{|\mu|^2}{E_{n'l'} - E_{nl}} = \sum_{nl \neq n'l'} \frac{|\langle nl | \hat{d} | n'l' \rangle|^2}{E_{n'l'} - E_{nl}} = \sum_{nl \neq n'l'} \frac{|\langle nl | e\hat{r} | n'l' \rangle|^2}{E_{n'l'} - E_{nl}},$$

where $\hat{d}$ is the electric dipole moment. The two coupled states are the electron wave functions denoted by their corresponding quantum numbers. For $n \sim n'$ the

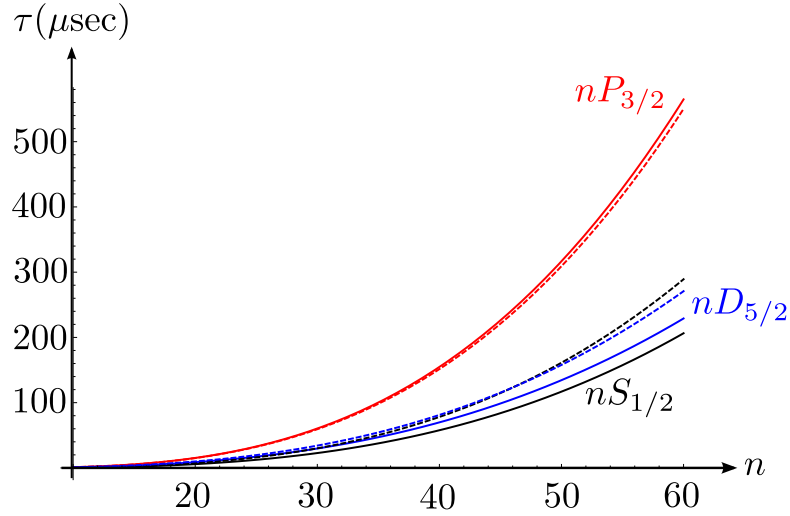


Figure 1.7.: ^{85}Rb radiative lifetimes τ in μsec as a function of the principle quantum number n . The solid lines represent the theoretical radiative times, whereas the dashed lines represent the experimental values of the radiative times. The black lines are for $nS_{1/2}$ state, the red lines are for $nP_{3/2}$ and the blue lines are for $nD_{5/2}$. It can be observed that nP states have longer lifetimes than nS and nD states. This fact is due to their small oscillator strengths connecting to the lower states, which leads to a smaller Einstein radiative rate coefficient when compared to nS and nD states; and therefore to longer lifetimes [2].

transition dipole moment scales as $\mu \propto n^2$, whereas for $n \gg n'$ the transition dipole moment has the scaling $\mu \propto n^{-3/2}$ [59]. As a results, the corresponding polarisability scales as n^7 as the energy level spacing scales n^{-3} which yields to very strong interactions between the Rydberg atoms.

Having demonstrated the mathematical quantum derivation of the total wave function of the hydrogen atom, one can use combinations of radial matrix elements and energy separations which is possible to deduce the n scaling of many properties of hydrogen (Rydberg) atoms as are stated in Table (1.4).

1.3.3. Effective two-level atom description

Rydberg atoms have been produced by several kinds of methods, electron impact excitation, charge exchange excitation and photoexcitation. Electron impact excitation uses collimated beams of fast electrons incident on ground state atoms producing an increase in the internal energy of the atoms due to the inelastic scat-

Property	Symbol	n dependence
Binding energy	E_{nl}	n^{-2}
Orbital radius	r	n^2
Expectation value of orbital radius	$\langle r \rangle$	n^2
Radiative lifetime	τ	n^3
Dipole matrix elements $n \sim n'$	$\mu_{n \sim n'}$	n^2
Dipole matrix elements $n \gg n'$	$\mu_{n \gg n'}$	$n^{-3/2}$
Energy level spacing	$E_{n'l'} - E_{nl}$	n^{-3}
Polarisability	α_{polar}	n^7
Van der Waals coefficient	C_6	n^{11}

Table 1.4.: Rydberg atom properties and their n -scaling.

tering [60, 2]. Charge exchange excitation relies on a beam of ions colliding with neutral atoms of different species resulting in the formation of a beam of highly excited atoms [61, 2]. Both of these methods have a common disadvantage of being nonselective methods, i.e. they are unable to select a specific Rydberg state to be populated where nearly all energetically possible states being produced [2]. This is because, during the collision between the charged particles, the amount of energy of the incident particles being transferred to the target valence electrons is uncontrollable, thus leading to the electrons being excited to different Rydberg states according to the energy absorbed [37]. After the discovery of dye lasers in 1970, photoexcitation has become the preferable method for producing Rydberg atoms. Photoexcitation differs from collisional excitation in a fundamental way; the exciting photon is absorbed by the target atom. As a result, specifying the energy of the absorbed photon specifies the Rydberg state produced [2].

In practice, it is very difficult to produce Rydberg atom via a single laser due to restriction of laser frequencies to meet the transition frequency between the electronic ground state and the target Rydberg state. For instance, for a single photon excitation of rubidium to Rydberg states one would have to use light at 287 nm which is difficult to produce and would also not allow access to the desired S -states [62]. Also, due to selection rules, exciting an atom from the ground state, i.e. $|nS\rangle_g$, to a highly excited $|nS\rangle_r$ state is not allowed since the difference in orbital angular momentum of the two states has to be $\Delta l = \pm 1$. Therefore, Rydberg states in ultracold atom experiments are often populated through a two-photon process [37] as shown in Fig(1.8, a).

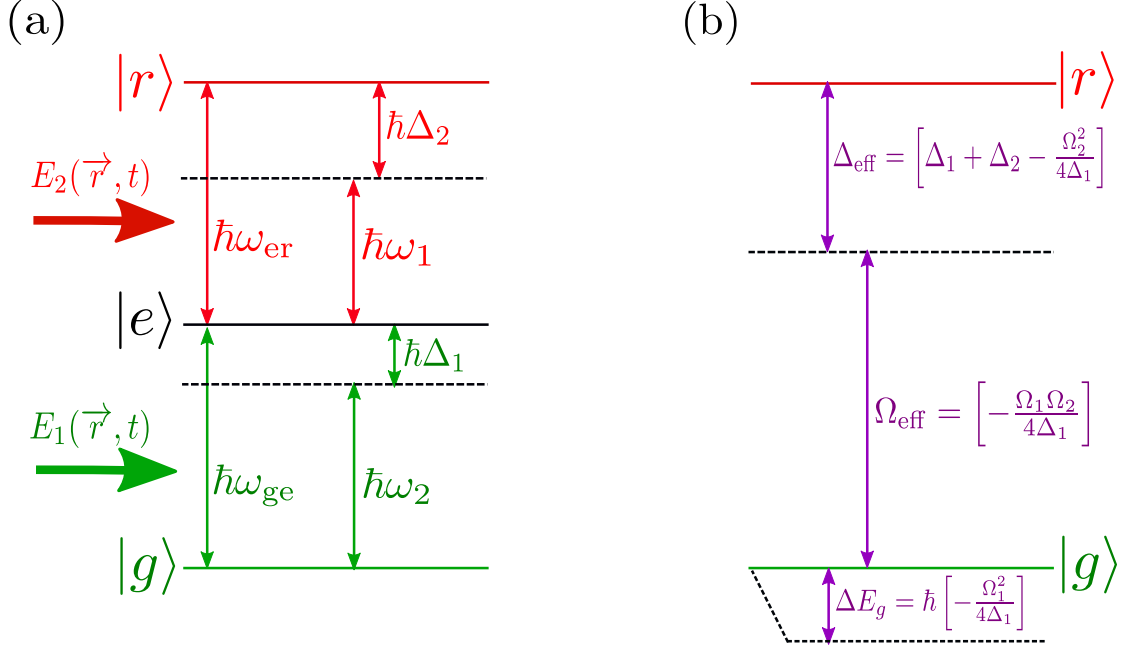


Figure 1.8.: (a) a ladder-type three-level atom where $|g\rangle$ is the ground state and $|e\rangle$ is the intermediate state and $|r\rangle$ is the Rydberg state. (b) the effective two-level atom after the adiabatic elimination of the intermediate state $|e\rangle$.

To understand the two-photon excitation process, we need to study the interaction between a ladder-type three-level atom with $|g\rangle$ the ground state, $|e\rangle$ the intermediate state and $|r\rangle$ the Rydberg state with two driving lasers, $\vec{E}_1(\vec{r}, t)$ with frequency ω_1 being applied between $|g\rangle$ and $|e\rangle$, and $\vec{E}_2(\vec{r}, t)$ with frequency ω_2 being applied between $|e\rangle$ and $|r\rangle$. The total Hamiltonian of the system is written as

$$\hat{H} = \hat{H}_{\text{atom}} + \hat{H}_{\text{int1}} + \hat{H}_{\text{int2}}, \quad (1.68)$$

where $\hat{H}_{\text{atom}}$ is the Hamiltonian of the three-level atom, $\hat{H}_{\text{int1}}$ is the Hamiltonian describing the interaction between $\vec{E}_1(\vec{r}, t)$ and both states $|g\rangle$ and $|e\rangle$, and $\hat{H}_{\text{int2}}$ is the Hamiltonian describing the interaction between $\vec{E}_2(\vec{r}, t)$ and the states $|e\rangle$ and $|r\rangle$.

The Hamiltonian of the three-level atom is

$$\hat{H}_{\text{atom}} = E_g|g\rangle\langle g| + E_e|e\rangle\langle e| + E_r|r\rangle\langle r|,$$

where the basis states $\{|g\rangle, |e\rangle, |r\rangle\}$ are eigenstates of $\hat{H}_{\text{atom}}$. The ground state en-

ergy is assumed to be equal to zero $E_g = 0$, therefore, the energy of $|e\rangle$ corresponds to the energy gap between both $|g\rangle$ and $|e\rangle$ which equals to $\hbar\omega_{ge}$, and the Rydberg state energy corresponds to the energy gap between both $|g\rangle$ and $|r\rangle$ which equals to $\hbar(\omega_{ge} + \omega_{er})$. The three-level Hamiltonian can be written in a 3×3 matrix representation as

$$\hat{H}_{\text{atom}} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega_{ge} & 0 \\ 0 & 0 & \omega_{ge} + \omega_{er} \end{pmatrix}. \quad (1.69)$$

The first laser field $\vec{E}_1(\vec{r}, t)$ with a frequency ω_1 that couples $|g\rangle$ and $|e\rangle$ can be written in the dipole approximation

$$\vec{E}_1(\vec{r}, t) = \hat{\epsilon}_1 E_{01} \cos(\omega_1 t),$$

where E_{01} is the electric field amplitude and $\hat{\epsilon}_1$ is the unit polarisation vector. The first interaction Hamiltonian is therefore,

$$\hat{H}_{\text{int1}} = \sum_{i,j} \hat{d} \cdot \vec{E}_1(\vec{r}, t) \cdot |i\rangle\langle j| = \sum_{i,j} e\hat{r} \cdot \hat{\epsilon}_1 E_{01}(\vec{r}) \cos(\omega_1 t) \cdot |i\rangle\langle j|,$$

where $i, j = |g\rangle, |e\rangle$ and $\hat{d} = e\hat{r}$ is the dipole moment operator. Assuming that Rabi frequency is a real quantity, i.e., $\Omega_1 \in \mathbb{R}$, we can rewrite the Hamiltonian in the matrix representation after taking into accounts that $|g\rangle$ and $|e\rangle$ are the only coupling states with $\vec{E}_1(\vec{r}, t)$, then the matrix of $\hat{H}_{\text{int1}}$ takes the form of

$$H_{\text{int1}} = \hbar \begin{pmatrix} 0 & \Omega_1 \cos(\omega_1 t) & 0 \\ \Omega_1 \cos(\omega_1 t) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (1.70)$$

where the Rabi frequency explaining this coupling is given by

$$\Omega_1 = \frac{e\hat{\epsilon}_1 E_{01}}{\hbar} \langle g | \hat{r} | e \rangle = \frac{e\hat{\epsilon}_1 E_{01}}{\hbar} \langle e | \hat{r} | g \rangle.$$

Following the same treatment, the Hamiltonian which describes the interaction between the second laser field $\vec{E}_2(\vec{r}, t)$ with frequency ω_2 and the states $|e\rangle$ and $|r\rangle$

takes the matrix

$$\hat{H}_{\text{int}2} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \Omega_2 \cos(\omega_2 t) \\ 0 & \Omega_2 \cos(\omega_2 t) & 0 \end{pmatrix}, \quad (1.71)$$

where,

$$\Omega_2 = \frac{e\hat{\epsilon}_2 E_{02}}{\hbar} \langle e|\hat{r}|r\rangle = \frac{e\hat{\epsilon}_2 E_{02}}{\hbar} \langle r|\hat{r}|e\rangle.$$

The total Hamiltonian is the sum of Eq.(1.69,1.70,1.71)

$$\hat{H} = \hbar \begin{pmatrix} 0 & \Omega_1 \cos(\omega_1 t) & 0 \\ \Omega_1 \cos(\omega_1 t) & \omega_{\text{ge}} & \Omega_2 \cos(\omega_2 t) \\ 0 & \Omega_2 \cos(\omega_2 t) & \omega_{\text{ge}} + \omega_{\text{er}} \end{pmatrix}. \quad (1.72)$$

As has been treated before, the time-dependance can be eliminated by using the rotating frame by means of a unitary transformation which in the case of a three-level atom has the form

$$\hat{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-i\omega_1 t} & 0 \\ 0 & 0 & e^{-i(\omega_1 + \omega_2)t} \end{pmatrix},$$

which leads us to get the effective Hamiltonian. Applying the rotating wave approximation, the total time-independent effective Hamiltonian for the three-level system is

$$\hat{\mathcal{H}} \approx \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_1 & 0 \\ \Omega_1 & 2\Delta_1 & \Omega_2 \\ 0 & \Omega_2 & 2(\Delta_1 + \Delta_2) \end{pmatrix}, \quad (1.73)$$

where $\Delta_1 = \omega_{\text{ge}} - \omega_1$ and $\Delta_2 = \omega_{\text{er}} - \omega_2$ are the detunings.

Since we are only interested in exciting the atom to the Rydberg state, ideally, one would make the intermediate state remain unpopulated. This is done by making the first laser far-detuned, i.e. $\Delta_1 \gg \Omega_1, \Omega_2$ [37]. Assuming that $A(t)$, $B(t)$ and $C(t)$ are the time-dependent amplitudes for $|g\rangle$, $|e\rangle$ and $|r\rangle$, respectively, of the

three-level atom wave function, then by applying the time-dependent Schrödinger equation allows us to write the following differential equations:

$$i\hbar\dot{A}(t) = \frac{\hbar}{2}\Omega_1 B(t) \quad (1.74a)$$

$$i\hbar\dot{B}(t) = \frac{\hbar}{2} [\Omega_1 A(t) + \Omega_2 C(t) + 2\Delta_1 B(t)] \quad (1.74b)$$

$$i\hbar\dot{C}(t) = \frac{\hbar}{2} [\Omega_2 B(t) + 2(\Delta_1 + \Delta_2)C(t)], \quad (1.74c)$$

Presuming that the detuning Δ_1 in the intermediate state $|e\rangle$ is very large comparing to Rabi frequency related to the first mode Ω_1 , then we can eliminate the state adiabatically by setting $i\hbar\dot{B}(t) \approx 0$ and hence ensuring that the population in the intermediate state is unchanged:

$$i\hbar\dot{B}(t) \approx 0 \quad \implies \quad B(t) = -\frac{\Omega_1}{2\Delta_1}A(t) - \frac{\Omega_2}{2\Delta_1}C(t), \quad (1.75)$$

thus, substituting Eq.(1.75) into Eq.(1.74a,1.74c) we get:

$$i\hbar\dot{A}(t) = \frac{\hbar}{2} \left[-\frac{\Omega_1^2}{2\Delta_1}A(t) - \frac{\Omega_1\Omega_2}{2\Delta_1}C(t) \right], \quad (1.76)$$

$$i\hbar\dot{C}(t) = \frac{\hbar}{2} \left[-\frac{\Omega_1\Omega_2}{2\Delta_1}A(t) + \left(2(\Delta_1 + \Delta_2) - \frac{\Omega_2^2}{2\Delta_1} \right) C(t) \right]. \quad (1.77)$$

As the intermediate state has been adiabatically eliminated, then Eq.(1.76) and Eq.(1.77) represent the effective two-level atom as shown in Fig.(1.8, b) where the time-dependent Schrödinger equation for this system can be written as

$$i\hbar \begin{pmatrix} \dot{A}(t) \\ \dot{C}(t) \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} -\frac{\Omega_1^2}{2\Delta_1}A(t) - \frac{\Omega_1\Omega_2}{2\Delta_1}C(t) \\ -\frac{\Omega_1\Omega_2}{2\Delta_1}A(t) + \left(2(\Delta_1 + \Delta_2) - \frac{\Omega_2^2}{2\Delta_1} \right) C(t) \end{pmatrix}, \quad (1.78)$$

and thus the effective two-level atom Hamiltonian is given by,

$$\begin{aligned}\hat{\mathcal{H}}_{\text{eff}} &= \frac{\hbar}{2} \begin{pmatrix} -\frac{\Omega_1^2}{2\Delta_1} & -\frac{\Omega_1\Omega_2}{2\Delta_1} \\ -\frac{\Omega_1\Omega_2}{2\Delta_1} & 2(\Delta_1 + \Delta_2) - \frac{\Omega_2^2}{2\Delta_1} \end{pmatrix} \\ &= \frac{\hbar}{2} \left(-\frac{\Omega_1^2}{2\Delta_1} \right) \mathbb{I} + \frac{\hbar}{2} \begin{pmatrix} 0 & -\frac{\Omega_1\Omega_2}{2\Delta_1} \\ -\frac{\Omega_1\Omega_2}{2\Delta_1} & 2(\Delta_1 + \Delta_2 + \frac{\Omega_1^2 - \Omega_2^2}{4\Delta_1}) \end{pmatrix},\end{aligned}$$

where the first term represents a constant energy value which does not alter the two level description and it can be considered as an energy reference for the system, with $\mathbb{I}$ being the unit matrix. In the second term, $\Omega_{\text{eff}} = -\frac{\Omega_1\Omega_2}{2\Delta_1}$ is the effective Rabi frequency, and $\Delta_{\text{eff}} = \Delta_1 + \Delta_2 + \frac{\Omega_1^2 - \Omega_2^2}{4\Delta_1}$ is the effective detuning for the effective two-level atom. As a result, the effective Hamiltonian for an effective two-level atom is reduced to

$$\hat{\mathcal{H}}_{\text{eff}} = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_{\text{eff}} \\ \Omega_{\text{eff}} & 2\Delta_{\text{eff}} \end{pmatrix}. \quad (1.79)$$

From now on, we will denote the effective Rabi frequency by Ω and the effective detuning by Δ . In terms of the Pauli matrix $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and by introducing a projection operator, $\hat{\chi} = |r\rangle\langle r| = (\mathbb{I} + \sigma_z)/2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ that projects onto the Rydberg state, we can rewrite the effective two-level atom Hamiltonian as,

$$\hat{\mathcal{H}}_{\text{eff}} = \frac{\hbar}{2} (\Omega \sigma_x + 2\Delta \cdot \hat{\chi}). \quad (1.80)$$

1.3.4. Interacting Rydberg atoms

Interactions are at the heart of an interesting physics, to understand and control them is an ultimate goal in many fields of physics. This is especially true for Rydberg atoms, as most proposals including Rydberg atoms are based on their strong interactions [54]. One of the main advantages of Rydberg atoms over other systems, is the ability to control the strength, sign and spatial dependence through choice of state. In addition, interactions can be turned off by returning population

to the ground state [58]. In this subsection, we discuss the interaction between two Rydberg atoms in the absence of an external electromagnetic field.

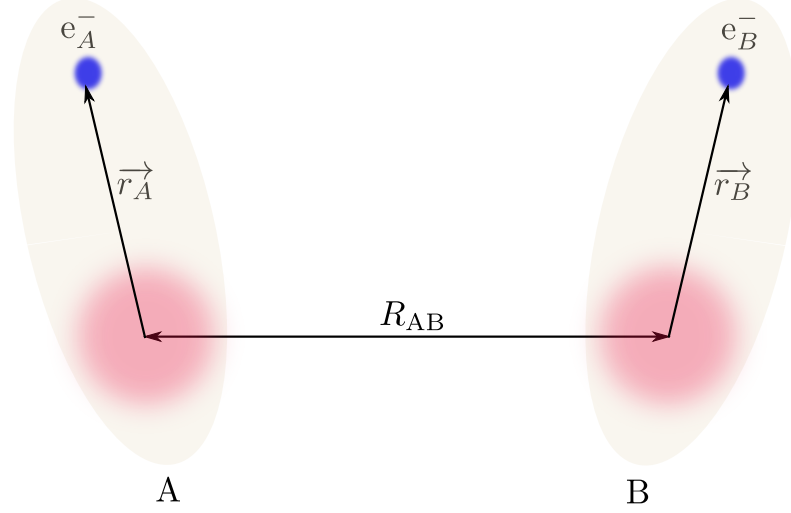


Figure 1.9.: A Sketch of two nearby Rydberg atoms A and B whose nuclei are separated by a distance R_{AB} . $\vec{r}_A$ and $\vec{r}_B$ are the vectors describing the positions of the valence electrons e_A^-, e_B^- of atoms A and B respectively.

Suppose there are two Rydberg atoms whose nuclei are separated by a distance R_{AB} , shown schematically in Fig(1.9). In the approximation where the ionic core is assumed to be a point particle, the full Coulomb interaction potential reads as [36]

$$V_{AB}(R_{AB}) = \frac{e^2}{4\pi\epsilon_0 |\vec{R}_{AB}|} - \frac{e^2}{4\pi\epsilon_0 |\vec{R}_{AB} - \vec{r}_B|} - \frac{e^2}{4\pi\epsilon_0 |\vec{R}_{AB} - \vec{r}_A|} + \frac{e^2}{4\pi\epsilon_0 |\vec{R}_{AB} + \vec{r}_B - \vec{r}_A|}, \quad (1.81)$$

where $\vec{r}_A$ and $\vec{r}_B$ are the vectors describing the positions of the valence electrons relative to their nuclei of atoms A and B , respectively. The first term in Eq.(1.81) describes the interaction between the two nuclei, the second and the third are between each nucleus and the valence electron of the other atom and the final term being that between the two valence electrons. If we assume that $\vec{R}_{AB} \gg \vec{r}_A, \vec{r}_B$ where $\vec{r}_A \equiv |\vec{r}_A|$ and $\vec{r}_B \equiv |\vec{r}_B|$, this expression may be Taylor expanded and yields to [46]

$$V_{dd}(R_{AB}) = \frac{e^2}{4\pi\epsilon_0 R_{AB}^3} \cdot \left[\vec{r}_A \cdot \vec{r}_B - 3 \left(\vec{r}_A \cdot \frac{\vec{R}_{AB}}{R_{AB}} \right) \left(\vec{r}_B \cdot \frac{\vec{R}_{AB}}{R_{AB}} \right) \right], \quad (1.82)$$

which is the so-called dipole-dipole interaction. To see the interaction strength and how it scales with the principal quantum number n , we illustrate it with a simple model. Due to spin-orbit coupling, a Rydberg state is specified by four quantum numbers: n, l, j, m_j as it was discussed in section (1.3). But for simplicity, we only keep track of n and l [46]. Therefore, we assume that both atoms are in the same Rydberg state $|n, l\rangle$. For each atom, we adopt the two-level approximation where for instance, the first Rydberg atom has two energy levels, the initial Rydberg state $|n, l\rangle$ and another nearby state $|n', l'\rangle$ that is electric dipole coupled to the initial Rydberg state, i.e. a dipole transition is allowed between the two states due to selection rules, and hence, $\Delta l = \pm 1$. The second Rydberg atom, has its second energy level denoted as $|n'', l''\rangle$. The energy level scheme of the two Rydberg atoms are illustrated in Fig.(1.10).

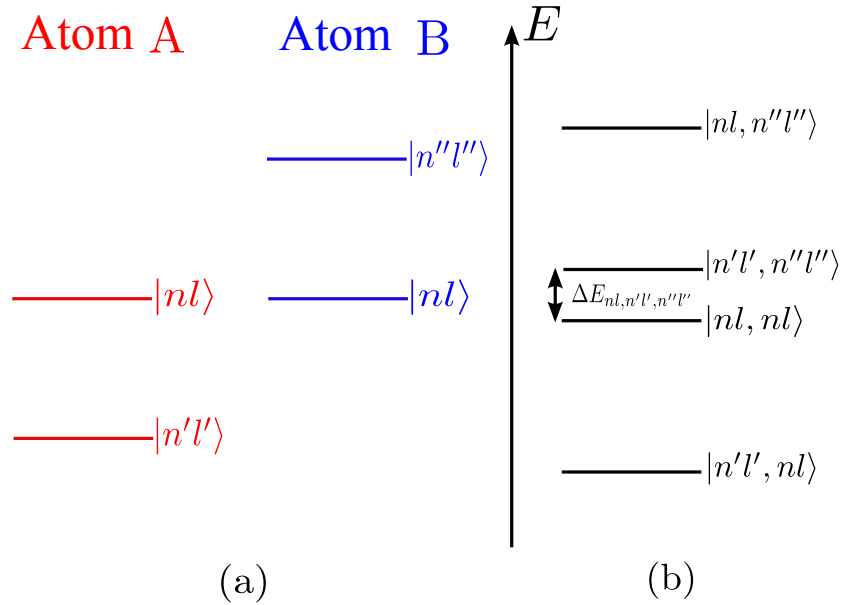


Figure 1.10.: (a) Two Rydberg atoms A and B with energy states labeled with their bare atomic states $|nl\rangle, |n'l'\rangle$ and $|nl\rangle, |n''l''\rangle$ respectively. (b) The pair energy states for both Rydberg atoms. In order for the two Rydberg atoms to interact, the choice of $|n'l'\rangle$ and $|n''l''\rangle$ has to satisfy the condition that Förster defect $E_{nl, n'l', n''l''}$ is very small, i.e. $|nl, nl\rangle$ and $|n'l', n''l''\rangle$ are near degenerate.

To calculate the energy shift due to the dipole-dipole interaction, it is necessary to transform from the bare atomic basis to a pair basis, i.e. direct product of the two single atomic states. The initial pair state $|nl, nl\rangle$ is coupled by $V_{dd}(R_{AB})$ to only

one state denoted by $|n'l', n''l''\rangle$. The energy of each pair state is simply the sum of the energy of the single atom. In order for the two Rydberg atoms to interact through the process discussed, the energy difference between the two states, $|nl, nl\rangle$ and $|n'l', n''l''\rangle$, also known as the Förster defect, denoted as

$$\Delta E_{nl, n'l', n''l''} = E_{|n'l'\rangle} + E_{|n''l''\rangle} - 2E_{|nl\rangle}, \quad (1.83)$$

has to be much smaller than the transition energy between $|nl, nl\rangle$ to the other two pair states, $|n'l', nl\rangle$ and $|nl, n''l''\rangle$. This is because a small Förster defect allows the transition from the initial pair state to the state $|n'l', n''l''\rangle$ while energetically forbids the transition to the other two states $|n'l', nl\rangle$ and $|nl, n''l''\rangle$ [37]. As a consequence, the system can be effectively described by a two-level Hamiltonian as,

$$\hat{H} = \begin{pmatrix} 0 & \langle nl, nl | V_{dd}(R_{AB}) | n'l', n''l'' \rangle \\ \langle n'l', n''l'' | V_{dd}(R_{AB}) | nl, nl \rangle & \Delta E_{nl, n'l', n''l''} \end{pmatrix}. \quad (1.84)$$

The eigenenergies of the system are found by diagonalising the Hamiltonian

$$U_{\pm} = \frac{\Delta E_{nl, n'l', n''l''} \pm \sqrt{\Delta E_{nl, n'l', n''l''}^2 + 4|\langle n'l', n''l'' | V_{dd}(R_{AB}) | nl, nl \rangle|^2}}{2}. \quad (1.85)$$

It is clear that the interaction energy of the pair states is now dependent upon the separation of the two atoms.

Two distinct limits of the interaction energy can be discussed based on Eq.(1.85) [58]

1. Short-range ($|\langle n'l', n''l'' | V_{dd}(R_{AB}) | nl, nl \rangle| \gg \Delta E_{nl, n'l', n''l''}$)

$$U_{\pm} \approx \pm |\langle n'l', n''l'' | V_{dd}(R_{AB}) | nl, nl \rangle| \approx \pm \frac{C_3}{R_{AB}^3},$$

where C_3 is the dispersion coefficient for the dipole-dipole interaction. For large n , the dipole matrix element between nearby Rydberg levels scales as n^2 . Thus $|\langle n'l', n''l'' | V_{dd}(R_{AB}) | nl, nl \rangle|$ contains two factors of n^2 , one for each

atom. Therefore, this coefficient scales as $C_3 \propto n^4$.

2. Long-range ($|\langle n'l', n''l'' | V_{\text{dd}}(R_{\text{AB}}) | nl, nl \rangle| \ll \Delta E_{nl, n'l', n''l''}$)

$$U_{\pm} \approx -\frac{|\langle n'l', n''l'' | V_{\text{dd}}(R_{\text{AB}}) | nl, nl \rangle|^2}{\Delta E_{nl, n'l', n''l''}} \approx \pm \frac{C_6}{R_{\text{AB}}^6},$$

this is the van der Waals (vdW) regime where the interaction is dominated by the Förster defect $\Delta E_{nl, n'l', n''l''}$. In this limit, the strength of the interaction is characterized by the dispersion coefficient for the van der Waals interaction C_6 which scales proportional to n^{11} as

$|\langle n'l', n''l'' | V_{\text{dd}}(R_{\text{AB}}) | nl, nl \rangle|^2 \propto |n^4|^2$ and the Förster (energy) defect $\Delta E_{nl, n'l', n''l''} \propto n^{-3}$. For more elaborate calculations of C_6 , see Ref [63]. The dramatic scaling with n leads to an interaction strength between two highly excited Rydberg atoms being in the region of Megahertz over micrometer distances [64]. Other feature of vdW interaction is that it quickly decays with increasing distance due to the inverse power law [37].

The transition between the $1/R_{\text{AB}}^3$ and $1/R_{\text{AB}}^6$ regimes occurs at a crossover distance R_C when $|\langle n'l', n''l'' | V_{\text{dd}}(R_{\text{AB}}) | nl, nl \rangle| \approx \Delta E_{nl, n'l', n''l''}$. When $R_{\text{AB}} < R_C$ the interaction has the dipolar form U_{dd} . When $R_{\text{AB}} > R_C$ the interaction has the van der Waals form U_{vdW} [46]. In this thesis, we restrict ourselves to regime where the interatomic distance is large enough such that Rydberg atoms always interact via vdW interaction.

1.3.5. Rydberg-dressed atoms

The most challenging problem in using Rydberg excitation in quantum gases and many-body systems is the mismatch in timescales; the lifetime of Rydberg atoms in low angular momentum l states is on the order of tens of microseconds [65]. For instance, for a Rydberg state $50S_{1/2}$ is approximately $\sim 100 \mu\text{sec}$ [2], whereas it typically takes three orders of magnitude longer for a typical experimental system of cold atoms to equilibrate [65]. This problem can be overcome by employing the following scheme. Because the Rydberg-Rydberg interactions are so strong due to the $C_6 \sim n^{11}$ scaling of the van der Waals (vdW) interaction, we can instead of

completely transferring a ground state atom to a certain $nS_{1/2}$ Rydberg state, we rather couple it off-resonantly by a two-photon laser transition [66]. To illustrate this idea, let us first write the wave function of the Rydberg-dressed atom which is mostly ground state with a small, adjustable Rydberg component β as [67]

$$|\psi_{\text{dressed}}\rangle = \alpha|g\rangle + \beta|r\rangle,$$

where α and β are the probability amplitudes for the ground and the Rydberg states, respectively. The radiative decay rate (spontaneous decay rate) due to the dressing Γ_{dressed} is proportional to the radiative decay rate of the Rydberg state Γ_r which was expressed in Eq.(1.50), and the dressing fraction β^2 which represents the probability for the atom to be in Rydberg state

$$\Gamma_{\text{dressed}} \sim |\langle g|\hat{d}|\psi_{\text{dressed}}\rangle|^2 \sim \beta^2 |\langle g|\hat{d}|r\rangle|^2 \sim \beta^2 \Gamma_r.$$

Therefore, as the lifetime of the dressed atom is the reciprocal of the radiative decay rate $\tau_{\text{dressed}} = 1/\Gamma_{\text{dressed}}$, one can write

$$\tau_{\text{dressed}} \sim \frac{1}{\beta^2} \cdot \tau_r. \quad (1.86)$$

As a result, this procedure of weakly dressing the atomic ground state with a small fraction β^2 of the Rydberg state enhances the overall lifetime of the system by $1/\beta^2$ [65]. We can imagine creating atoms that have only $\beta^2 \sim 0.01$ Rydberg character, which due to Rydberg atom exaggerated properties is still sufficient to create interesting physics, to increase the lifetimes to $\sim 100\tau_r$ where it may be possible for the system to come to equilibrium.

Furthermore, it is tempting to simply calculate the interaction energy resulting from the dressing between two Rydberg-dressed states as

$$E_{\text{int}} = \langle \psi_{\text{dressed}} | \hat{V}_{\text{int}} | \psi_{\text{dressed}} \rangle = \beta^2 \langle r | \hat{V}_{\text{int}} | r \rangle = \beta^2 E_r \propto \frac{\beta^2}{R_{12}^6}, \quad (1.87)$$

where V_{int} is the usual Van der Waals operator between Rydberg states and E_r is the full interaction energy between two Rydberg states. As we will see in the next subsection, this expression is in general invalid because the atom-atom wave

function contains much less than β^2 of the $|r\rangle|r\rangle$ state and as a result it does not give the "soft-core" shape of the dressing interaction. The correct procedure is to calculate the dressed states for two atoms simultaneously. The blockade effect will arise naturally out of the dressed eigenstates of this two-atom system [67].

The admixture fraction is controllable by adjusting the coupling laser detuning and intensity, and thus would also give a tunable interatomic interaction between atoms in ultracold gases which could be a useful feature in exploring the effects of long-range interactions [67]. Theory predicts that this approach also yields a unique type of long-range interactions between Rydberg-dressed ground state atoms that would enable the observation of interesting non-linear wave dynamics [68] and exotic many body phenomena such as supersolidity [69] in degenerate quantum gases [70].

1.3.6. Interacting Rydberg-dressed atoms

We consider a system that consists of two free, i.e. not trapped, atoms where a far off-resonant laser dressing the electronic ground state $|g\rangle$ with a Rydberg nS state $|r\rangle$. The laser excitation is achieved by a two photon process as illustrated in Fig(1.8, a). In the regime where the effective Rabi frequency Ω is much smaller than the detuning Δ , the laser admixes a fraction of the Rydberg state to the ground state. The Hamiltonian of the system can be represented by a 4×4 matrix form,

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} |g_1 g_2\rangle & |g_1 r_2\rangle & |r_1 g_2\rangle & |r_1 r_2\rangle \\ \begin{pmatrix} 0 & \Omega & \Omega & 0 \\ \Omega & 2\Delta & 0 & \Omega \\ \Omega & 0 & 2\Delta & \Omega \\ 0 & \Omega & \Omega & 4\Delta + V_{12} \end{pmatrix} \end{pmatrix} \begin{pmatrix} \langle g_1 g_2| \\ \langle g_1 r_2| \\ \langle r_1 g_2| \\ \langle r_1 r_2| \end{pmatrix}. \quad (1.88)$$

In our system, the electronic dynamics (Rydberg excitation and van der Waals interaction) take place on a timescale ($\sim \mu\text{sec}$) that is orders of magnitude faster than that of the external motion of ultracold atoms ($\sim \text{msec}$). This huge difference in these time scales permits the use of the Born-Oppenheimer approximation for treating the electronic Hamiltonian. Rydberg dressing implies a far off-resonant excitation, i.e. $|\Delta/\Omega| \gg 1$, which permits the adiabatic elimination of the atomic

Rydberg states. This can be done by using the perturbation theory to the fourth order by assuming as a start point that the Hamiltonian is composed of two matrices, an unperturbed Hamiltonian $\hat{H}_{\text{unperturbed}}$ and a perturbation $\hat{H}_{\text{perturbation}}$,

$$\hat{H} = \hat{H}_{\text{unperturbed}} + \hat{H}_{\text{perturbation}},$$

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega & \Omega & 0 \\ \Omega & 0 & 0 & \Omega \\ \Omega & 0 & 0 & \Omega \\ 0 & \Omega & \Omega & 0 \end{pmatrix} + \frac{\hbar}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2\Delta & 0 & 0 \\ 0 & 0 & 2\Delta & 0 \\ 0 & 0 & 0 & 4\Delta + V_{12} \end{pmatrix},$$

The effective Hamiltonian of the system is obtained by applying the perturbation theory to the fourth order which leads to⁸,

$$\hat{H}_{\text{eff}} = 2\hbar \left(\frac{\left(\frac{\Omega}{2}\right)^4}{\Delta^3} - \frac{\left(\frac{\Omega}{2}\right)^2}{\Delta} \right) + \frac{2\hbar \left(\frac{\Omega}{2}\right)^4}{\Delta^3} \left(\frac{V_{12}}{2\hbar\Delta + V_{12}} \right).$$

As the interaction between both Rydberg atoms is in the form of van der Waals interaction $V_{12} = C_6/|\vec{r}_1 - \vec{r}_2|^6$, then we obtain,

$$\hat{H}_{\text{eff}} = V_{\text{BO}} = 2\hbar \left(\frac{\left(\frac{\Omega}{2}\right)^4}{\Delta^3} - \frac{\left(\frac{\Omega}{2}\right)^2}{\Delta} \right) + V_{\text{SC}}(\vec{r}_1, \vec{r}_2), \quad (1.89)$$

where:

$$V_{\text{SC}}(\vec{r}_1, \vec{r}_2) = \frac{\zeta R_{\text{SC}}^6}{|\vec{r}_1 - \vec{r}_2|^6 + R_{\text{SC}}^6}, \quad (1.90)$$

represents the soft-core interaction sketched in Fig(1.11) with $\zeta = 2\hbar \left(\frac{\Omega}{2}\right)^4 / \Delta^3$ and $R_{\text{SC}} = (C_6/2\Delta)^{1/6}$ is the soft-core radius which depends on the laser detuning and the Rydberg state and it typically ranges from $1\mu\text{m}$ to a few μm . In the following we will neglect the constant term in Eq.(1.89) which represents the second and fourth order light shift. This effective Hamiltonian $\hat{H}_{\text{eff}}$, which also called Born-Oppenheimer potential surface V_{BO} , describes the dynamics of ground state Rydberg-dressed atoms in the regime where the effective Rabi frequency Ω is much smaller than the de-

⁸The derivation of the effective Hamiltonian is found in Appendix B

tuning Δ . the hallmark of the soft-core potential is the characteristic change of its behaviour in the vicinity of the distance R_{SC} : At large interatomic distance $|\vec{r}_1 - \vec{r}_2| \gg R_{\text{SC}}$, a small fraction $(\Omega/\Delta)^2$ that represents the probability for both atoms to be in the Rydberg states, is independently admixed to each ground state atom [69], such that the potential falls off rapidly with $1/|\vec{r}_1 - \vec{r}_2|^6$, originating from the van der Waals (vdW) interaction between Rydberg atoms in $|nS\rangle$ states with a reduced van der Waals coefficient $\tilde{C}_6 = \zeta R_{\text{SC}}^6 = (\Omega/2\Delta)^4 C_6$ [70]. However, at short distances $|\vec{r}_1 - \vec{r}_2| \ll R_{\text{SC}}$, the probability to find both atoms in the the Rydberg states decreases dramatically [65] with an energy due to interactions proportional to $\sim \hbar\Omega^4/8\Delta^3$ [67] and the interaction potential levels off to a constant value below the critical distance R_{SC} where it becomes independent of $|\vec{r}_1 - \vec{r}_2|$. This soft-core behaviour, i.e., $|\vec{r}_1 - \vec{r}_2|$ -independence, is a consequence of the *Rydberg blockade phenomenon*, which inhibits the simultaneous excitation of nearby atoms to Rydberg states. It can be easily noticed that the overall magnitude of the dressing effect is determined only by the laser parameters Ω and Δ [70].

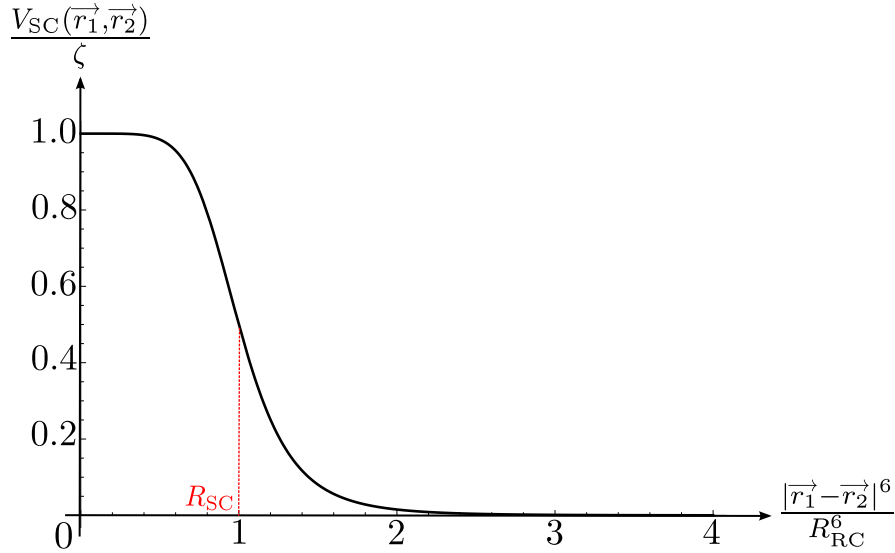


Figure 1.11.: The dimensionless soft-core interaction potential $V_{\text{SC}}(\vec{r}_1, \vec{r}_2)/\zeta$ which represents the resulting dressing induced interaction potential between ground state dressed Rydberg atoms as a function of the dimensionless distance $|\vec{r}_1 - \vec{r}_2|^6 / R_{\text{SC}}^6$. For large distances $|\vec{r}_1 - \vec{r}_2|/R_{\text{SC}} > R_{\text{SC}}$ the potential quickly decreases. For short distances $|\vec{r}_1 - \vec{r}_2|/R_{\text{SC}} < R_{\text{SC}}$ the potential saturates to a constant value.

It is very important to mention that the effective Rabi frequency Ω for systems

containing more than one atom is enhanced by factor of $\Omega_0\sqrt{N}$ with Ω_0 being the single-atom effective Rabi frequency and N is the total number of atoms in the system. This can be explained as follows. Since the simplest case of interacting dressed atoms is to consider only two atoms, then the Hamiltonian of the system, according to Eq.(1.80), can be written as

$$H = \frac{\hbar}{2} \sum_{i=1}^2 (\Omega_0 \sigma_x^i + 2\Delta n_i)$$

If we choose the basis of this Hamiltonian to be $\{|g_1 r_2\rangle, 1/\sqrt{2}(|g_1 r_2\rangle \pm |r_1 g_2\rangle), |r_1 r_2\rangle\}$, then to study the coupling⁹ between the ground state $|g_1 g_2\rangle$ and the single-excited state $1/\sqrt{2}(|g_1 r_2\rangle + |r_1 g_2\rangle)$, we calculate the following matrix element considering only the Rabi frequency term since detuning does not couple two states, it only changes their energies

$$\begin{aligned} I &= \left\langle g_1 g_2 \left| \frac{\hbar}{2} \Omega_0 (\sigma_x^1 + \sigma_x^2) \right| \frac{1}{\sqrt{2}} (|g_1 r_2\rangle + |r_1 g_2\rangle) \right\rangle \\ &= \frac{\hbar \Omega_0}{2\sqrt{2}} [\langle g_1 g_2 | (\sigma_x^1 + \sigma_x^2) | g_1 r_2 \rangle + \langle g_1 g_2 | (\sigma_x^1 + \sigma_x^2) | r_1 g_2 \rangle] \\ &= \frac{\hbar \Omega_0}{2\sqrt{2}} [1 + 1] \\ &= \frac{\hbar \Omega_0}{\sqrt{2}} \\ &= \frac{\hbar}{2} \Omega_0 \sqrt{2} \end{aligned} \tag{1.91}$$

It is clear that both states, $|g_1 g_2\rangle$ and $1/\sqrt{2}(|g_1 r_2\rangle + |r_1 g_2\rangle)$, do couple with a Rabi frequency larger than the one-atom frequency Ω_0 with a factor of $\Omega_0\sqrt{2}$. Likewise, if the system contains three atoms, then the enhanced Rabi frequency is $\Omega_0\sqrt{3}$, and similarly for N atoms where the resulting frequency is $\Omega_0\sqrt{N}$.

⁹Bearing in mind that the anti-symmetric state, $1/\sqrt{2}(|g_1 r_2\rangle - |r_1 g_2\rangle)$, is uncoupled and therefore can be ignored.

1.4. Outlook

In summary, we have presented in this introduction three key sections that are significantly related to the research topics in the upcoming chapters. In the first section the physics of non- and contact-interacting Bose-Einstein condensates (BECs) has been examined. The non-linear Gross-Pitaevskii equation (GPE) and its validity have been studied since the dynamics of a dilute BEC are usually governed by this equation. Later, the fundamentals of the interaction between a two-level atom and an electromagnetic field have been analysed where this study aimed to produce a periodic optical lattice potential. Lastly, the characteristics, properties and the nature of interactions between Rydberg atoms have been outlined. In the limit where the detuning is much larger than Rabi frequency, a very interesting phenomenon, known as Rydberg-dressing, occurs. Rydberg-dressed atoms, as we have seen, show a soft-core interaction shape that differs from the typical van der Waals interaction such that when the distance between two Rydberg-dressed atoms is much smaller than the soft-core radius, the interactions saturates to a constant value which is a consequence of Rydberg blockade.

In the following, our proceeding plan for the next chapters focuses on investigating the quantum dynamics of multiple BECs composed of interacting Rydberg-dressed atoms trapped in multi-well potential traps. In the second and third chapters, static traps are selected to examine these atoms using mean-field approach and extended Bose-Hubbard model, respectively. In the fourth chapter, a dynamical trapping potential is produced where both, the time-dependent linear and non-linear Schrödinger equations are used to probe the atoms' behaviours.

CHAPTER 2

Quantum dynamics of Bose-Einstein condensates trapped in
multi-well potentials in the mean-field regime

The characteristic feature of Bose-Einstein condensation (BEC) is the accumulation of a macroscopic number of particles in the energetically lowest quantum state of a given trapping potential [71]. The experimental observation of the BEC in a dilute gas of trapped atoms has generated much interest in the properties of this new state of matter [72], as well as considerable progress in the analysis of relevant models based on the non-linear Schrödinger (NLS)-type equations [73]. Many of these studies have been dealing with macroscopic non-linear structures that arise in BECs. One of the appealing features of this research area is the possibility to realise different potential traps of various shapes that confine the ultra-cold bosonic atoms which leads to exceptionally plentiful dynamical behaviours. For this reason, the analysis of the structure, stability and dynamical properties of non-linear matter-waves trapped in such tailored traps has become one of the most important topics for such studies. Recently, ultra-cold atoms in multi-well potentials have received much attention due to the tunability of their experimental parameters.

A prominent feature of quantum mechanics is the tunnelling through energetically forbidden regions. In solid state physics many investigations of the tunnelling phenomena have been done with *Superconducting Josephson Junctions* (SJJ). A SJJ consists of two superconductors separated by a thin insulating barrier. In such a junction the electron cooper pairs in the superconductors can tunnel through the barrier. We study a similar situation but instead of cooper pairs in superconductors, we consider Bose condensed atoms in a double-well potential which is usually called a *Bosonic Josephson Junction* (BJJ). In 2005, Albiez *et al.*, [74] reported the first realisation of a single bosonic Josephson junction, implemented by two weakly linked Bose-Einstein condensates in a double-well potential. The analogy between double Bose-Einstein condensates, separated by a barrier, and Josephson oscillations of superconductors was first suggested by Javanainen [75]. Likewise to the analogue of the double-well to the Josephson junction, the triple-well, as well, is the minimum system that can control the *source-gate-drain junction* where the left potential well behaves like the source, the middle as the gate, and the right potential well is equivalent to the drain. The simplest atom transistor utilises a three-well potential in which quantum mechanical tunnelling between “source” and “drain” wells is controlled by the number of atoms in the central “gate” well [76].

In a cold dilute Bose gas, atoms interact via short-range contact-interactions determined by the s -wave scattering length a as Eq.(1.14) showed, which can be experimentally varied with the help of Feshbach resonances [77]. In addition, trapped Rydberg-dressed atoms exhibit long-range interactions formulated by the soft-core interaction expressed in Eq.(1.90).

Our aim in this chapter is to study the quantum dynamics of an ensemble of N_T three-level ^{87}Rb Rydberg-dressed atoms trapped in multi-well potentials in the presence of repulsive, long-range (non-local) and non-linear interactions. The dynamics of these atoms, which form a BEC, are described within the mean-field theory by using the time-dependant non-linear Gross-Pitaevskii equation (GPE).

This chapter is an extension of the work detailed in reference [72] where they examined, via the mean-field theory using GPE, the quantum dynamics of two contact-interacting BECs trapped in a symmetric double-well potential trap. Our analysis in this chapter investigates the non-linear coherent dynamics considering two additional concepts:

1. The non-linear dynamics are probed inside multi-well potential traps.
2. Long-range interaction is added.

The chapter is structured as follows. In section (2.1) we begin by introducing the double-well potential trap where we present an optical setup to create a three-dimensional double-well potential in subsection (2.1.1). The mean-field description of the system is studied in subsection (2.1.5) leading, after obtaining the dynamical differential equations, to study the system in three distinct dynamical regimes, Rabi regime in subsection (2.1.6.1), Josephson regime in subsection (2.1.6.2) and Fock regime in subsection (2.1.6.3). With the same analysis, an extension of the study to an one-dimensional triple-well potential trap in section (2.2) and a two-dimensional quadruple-well potential trap in section (2.3) is presented. This chapter is finalized with a conclusion in section (2.4) that summarizes all the results being discussed.

2.1. Double-well potential

The double-well potential is the simplest case of a multi-well potential, and a plethora of phenomena have been observed and analysed in great detail for this system [78]. Recently, Bose-Einstein condensate in double-well potentials have been the subject of interesting and exciting research where they provide an ideal medium for the study of fundamental quantum many-body phenomena, such as macroscopic quantum tunnelling and macroscopic superposition states [79]. In this section we begin by constructing an optical setup for a three-dimensional double-well potential via laser fields. Next, the conditions that have to be fulfilled in order to reduce the dimensionality of the double-well potential trap are discussed. Since the phenomenon of tunnelling is an important consequence of quantum mechanics, a single rubidium atom tunnelling in the double-well potential under the two-mode approximation is studied analytically and numerically. A trapped BEC within a symmetric one-dimensional double-well potential via the mean-field theory is analysed using dynamical differential equations for both, the fractional population imbalance and relative phase. Later on, the condensate is studied within three distinct interacting regimes; Rabi (non-interacting limit), Josephson (linear interacting limit) and Fock (non-linear interacting limit) regimes.

2.1.1. Realisation of double-well potential via laser fields

There are many different methods to produce a double-well potential for Bose-Einstein condensates. The first realised double-well potential was obtained already in the early days of BEC using a harmonic confinement created by a magnetic trap and a focused blue detuned laser beam generating the tunnelling barrier [80]. Many other attempts have been made to realise double-well potentials [81, 71, 82]. Our work here based on creating a double-well potential for one rubidium atom ^{87}Rb using two crossed, focused and far-off-resonant Gaussian lasers beams¹.

We consider a typical V-type three-level ^{87}Rb atom as shown in Fig.(2.1) consisting of a singlet ground state $|5^2S_{\frac{1}{2}}\rangle$ and two excited states which are two of the hyperfine energy states of $|5^2P_{\frac{3}{2}}\rangle$. The atom is driven by two lasers; a far-off res-

¹Fully detailed analysis about the optical setup of the double-well potential is found in the Appendix C.

onant red-detuned Gaussian laser beam $\vec{E}_1(x, y, z)$ with a frequency ω_{l1} coupling the ground state with $|5^2P_{\frac{3}{2}}(F=3, m_F=-3)\rangle$ state, and a far-off resonant blue-detuned Gaussian laser beam $\vec{E}_2(x, y, z)$ with a frequency ω_{l2} that couples the ground state with the $|5^2P_{\frac{3}{2}}(F=3, m_F=-1)\rangle$ state. Both Gaussian laser beams can be written as

$$\begin{aligned}\vec{E}_1(x, y, z) &= E_{01}\hat{\epsilon}_1 \frac{w_1}{w_1(x)} \exp(ik_1x) \exp\left(-\frac{y^2+z^2}{w_1(x)^2}\right) \\ \vec{E}_2(x, y, z) &= E_{02}\hat{\epsilon}_2 \frac{w_2}{w_2(x)} \exp(ik_2x) \exp\left(-\frac{y^2+z^2}{w_2(x)^2}\right),\end{aligned}\quad (2.1)$$

where, $E_{0i}, w_i, k_i, \hat{\epsilon}_i$ are the amplitudes, waists, wave vectors and the unit polarisations, respectively. $w_i(x)$ is the beam width which is given by $w_i(x) = w_i\sqrt{1 + (x/x_{ri})^2}$ where x_{ri} is Rayleigh length, with $i = 1, 2$.

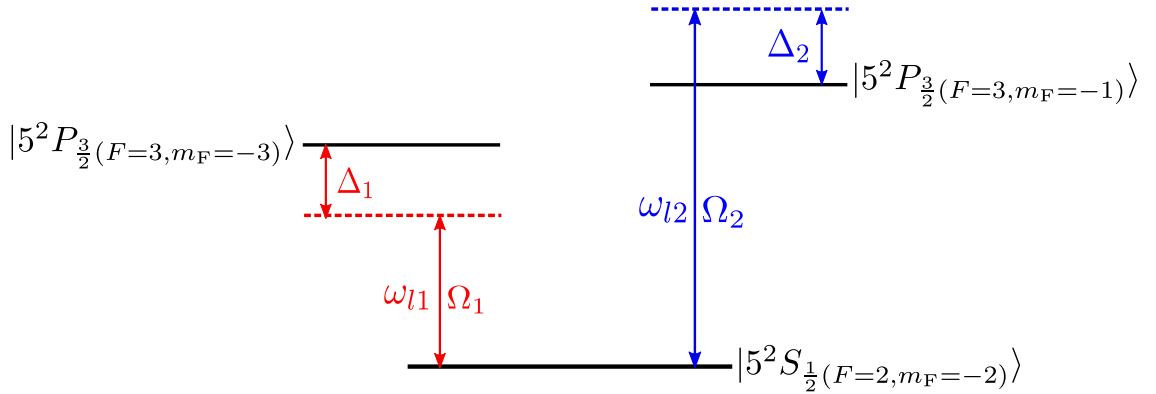


Figure 2.1.: V-type three-level ^{87}Rb atom where the ground state $|5^2S_{\frac{1}{2}}(F=2, m_F=-2)\rangle$ and the excited state $|5^2P_{\frac{3}{2}}(F=3, m_F=-3)\rangle$ are coupled by the far red-detuned off-resonant laser beam having a frequency of ω_{l1} with a detuning $\Delta_1 > 0$. However, the far blue-detuned off-resonant laser beam couples the same ground state with the second excited state $|5^2P_{\frac{3}{2}}(F=3, m_F=-1)\rangle$ having a frequency equals to ω_{l2} and a detuning $\Delta_2 < 0$.

The Hamiltonian in the rotating wave approximation describing this atom can be expressed as a 3×3 matrix in the basis $\{|5^2S_{\frac{1}{2}}\rangle, |5^2P_{\frac{3}{2}}(m_F=-3)\rangle, |5^2P_{\frac{3}{2}}(m_F=-1)\rangle\}$

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_1 & \Omega_2 \\ \Omega_1 & 2\Delta_1 & 0 \\ \Omega_2 & 0 & 2\Delta_2 \end{pmatrix}, \quad (2.2)$$

where both Rabi frequencies are assumed to be real values, i.e., $\Omega_{1,2} \in \mathbb{R}$, and given

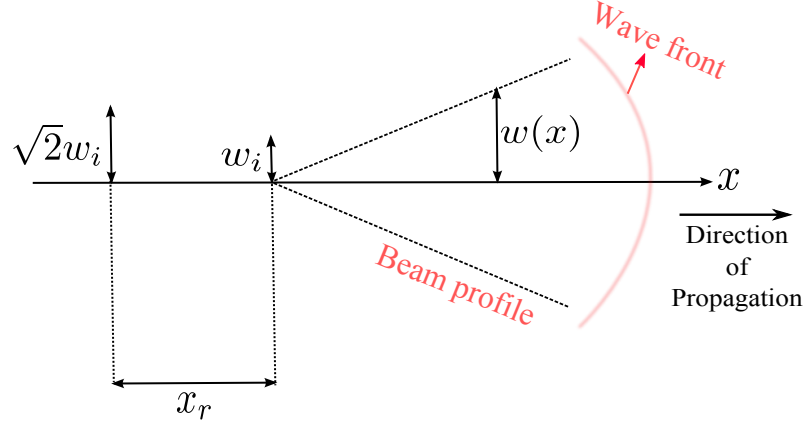


Figure 2.2.: The Gaussian laser beam where the Gaussian beam width $w_i(x)$ is illustrated as a function of the propagation axis x where w_i is the beam waist with $i = 1, 2$ referring to either of the Gaussian beams used to create the double-well potential trap, and x_r is the Rayleigh range.

by

$$\Omega_1 = \frac{eE_{01}\hat{\epsilon}_1}{\hbar} \langle 5^2 S_{\frac{1}{2}}(F=2, m_F=-2) | \vec{r} | 5^2 P_{\frac{3}{2}}(F=3, m_F=-3) \rangle$$

$$\Omega_2 = \frac{eE_{02}\hat{\epsilon}_2}{\hbar} \langle 5^2 S_{\frac{1}{2}}(F=2, m_F=-2) | \vec{r} | 5^2 P_{\frac{3}{2}}(F=3, m_F=-1) \rangle.$$

To create conservative potentials for coherent manipulation, spontaneous decay of the excited state has to be avoided [83]. Thus we can make the excited state probability small enough by assuming that the detuning is larger than the Rabi frequency $|\Delta_{1,2}| \gg \Omega_{1,2}$. Based on the study of two-level atom's interaction with light that has been presented in section (1.2), the problem here can be readily extended to three-level atom. Therefore, applying the second order perturbation theory on the Hamiltonian in Eq.(2.2) leads to

$$\begin{aligned} V_{\text{dw}} &= \hat{H}_{\text{nn}}^{(0)} + \hat{H}_{\text{nn}}^{(1)} + \hat{H}_{\text{nn}}^{(2)} \\ &= E_{|S\rangle} + \langle S | \hat{H}_{\text{perturbed}} | S \rangle + \left[\frac{|\langle S | \hat{H}_{\text{perturbed}} | P_{m_F=-3} \rangle|^2}{E_{|P_{m_F=-3}\rangle} - E_{|S\rangle}} + \frac{|\langle S | \hat{H}_{\text{perturbed}} | P_{m_F=-1} \rangle|^2}{E_{|P_{m_F=-1}\rangle} - E_{|S\rangle}} \right] \\ &= 0 + 0 + \left[\frac{\left(\frac{\hbar\Omega_1}{2} \right)^2}{\hbar\Delta_1} + \frac{\left(\frac{\hbar\Omega_2}{2} \right)^2}{\hbar\Delta_2} \right] = \frac{|\vec{d}_1 \cdot \vec{E}_1(x, y, z)|^2}{4\hbar\Delta_1} + \frac{|\vec{d}_2 \cdot \vec{E}_2(x, y, z)|^2}{4\hbar\Delta_2}. \end{aligned}$$

Since the dipole moments of the atom are given by $\vec{d}_i = e\langle S|\vec{r}|P_j\rangle$, where: $i = 1, 2$ and $j = m_F = -3, -1$, respectively, and the electric fields for both lasers are given by $\vec{E}_i = \hat{e}_i E_{0i}$, hence, if we assume that $\vec{d}_i$ and $\vec{E}_i$ are circularly polarised, therefore the ground state energy shift can be written

$$V_{\text{dw}} \approx A_1|E_1(x, y, z)|^2 + A_2|E_2(x, y, z)|^2, \quad (2.3)$$

where: $A_i = \frac{|d_i|^2}{4\hbar\Delta_i}$ with $i = 1, 2$.

To get a more applicable double-well potential trap expression, the Gaussian beams in Eqs.(2.1) can be expanded in the vicinity of the focus $(x_0, y_0, z_0) = (0, 0, 0)$ using Taylor expansion in higher dimensions, then inserting the approximated laser beams into Eq.(2.3) leads to the three-dimensional double-well potential trap

$$V_{\text{dw}}(x, y, z) = \alpha - \beta x^2 + \gamma x^4 - \delta (y^2 + z^2), \quad (2.4)$$

where,

$$\begin{aligned} \alpha &= A_1 E_{01}^2 + A_2 E_{02}^2 & \beta &= \frac{A_1 E_{01}^2}{x_{r1}^2} + \frac{A_2 E_{02}^2}{x_{r2}^2} \\ \gamma &= \frac{A_1 E_{01}^2}{x_{r1}^4} + \frac{A_2 E_{02}^2}{x_{r2}^4} & \delta &= \frac{2A_1 E_{01}^2}{w_1^2} + \frac{2A_2 E_{02}^2}{w_2^2}. \end{aligned}$$

It is worth mentioning that our system is engineered so that $(\beta, \gamma > 0, \delta < 0)$, which makes this expression produces a double-well potential with two minima. However, if $(\beta \leq 0)$, it creates an anharmonic potential with only one minimum.

2.1.2. Quasi one-dimensional double-well trap

Up to this point, we have put an optical setup to create a three-dimensional double-well potential using two Gaussian laser beams. However, in the following, we will concentrate on investigating the properties of quasi one-dimensional double-well potential since it is the simplest case. Let us discuss the condition that allows us to reduce the dimensionality of a three-dimensional potential to a quasi one-

dimensional trap.

As a first step, we get the trapping frequencies ω_x, ω_y and ω_z for the three-dimensional double-well potential in Eq.(2.4). Since the potential can be approximated as harmonic oscillator in the vicinity of its minima $(x_{\min}, y_{\min}, z_{\min})$, then we apply the quadratic Taylor expansion, the so-called *harmonic approximation*, and then compare it with the harmonic oscillator expression, which yields to

$$\frac{1}{2}m_{\text{Rb}}\omega_x^2(x - x_{\min})^2 = \frac{1}{2!} \left. \frac{d^2V_{\text{dw}}(x)}{dx^2} \right|_{x=x_{\min}} (x - x_{\min})^2, \quad (2.5)$$

and the same goes for y and z , with m_{Rb} being the atomic mass of the rubidium atom ^{87}Rb . The minima of the three-dimensional double-well potential $(x_{\min}, y_{\min}, z_{\min})$ are calculated by setting the first derivatives of the double-well potential to zero

$$\begin{aligned} \frac{dV_{\text{dw}}(x, y, z)}{dx} = 0 & \implies x_{\min} = \pm \sqrt{\frac{\beta}{2\gamma}} \\ \frac{dV_{\text{dw}}(x, y, z)}{dy} = 0 & \implies y_{\min} = 0 \\ \frac{dV_{\text{dw}}(x, y, z)}{dz} = 0 & \implies z_{\min} = 0. \end{aligned} \quad (2.6)$$

Therefore, by inserting Eq.(2.6) into Eq.(2.5) we write the trapping frequencies as

$$\omega_x = \sqrt{\frac{4\beta}{m_{\text{Rb}}}} \quad \omega_y = \sqrt{\frac{2\delta}{m_{\text{Rb}}}} \quad \omega_z = \sqrt{\frac{2\delta}{m_{\text{Rb}}}}. \quad (2.7)$$

For sufficiently large trapping frequencies and thus strong confinements on the y and z axes (in the yz plane) where $\omega_y \approx \omega_z \gg \omega_x$, the high-energy modes of excitations on y and z axes become heavily suppressed where the atomic motion in these both axes can be considered as "frozen" into their relevant harmonic oscillator ground state since they have large energy spacings of approximately $\hbar\omega_{y,z}$. In this regime, the dynamics on the x axis which are of relatively low energy, dominate the system where the atoms can be excited more easily to higher energy states as the energy spacing $\hbar\omega_x$ is much smaller compared to the excitations along the y, z axes. Therefore, this allows us to study only the quasi-one dimensional motion of the trapped atoms along the x axis. Moreover, the wave function of the system

is factorised into the product of x component and y, z components, $\psi(x, y, z) = \psi(x)\psi(y, z)$. Here, $\psi(y, z)$ has the expression of the ground state of the harmonic oscillator expressed in Eq.(1.4).

Consequently, our potential can be regarded as a quasi one-dimensional double-well potential along the x axis as shown in Fig.(2.3), and its quasi one-dimensional expression is formulated as

$$V_{\text{dw}}(x) \approx \alpha - \beta x^2 + \gamma x^4. \quad (2.8)$$

2.1.3. Numerical approach to study one rubidium atom in a quasi one-dimensional double-well potential

Consider one rubidium atom trapped in a quasi one-dimensional double-well potential, then the time-independent one-dimensional Schrödinger equation is given by

$$\hat{H}\psi(x) = E\psi(x) \implies \left[-\frac{\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{dx^2} + V_{\text{dw}}(x) \right] \psi(x) = E\psi(x), \quad (2.9)$$

where $\psi(x)$, E and m_{Rb} are the wave function, the energy and the mass of the rubidium atom, respectively. The problem is simplified by transforming the Schrödinger equation into a dimensionless eigenvalue equation. A simple strategy is to define a dimensionless coordinate $q = \frac{x}{\xi_x}$, where $\xi_x = (\hbar/m_{\text{Rb}}\omega_x)^{1/2}$ is the local harmonic oscillator length of one well, and we assume that $q \in [q_{\min}, q_{\max}]$ with the interval $[q_{\min}, q_{\max}]$ sufficiently large such that the wave function and all its derivatives of interest vanish at the boundaries. Then we can write

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{d(q\xi_x)^2} + V_{\text{dw}}(q\xi_x) \right] \psi(q\xi_x) = E\psi(q\xi_x) \\ & \left[-\frac{\hbar^2}{2m_{\text{Rb}}\xi_x^2} \frac{d^2}{dq^2} + \left(-\beta(q\xi_x)^2 + \gamma(q\xi_x)^4 \right) \right] \psi(q\xi_x) = E\psi(q\xi_x). \end{aligned}$$

In the following, we rescale this equation in the energy unit of $\hbar^2/2m_{\text{Rb}}\xi_x^2$, thus defining a new solution $\phi(q) = \psi(q\xi_x)$ yields

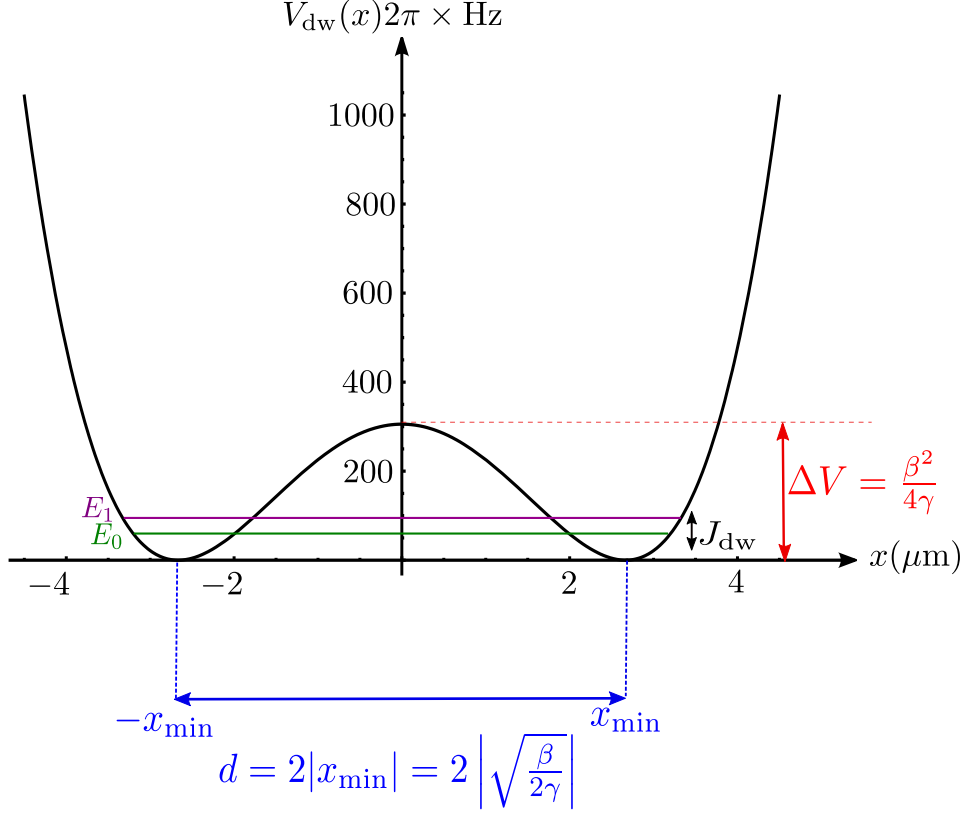


Figure 2.3.: A symmetric quasi one-dimensional double-well potential on the x axis $V_{\text{dw}}(x) = \alpha - \beta x^2 + \gamma x^4$, where $\beta = 5.69 \times 10^{-20} \hbar \cdot \text{Hz} \cdot \text{m}^{-2}$ and $\gamma = 4 \times 10^{-9} \hbar \cdot \text{Hz} \cdot \text{m}^{-4}$. α is considered as an energy shift for the double-well trap. This potential has two minima $\pm x_{\text{min}}(\mu\text{m}) \approx \pm 2.6 \mu\text{m}$ where the separation between both wells is d . ΔV is the double-well potential barrier height which is calculated as $\Delta V = V_{\text{dw}}(x=0) - V_{\text{dw}}(x=x_{\text{min}}) = \beta^2/4\gamma \approx 2\pi \times 305.551 \text{Hz}$. If the barrier is high enough, the Bose-Einstein condensate is split into two localised matter-wave packets, and if the barrier is not too high, particles can tunnel from well to well leading to a coherent coupling. E_0 (solid green line) and E_1 (solid purple line) are the ground-state and the first excited state eigen-energies of the double-well potential, respectively. The tunnelling rate $J_{\text{dw}} = E_1 - E_0$ in a symmetric double-well potential represents the difference between the first pair of the energy levels.

$$\left[-\frac{d^2}{dq^2} - \frac{2m_{\text{Rb}}\xi_x^4\beta}{\hbar^2}q^2 + \frac{2m_{\text{Rb}}\xi_x^6\gamma}{\hbar^2}q^4 \right] \phi(q) = \frac{2m_{\text{Rb}}\xi_x^2 E}{\hbar^2} \phi(q).$$

New dimensionless parameters can be defined

$$\frac{2m_{\text{Rb}}\xi_x^4\beta}{\hbar^2} = \tilde{\beta} \quad \frac{2m_{\text{Rb}}\xi_x^6\gamma}{\hbar^2} = \tilde{\gamma} \quad \frac{2m_{\text{Rb}}\xi_x^2 E}{\hbar^2} = \epsilon. \quad (2.10)$$

Therefore, the dimensionless form of the Schrödinger equation describing one rubid-

ium atom trapped in a double-well potential is

$$\left[-\frac{d^2}{dq^2} - \tilde{\beta}q^2 + \tilde{\gamma}q^4 \right] \phi(q) = \epsilon \phi(q). \quad (2.11)$$

A conventional numerical approach to the solution of the Schrödinger equation Eq.(2.11) has been the *finite-difference discretisation method* (FDDM). This scheme is almost standard in numerical methods that are based on computational grids as it is considered an important and one of the simplest forms of discretisation [84]. It provides the best possible accuracy and efficient solutions to the time-independent differential equations in one-dimensional space geometry when the equations contain second-order spatial derivatives. With this method, the spatial parameter q is divided into N discrete and equally spaced mesh points $q_i = q_0 + j\Delta q$, with $j = 0, 1, 2, \dots, N-1$, where $q_{\min} = q_0$ and $q_{\max} = q_N$, hence, the wave function $\phi(q)$ is solved within those discrete spacings. In this way, the interval $[q_{\min}, q_{\max}]$ is divided into N subintervals of size $\Delta q = \frac{q_{\max} - q_{\min}}{N} + 1$. It is noteworthy that the mesh size is determined by the opposing requirements of greater accuracy on one hand (hence, smaller mesh size) and a rapid computational times on the other hand (hence large mesh size) [84]. By implementing the three-point finite-difference discretisation method on the second-order spatial derivative in Eq.(2.11), we obtain

$$\begin{aligned} & -\frac{d^2}{dq^2} \phi(q) + \left(-\tilde{\beta}q^2 + \tilde{\gamma}q^4 \right) \phi(q) = \epsilon \phi(q), \\ & -\frac{\phi(q_{n+1}) - 2\phi(q) + \phi(q_{n-1}))}{\Delta q^2} + \left(-\tilde{\beta}q^2 + \tilde{\gamma}q^4 \right) \phi(q) = \epsilon \phi(q), \\ & \underbrace{-\frac{1}{\Delta q^2} \phi(q_{n+1}) - \frac{1}{\Delta q^2} \phi(q_{n-1}))}_{\text{off-diagonal}} + \underbrace{\left[\frac{2}{\Delta q^2} - \tilde{\beta}q^2 + \tilde{\gamma}q^4 \right]}_{\text{diagonal}} = \epsilon \phi(q). \end{aligned} \quad (2.12)$$

The eigenstates and the eigenenergies of the rubidium atom in the double-well potential are calculated using this discretised equation where the first two terms represent the off-diagonal elements of the Hamiltonian matrix, whereas, the third term between squared brackets represents the diagonal ones. Fig.(2.4) shows the ground state and the the first three excited states of the rubidium atom in the double-well

potential trap.

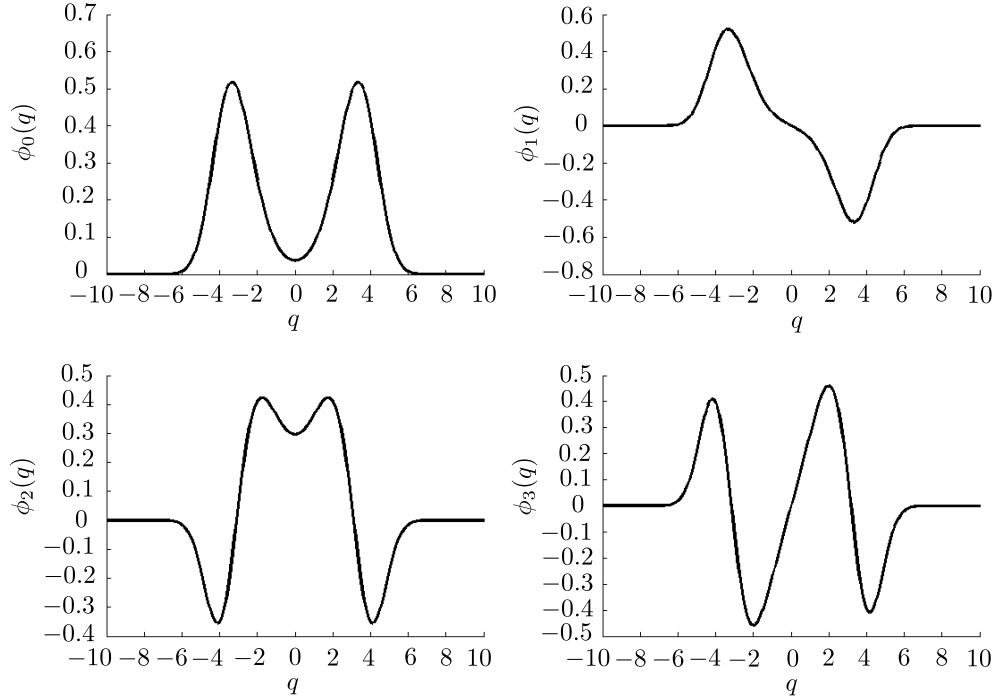


Figure 2.4.: The normalized ground state $\phi_0(q)$ and the first three excited states $\phi_1(q)$, $\phi_2(q)$, $\phi_3(q)$, respectively, of a one rubidium atom trapped in a quasi one-dimensional double-well potential $\tilde{V}_{\text{dw}}(q)$ as a function of the dimensionless spatial variable q where $\tilde{\beta} = 0.5$ and $\tilde{\gamma} = 0.0204$.

2.1.4. Two-mode approximation for a single-atom tunnelling

The geometry of the double-well potential leads to an energy spectrum, in which the energy difference between the first two single atom states, i.e., $E_1 - E_0$, is much smaller than the difference to all energetically higher lying states² as Fig.(2.5) illustrates. The difference in energy $E_1 - E_0$ is known as the *ground state energy splitting*. Higher energy levels are also paired in this way (e.g. E_2 is far from E_1 but close to E_3) and the energy splittings between these pairs are known as *higher state energy*

²If there is a particle moving in one-dimensional n -well potential, the bound states split into sets of n levels that the separation among the levels is equally spaced and it is much smaller than the separation among the sets. The energy separation among these sets becomes better defined the deeper the potential wells are [85].

splittings (e.g. $E_3 - E_2$)³. Thus, the system can be reduced to only two orbitals in which the atoms are located, this is the so-called *two-mode approximation*.

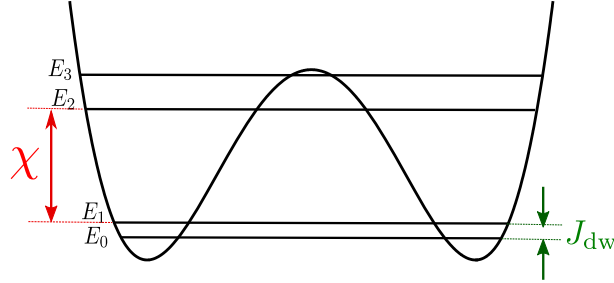


Figure 2.5.: Two-mode approximation condition is $\chi \gg J_{\text{dw}}$.

It has limited validity in the case of a low potential barrier, when it is not allowed to neglect higher excitation modes and strong atom-atom interactions. In this case, each energy level splits into two and these two levels correspond to the motion of the particle in the two wells at the same time [86]. However, it becomes increasingly accurate by raising the potential barrier, then the energy levels would roughly correspond to the motion of an atom in one of the two wells which are approximately harmonic oscillator potentials [6]. For that reason, the state of the double-well potential trap is determined by the population and the phase of these two modes [87] as we will see later on. Therefore, the tunnelling time or quantum oscillation period is inversely proportional to the energy splitting [88].

2.1.4.1. Numerical calculation of tunnelling rate

In the following, we will study the tunnelling rate numerically, i.e., the energy difference between the first two eigenenergies which are obtained from the numerically discretised Schrödinger equation in Eq.(2.12), and analytically, i.e., within the Gaussian approximation for both, the right and left wave functions, and afterwards, it would be certainly interesting to compare between both methods.

As was indicated in the subsection (2.1.3), based on the numerically discretised Schrödinger equation in Eq.(2.12) for one rubidium atom trapped in a double-well potential, the first two eigenstates, i.e., the symmetric ground $|\phi_{\text{sym}}\rangle = |\phi_0\rangle$ and

³Above the potential barrier, the wave function becomes more and more similar to an oscillator wave function, and therefore, the energy difference between these states becomes equally spaced.

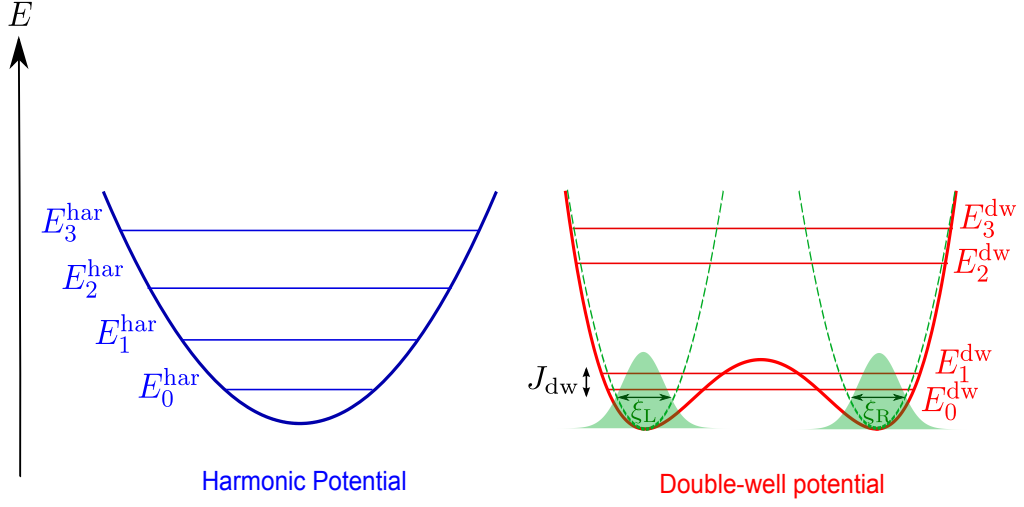


Figure 2.6.: Level spacing between the energy states in a harmonic potential in comparison to the double-well potential.

the anti-symmetric first excited states $|\phi_{\text{antisym}}\rangle = |\phi_1\rangle$ and their corresponding energies E_0^{dw} , E_1^{dw} , respectively as Fig(2.6) shows, can be obtained. Moreover, the two localised modes, i.e., the left and right orbitals, can be constructed as linear combinations from both eigenstates,

$$|\phi_{\text{Right}}\rangle = \frac{|\phi_{\text{sym}}\rangle - |\phi_{\text{antisym}}\rangle}{\sqrt{2}} \quad |\phi_{\text{Left}}\rangle = \frac{|\phi_{\text{sym}}\rangle + |\phi_{\text{antisym}}\rangle}{\sqrt{2}}. \quad (2.13)$$

The orbitals ϕ_{Left} , ϕ_{Right} are orthogonal to one another and satisfy $\phi_{\text{Left}}(-x) = \phi_{\text{Right}}(x)$. For sufficiently high barriers the orbitals ϕ_{Left} and ϕ_{Right} are localised in the left and the right wells of the double-well potential [89]. Therefore, the system which is prepared in the left orbital $|\phi_{\text{Left}}\rangle$ will evolve into the right localised orbital $|\phi_{\text{Right}}\rangle$ and back with a frequency $J_{\text{dw}}^{\text{Num}}/\hbar$ where $J_{\text{dw}}^{\text{Num}}$ is the numerical tunnelling rate and is defined by the energy difference between the eigenstates $|\phi_{\text{sym}}\rangle$ and $|\phi_{\text{antisym}}\rangle$.

Hence, the tunnelling rate can be easily calculated as:

$$J_{\text{dw}}^{\text{Num}} = \langle \phi_{\text{antisym}} | \hat{H} | \phi_{\text{antisym}} \rangle - \langle \phi_{\text{sym}} | \hat{H} | \phi_{\text{sym}} \rangle = -2 \langle \phi_{\text{Left}} | \hat{H} | \phi_{\text{Right}} \rangle, \quad (2.14)$$

where $\hat{H} = -\hbar^2/2m + V_{\text{dw}}(x)$ is the one-atom Hamiltonian trapped in the symmetric quasi one-dimensional double-well potential $V_{\text{dw}}(x)$. Table(2.1) shows the numerical eigenenergies for the first two eigenstates (note that they are quasi degenerate) and

the energy difference between both of them that presents the numerical tunnelling rate.

Ground state energy $E_0^{\text{dw}} = \langle \phi_{\text{sym}} \hat{H} \phi_{\text{sym}} \rangle$	First excited state energy $E_1^{\text{dw}} = \langle \phi_{\text{antisym}} \hat{H} \phi_{\text{antisym}} \rangle$	Numerical tunnelling rate $J_{\text{dw}}^{\text{Num}} = E_1^{\text{dw}} - E_0^{\text{dw}}$
$2\pi \times 95.1 \text{ Hz}$	$2\pi \times 95.5 \text{ Hz}$	$2\pi \times 0.4 \text{ Hz}$

Table 2.1.: The numerical value of the tunnelling rate $J_{\text{dw}}^{\text{Num}}$ is calculated as the energy difference between the ground state E_0^{dw} and the first excited state E_1^{dw} energies which are evaluated numerically using Eq.(2.12) with $\tilde{\beta} = 0.5$ and $\tilde{\gamma} = 0.0204$.

2.1.4.2. Tunnelling rate calculated using local harmonic approximation

For a symmetric and quasi one-dimensional double-well potential expressed in Eq.(2.8), when the potential is strong enough compared to other energies such that the on-site wave functions are fixed, being independent of the number of atoms on each site and for a high enough ΔV we may assume these wave functions to be Gaussians with widths $\xi_{L,R}$ and are given by

$$\langle x | G_R(x) \rangle = G_R(x) = \left(\frac{1}{\xi_R^2 \pi} \right)^{\frac{1}{4}} \exp \left[-\frac{(x - x_{\min})^2}{2\xi_R^2} \right] \quad (2.15a)$$

$$\langle x | G_L(x) \rangle = G_L(x) = \left(\frac{1}{\xi_L^2 \pi} \right)^{\frac{1}{4}} \exp \left[-\frac{(x + x_{\min})^2}{2\xi_L^2} \right], \quad (2.15b)$$

where: $G_i(x)$ are the localised Gaussian wave functions that represent the ground states of each local harmonic oscillators, and $\xi_i = \sqrt{\hbar/m_{\text{Rb}}\omega_x} = \xi$ are the Gaussian widths for the left and right wells, with $i = R, L$. Both widths are equal as we study a symmetric double-well potential. $(1/\xi_i^2 \pi)^{\frac{1}{4}}$ are the normalisation constants and they are calculated based on the normalization condition

$$\int_{-\infty}^{\infty} |G_i(x)|^2 dx = 1.$$

We limit to the case where ξ is small enough with respect to the separation between both wells d so that the sites are well defined [90], this is the so-called *Gaussian*

approximation. It is important to remark that if the overlap of the localised wave functions cannot be neglected, terms involving non-diagonal interaction appear in the Hamiltonian [85]. Therefore, the tunnelling rate $J_{\text{dw}}^{\text{Gauss}}$ can be expressed by,

$$J_{\text{dw}}^{\text{Gauss}} = -\langle G_L(x) | \hat{H}(x) | G_R(x) \rangle = - \int_{-\infty}^{+\infty} dx G_L(x) \hat{H}(x) G_R(x), \quad (2.16)$$

where $\hat{H}(x)$ is the Hamiltonian which describes one atom tunnels back and forth between both the right and left Gaussian localised states and is given by:

$$\hat{H}(x) = \frac{-\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{dx^2} + V_{\text{dw}}(x).$$

A more pragmatic analytical technique to investigate the one-atom tunnelling rate between both wells when calculating the matrix element $\langle G_L(x) | \hat{H}(x) | G_R(x) \rangle$ is to approximate the double-well potential $V_{\text{dw}}(x)$ in the Hamiltonian to be referring only to the overlapping area between the left and right wells⁴,

$$\begin{aligned} \langle G_L(x) | \hat{H}(x) | G_R(x) \rangle &= \left\langle G_L(x) \left| \frac{-\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{dx^2} + V_{\text{dw}}(x) \right| G_R(x) \right\rangle \\ &\approx \left\langle G_L(x) \left| \frac{-\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{dx^2} - \beta x^2 \right| G_R(x) \right\rangle. \end{aligned} \quad (2.17)$$

Inserting the above data into Eq.(2.16), we calculate the tunnelling rate of one trapped rubidium atom in a double-well potential as

$$J_{\text{dw}}^{\text{Gauss}} = -\langle G_L(x) | \hat{H}(x) | G_R(x) \rangle = - \int_{-\infty}^{+\infty} dx G_L(x) \hat{H}(x) G_R(x).$$

Thus,

$$\begin{aligned} J_{\text{dw}}^{\text{Gauss}} &= - \left(\frac{1}{\xi_L^2 \pi} \right)^{\frac{1}{4}} \left(\frac{1}{\xi_R^2 \pi} \right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} dx \exp \left[-\frac{(x + x_{\text{min}})^2}{2\xi_L^2} \right] \left(\frac{-\hbar^2}{2m_{\text{Rb}}} \frac{d^2}{dx^2} - \beta x^2 \right) \\ &\quad \exp \left[-\frac{(x - x_{\text{min}})^2}{2\xi_R^2} \right]. \end{aligned}$$

A detailed analytical calculation for the tunnelling rate $J_{\text{dw}}^{\text{Guass}}$ can be found in Ap-

⁴This potential can be obtained by applying the harmonic approximation on the quasi one-dimensional double-well potential $V_{\text{dw}}(x)$ in the vicinity of $x_0 = 0$.

pendix D, where we have obtained that the tunnelling rate can be expressed as

$$J_{\text{dw}}^{\text{Gauss}} = -\frac{\xi^2}{\sqrt{\pi}} \exp\left[-\frac{x_{\min}^2}{\xi^2}\right] \left\{ \frac{-\hbar^2}{2m_{\text{Rb}}} \frac{1}{\xi^4} N1 - \beta N2 \right\}, \quad (2.18)$$

where:

$$N1 = -\frac{\sqrt{\pi}}{2} + \frac{x_{\min}}{\xi} \left[\frac{x_{\min}}{\xi} \sqrt{\pi} - 2 \right] \quad N2 = \frac{\sqrt{\pi}}{2},$$

are dimensionless values. Important and essential relations can be concluded from Eq.(2.18) that the tunnelling rate:

1. is proportional to the square of the Gaussian width $J_{\text{dw}}^{\text{Gauss}} \propto \xi^2$, meaning that the tunnelling rate gets stronger as the Gaussian width gets larger.
2. is inversely proportional to the mass of the atom as $J_{\text{dw}}^{\text{Gauss}} \propto 1/m_{\text{Rb}}$.
3. decreases with increasing separation between the minima (wells) as $d = 2|x_{\min}|$ and $J_{\text{dw}}^{\text{Gauss}} \propto e^{-x_{\min}^2}$.
4. decreases with increasing the barrier height as $\Delta V = \beta^2/4\gamma$.

Table(2.2) reveals the analytical tunnelling rate value computed from Eq.(2.18) for one rubidium atom with mass m_{Rb} and after taking certain strengths for the double-well potential variables β and γ .

$m_{\text{Rb}} = 1.443 \times 10^{-25} \text{ Kg}$ $\beta = 5.69 \times 10^{-20} \hbar \text{ Hz } m^{-2}$ $\gamma = 4 \times 10^{-9} \hbar \text{ Hz } m^{-4}$	$J_{\text{dw}}^{\text{Gauss}} = 2\pi \times 0.00753 \text{ Hz}$
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Table 2.2.: The analytical value of the tunnelling rate $J_{\text{dw}}^{\text{Gauss}}$ which is calculated under the Gaussian approximation from Eq.(2.18), where the Gaussian width for either the left or the right orbital is taken to be $\xi = \sqrt{\hbar/m_{\text{Rb}}\omega_x} = \sqrt{\hbar/\sqrt{4m_{\text{Rb}}\beta}}$ and the double-well minimum $x_{\min} = \sqrt{\beta/2\gamma}$.

2.1.4.3. Comparison of the numerical and analytical approaches

It is interesting to compare between the numerical tunnelling rate $J_{\text{dw}}^{\text{Num}}$ expressed in Eq.(2.14) which is defined as the energy difference between the ground state and first excited state energies that can be gained from the numerically discretised

Schrödinger equation in Eq.(2.12), and the analytical tunnelling rate $J_{\text{dw}}^{\text{Gauss}}$ calculated from Eq.(2.18) obtaining from the Gaussian approximation for the left and right wave functions of the double-well potential which are formulated in Eq.(2.15). It is obviously noticeable that the numerical tunnelling rate $J_{\text{dw}}^{\text{Num}}$ is relatively larger than the one obtained from the Gaussian approximation $J_{\text{dw}}^{\text{Gauss}}$. This can be more explained by plotting numerically the left and right orbitals from Eq.(2.13), i.e., $|\phi_{\text{Left}}\rangle$ and $|\phi_{\text{Right}}\rangle$, and analytically using Eq.(2.15), i.e., $|G_L(x)\rangle$ and $|G_R(x)\rangle$ as illustrated in Fig.(2.7). It can be observed that the overlapping area between the left and right Gaussians in the solid blue and red lines, respectively, is nearly vanishing leading to a very small tunnelling rate. However, both numerical orbitals in the dashed blue and red lines show a non-vanishing overlapping area which refers to a relatively larger numerical tunnelling rate comparing to the corresponding analytical value. It is worth noting that this discrepancy between both values can be minimised by increasing the height of the double-well's potential barrier ΔV which leads to an increasingly weakly linked BECs and hence reduced tunnelling rates.

2.1.5. Mean-field description of two BECs in a double-well potential

A system of interacting bosons confined within an external potential at zero temperature can be described by a macroscopic wave function as the atoms occupy the same quantum mechanical wave function. Mean-field approaches are commonly developed for interacting systems in order to overcome the problem of solving exactly the full many-body Schrodinger equation. Apart from the convenience of avoiding heavy numerical work, mean-field theories allow one to understand the behaviour of a system in terms of a set of parameters having a clear physical meaning. Actually most of the results reviewed in this chapter show that the mean-field approach is very effective in providing quantitative predictions for the dynamical properties of these trapped gases [24]. The relevant model is a non-linear evolution equation, the so-called Gross-Pitaevskii equation (GPE) which is a universal model describing the evolution of systems in non-linear media. In the case of BECs, the non-linearity in the GP equation is introduced by the interatomic interactions, accounted for through an effective mean-field [28]. On the other hand, a theme that has also been progres-

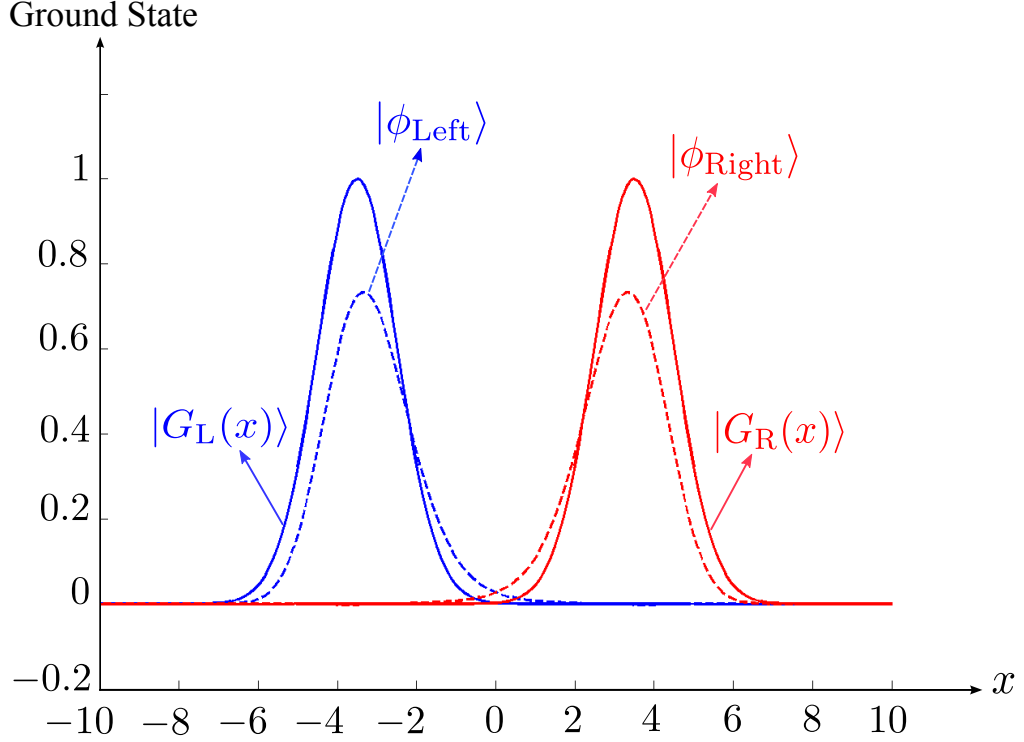


Figure 2.7.: The left and the right modes of the double-well potential as a function of the spatial variable x calculated: analytically under the Gaussian approximation, where the solid red and blue lines represent the Gaussian right $|G_R(x)\rangle$ and the Gaussian left $|G_L(x)\rangle$ orbitals, respectively. However, the dashed red and blue lines represent the numerical right $|\phi_{\text{Right}}\rangle$ and left $|\phi_{\text{Left}}\rangle$ wave functions which are obtained as a linear superposition as explained in Eq.(2.13).

sively becoming of increasing importance is the effects of the long-range interactions [91] which will be considered as an additional non-linearity in our systems.

In this subsection we use the mean-field theory to study the atomic tunnelling of N_T^{dw} interacting bosonic Rydberg-dressed rubidium atoms at zero temperature between two BECs in a quasi-one dimensional double-well potential trap. This induces a coherent, oscillating flux of atoms between wells, that is a signature of the macroscopic superposition of states in which the condensates evolve [72]. Sparked by the prospect that this unique model in many-body quantum physics could become experimentally accessible there has recently been a wave of theoretical interest in trapped one-dimensional gases [92].

Consider N_T^{dw} interacting bosonic Rydberg-dressed rubidium atoms confined in a symmetric quasi one-dimensional double-well potential trap at zero temperature

formulating two trapped Bose-Einstein condensates. This system can be described by a macroscopic wave function $\psi(x, t)$ having the meaning of an order parameter, normalised to the total number of atoms and satisfies the Gross-Pitaevskii equation

$$i\hbar \frac{d\psi(x, t)}{dt} = -\frac{\hbar^2}{2m_{\text{Rb}}} \nabla^2 \psi(x, t) + \left[V_{\text{dw}}(x) + \int_{-\infty}^{+\infty} dx' \psi^\dagger(x', t) V_{\text{int}}(x, x') \psi(x', t) \right] \psi(x, t), \quad (2.19)$$

where $V_{\text{dw}}(x)$ and $V_{\text{int}}(x, x')$ are the double-well potential and the overall interaction between atoms in trap, respectively. In our study, this interaction has two parts, the s-wave contact-interaction (or interatomic scattering pseudopotential) $V_{\text{SW}}(x, x')$ which is a short-range interaction, and the soft-core interaction $V_{\text{SC}}(x, x')$ which has a long-ranged behaviour. Thus, the total interaction is expressed as following

$$V_{\text{int}}(x, x') = V_{\text{SW}}(x, x') + V_{\text{SC}}(x, x') = g_{1\text{D}} \delta(x, x') + \frac{\zeta R_C^6}{|x - x'|^6 + R_C^6}, \quad (2.20)$$

with $\delta(x, x')$ being the Delta-function. The effective and the modified one-dimensional coupling constant becomes $g_{1\text{D}} = \frac{2\hbar^2 a}{m_{\text{Rb}} \xi_\perp^2} \left(1 - \frac{|\zeta(1/2)|a}{\sqrt{2}\xi_\perp} \right)^{-1}$ where a is the s -wave scattering length, and $\xi_\perp = (\hbar/m_{\text{Rb}}\omega_\perp)^{1/2}$ denotes the transverse confinement length (in the plane yz) in terms of the frequency of the transverse harmonic confinement, $\omega_\perp$. Here $\zeta(1/2)$ is the Riemann zeta function [93]. Inserting the total interaction into Eq.(2.19) gives the one-dimensional time-dependant GP-equation

$$i\hbar \frac{d\psi(x, t)}{dt} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, t) + \left[V_{\text{dw}}(x) + g_{1\text{D}} |\psi(x, t)|^2 + \int_{-\infty}^{+\infty} dx' |\psi(x', t)|^2 V_{\text{SC}}(x, x') \right] \psi(x, t). \quad (2.21)$$

Being interested in the dynamical properties of the weakly linked BECs within the two-mode representation, as was discussed in subsection (2.1.4), the wave function of the condensate $\psi(x, t)$, which is normalised to the total number of atoms ,i.e., $N_{L,R} = |\psi_{L,R}(t)|^2$, is defined as

$$\begin{aligned}
\psi(x, t) &= \sum_{i=L,R} \psi_i(t) \phi_i(x) \\
&= \psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x),
\end{aligned} \tag{2.22}$$

where, $\psi_L(t), \psi_R(t)$ are the complex time-dependent amplitudes and $\phi_L(x), \phi_R(x)$ are the localised wave functions for the left and right well, respectively. Inserting the new approximated wave function in Eq.(2.21) we obtain

$$\begin{aligned}
i\hbar \frac{d}{dt} [\psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x)] &= -\frac{\hbar^2}{2m_{\text{Rb}}} \nabla^2 [\psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x)] \\
&+ [V_{\text{dw}}(x) + g |[\psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x)]|^2 \\
&+ \int_{-\infty}^{+\infty} dx' |[\psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x)]|^2 V_{\text{SC}}(x, x')] [\psi_L(t) \phi_L(x) + \psi_R(t) \phi_R(x)].
\end{aligned} \tag{2.23}$$

2.1.5.1. Differential equations of the time-dependent amplitudes

To get the equations of motion for both condensates, i.e. the differential equations of the time-dependent amplitudes $\psi_L(t), \psi_R(t)$, we project Eq.(2.23) onto the single well states $\phi_L(x)$ and $\phi_R(x)$ by multiplying from the left with $\phi_L^*(x)$ and $\phi_R^*(x)$ and integrate over the space x , bearing in mind that the normalisation and orthogonal conditions have to be fulfilled⁵

$$\int_{-\infty}^{+\infty} dx \phi_{L,R}^*(x) \phi_{L,R}(x) \approx 1 \quad \int_{-\infty}^{+\infty} dx \phi_{L,R}^*(x) \phi_{R,L}(x) \approx 0.$$

As a result, we write the differential equations of the time-dependent amplitudes for the left and right wells as

⁵Since the wells are deep enough, this makes $\phi_{L,R}(x)$ very greatly localised and we can safely impose the condition that the overlap between the localised probability amplitudes can be neglected, i.e., $\int_{-\infty}^{+\infty} dx \phi_i(x) \phi_j(x) \approx \delta_{ij}$ where $i, j = L, R$ and it is a very reasonable approximation.

$$i\hbar \frac{d\psi_L(t)}{dt} = \left[E_L^0 + U_L N_L + \eta_{L1} N_L + (\eta_{L3} + \eta_{L6}) N_R \right] \psi_L(t) - \left[J + (\eta_{L2} + \eta_{L5}) N_L + \eta_{L4} N_R \right] \psi_R(t) \quad (2.24a)$$

$$i\hbar \frac{d\psi_R(t)}{dt} = \left[E_R^0 + U_R N_R + \eta_{R1} N_R + (\eta_{R3} + \eta_{R6}) N_L \right] \psi_R(t) - \left[J + (\eta_{R2} + \eta_{R5}) N_R + \eta_{R4} N_L \right] \psi_L(t), \quad (2.24b)$$

where we have denoted⁶,

$$E_{L,R}^0 = \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2}{2m_{\text{Rb}}} |\nabla \phi_{L,R}(x)|^2 + V_{\text{dw}}(x) |\phi_{L,R}(x)|^2 \right]$$

$$J = - \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2}{2m_{\text{Rb}}} \nabla \phi_L(x) \nabla \phi_R(x) + V_{\text{dw}}(x) \phi_L(x) \phi_R(x) \right]$$

$$U_{L,R} = g_{1\text{D}} \int_{-\infty}^{+\infty} dx |\phi_{L,R}(x)|^4,$$

as $E_{L,R}^0$ is the zero point energy, J is the interwell coupling constant (tunnelling amplitude) which describes the dynamics of the tunnelling between both condensates and $U_{L,R}$ is the atomic and non-linear self-interaction energy in the left, right wells, respectively. It is worth noting that the first two terms, i.e., $E_{L,R}^0$ and J , describe a single-atom dynamics within the trap. However, $U_{L,R}$ relates to atom-atom short-range interaction. The total number of atoms in the double-well trap is conserved $N_T^{\text{dw}} = N_L + N_R = \text{constant}$, with $N_{L,R} = |\psi_{L,R}(t)|^2$.

Additional matrix elements emerge as a consequence of including the long-range interaction, which will play a fundamental role in our discussion below where they are interpreted as follows:

⁶Using the Laplacian property $-\int f(r) \nabla^2 u(r) dr = \int \nabla f(r) \nabla u(r) dr$.

$$\eta_{L1,R1} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R}(x')|^2 |\phi_{L,R}(x)|^2 \quad (2.25a)$$

$$\eta_{L2,R2} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R}(x')|^2 \phi_{L,R}^*(x) \phi_{R,L}(x) \quad (2.25b)$$

$$\eta_{L3,R3} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{R,L}(x')|^2 |\phi_{L,R}(x)|^2 \quad (2.25c)$$

$$\eta_{L4,R4} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{R,L}(x')|^2 \phi_{L,R}^*(x) \phi_{R,L}(x) \quad (2.25d)$$

$$\eta_{L5,R5} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R}(x)|^2 \phi_{L,R}(x') \phi_{R,L}(x') \quad (2.25e)$$

$$\eta_{L6,R6} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R}(x') \phi_{R,L}(x') \phi_{L,R}^*(x) \phi_{R,L}(x). \quad (2.25f)$$

Due to the symmetry of the soft-core interaction $V_{\text{SC}}(x, x')$, the previous overlapping integrals hold even if the subscripts L and R are swapped, or the spatial variables x and x' are interchanged. Additionally, it can be noticed that $\eta_{L2,R2} = \eta_{L4,R4} = \eta_{L5,R5}$. Fig.(2.8) shows how the overlap integrals $\eta_{Li,Ri}/\zeta$, with $i = 1, 2, \dots, 6$, change as a function of the soft-core interaction radius R_{SC} . In the near-local interaction regime, i.e., for small R_{SC} , the integral $\eta_{L1,R1}/\zeta$ in the solid blue line is the dominant term. However, in the non-local interaction regime, i.e, for large R_{SC} , the integral $\eta_{L3,R3}/\zeta$ in the dotted-dashed red line becomes comparable to $\eta_{L1,R1}/\zeta$ and both of them are on the same order of magnitude. The rest of the integrals $\eta_{L2,R2}/\zeta$, $\eta_{L4,R4}/\zeta$, $\eta_{L5,R5}/\zeta$ and $\eta_{L6,R6}/\zeta$ remain negligible for any value of R_{SC} . Therefore, we keep hold of only both $\eta_{L1,R1}/\zeta$ and $\eta_{L3,R3}/\zeta$ for the case of large R_{SC} leading to the simplified time-dependent amplitudes differential equations:

$$\begin{aligned} i\hbar \frac{d\psi_L(t)}{dt} &= \left[E_L^0 + U_L N_L + \eta_{L1} N_L + \eta_{L3} N_R \right] \psi_L(t) - J \psi_R(t) \\ i\hbar \frac{d\psi_R(t)}{dt} &= \left[E_R^0 + U_R N_R + \eta_{R1} N_R + \eta_{R3} N_L \right] \psi_R(t) - J \psi_L(t). \end{aligned}$$

We can re-organise these equations even more by inserting the fact that the overall atom population in the double-well trap is conserved and satisfies $N_T^{\text{dw}} = N_L + N_R$, then:

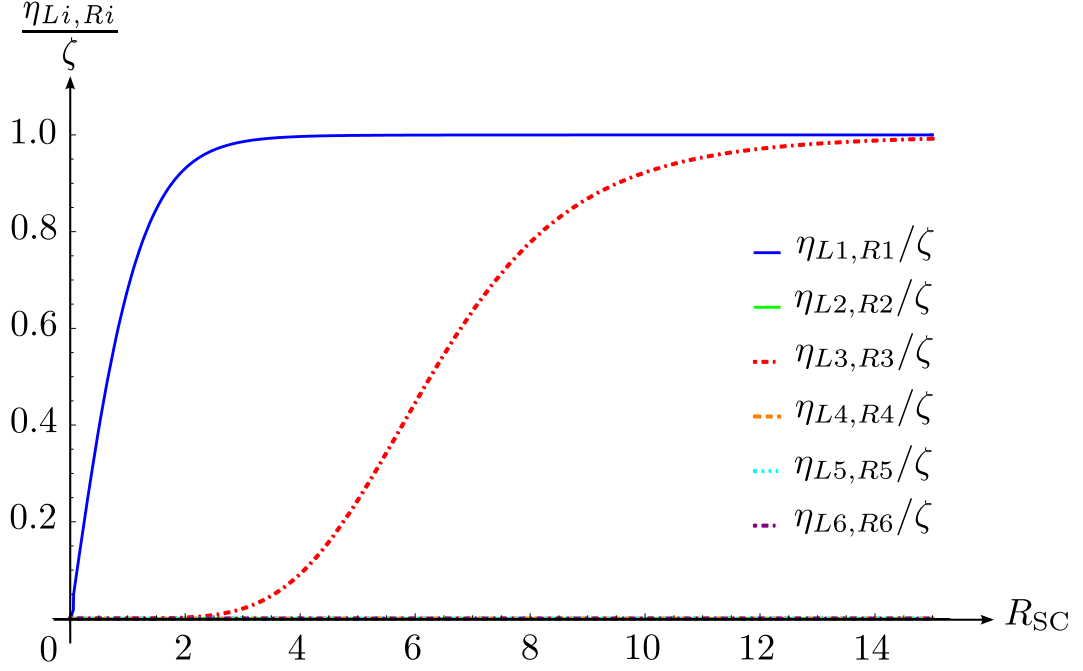


Figure 2.8.: The matrix elements $\eta_{Li,Ri}/\zeta$ where $i = 1, 2, \dots, 6$ are shown as a function of the soft-core interaction radius R_{SC} , where the dimensionless double-well minimum is $\min = \sqrt{\frac{\tilde{\beta}}{2\tilde{\gamma}}}$ with $\tilde{\beta} = 0.5$ and $\tilde{\gamma} = 0.025$. The Gaussian width for either the left or the right orbital is taken to be $\sigma \approx 1$.

$$i\hbar \frac{d\psi_L(t)}{dt} = \left[\mathcal{E}_L^0 + U_L N_L + (\eta_{L1} - \eta_{L3}) N_L \right] \psi_L(t) - J\psi_R(t) \quad (2.26a)$$

$$i\hbar \frac{d\psi_R(t)}{dt} = \left[\mathcal{E}_R^0 + U_R N_R + (\eta_{R1} - \eta_{R3}) N_R \right] \psi_R(t) - J\psi_L(t), \quad (2.26b)$$

where: $\mathcal{E}_L^0 = E_L^0 + \eta_{L3} N_T^{\text{dw}}$, $\mathcal{E}_R^0 = E_R^0 + \eta_{R3} N_T^{\text{dw}}$.

It is worth mentioning that Eq.(2.25a) represents the “local long-range interaction” which appears between atoms inside the same well (either left or right). However, Eq.(2.25c) represents the “non-local long-range interaction” appearing between atoms via both wells.

2.1.5.2. Tunnelling dynamics

In the following, we will analyse the tunnelling dynamics in terms of two time-dependent variables; the fractional population imbalance $Z(t)$ and the relative phase $\Phi(t)$ between the left and right wells, given by

$$Z(t) = \frac{N_L(t) - N_R(t)}{N_L(t) + N_R(t)} = \frac{N_L(t) - N_R(t)}{N_T^{\text{dw}}(t)} \quad Z(t) \in [-1, +1] \quad (2.27)$$

$$\Phi(t) = \theta_R(t) - \theta_L(t) \quad \Phi(t) \in [0, 2\pi], \quad (2.28)$$

where $N_{L(R)}(t)$ corresponds to the number of atoms on the left (right) well, and $\theta_{L(R)}(t)$ is the phase of the condensate on the left (right) well.

Since $\psi_{L(R)}(t)$ represents the time-amplitude of the left (right) condensate in the double-well potential that has the meaning of an order parameter, then using “Madelung representation” allows us to write:

$$\psi_{L(R)}(t) = \sqrt{N_{L(R)}} e^{i\theta_{L(R)}}. \quad (2.29)$$

To obtain the fractional population imbalance differential equation which can be done initially by obtaining the differential equations of the atom numbers in the left and right wells. To begin with the differential equation of the left atom number, we substitute the previous expression Eq.(2.29) into Eq.(2.26a) where we get after multiplying it by $\sqrt{N_L}$ the following

$$\frac{i\hbar}{2} e^{i\theta_L} \frac{dN_L}{dt} - \hbar N_L e^{i\theta_L} \frac{d\theta_L}{dt} = \left[\mathcal{E}_L^0 + U_L N_L + (\eta_{L1} - \eta_{L3}) N_L \right] N_L e^{i\theta_L} - J \sqrt{N_L N_R} e^{i\theta_R},$$

separating both the imaginary and the real parts via Euler’s formula $e^{i\theta} = \cos \theta + i \sin \theta$, gives us,

The imaginary part:

$$\begin{aligned} \frac{\hbar}{2} \frac{dN_L}{dt} \cos \theta_L - \hbar N_L \frac{d\theta_L}{dt} \sin \theta_L = & \left[\mathcal{E}_L^0 + U_L N_L + (\eta_{L1} - \eta_{L3}) N_L \right] N_L \sin \theta_L \\ & - J \sqrt{N_L N_R} \sin \theta_R, \end{aligned} \quad (2.30)$$

and the real part:

$$\begin{aligned} -\frac{\hbar}{2} \frac{dN_L}{dt} \sin \theta_L - \hbar N_L \frac{d\theta_L}{dt} \cos \theta_L = & \left[\mathcal{E}_L^0 + U_L N_L + (\eta_{L1} - \eta_{L3}) N_L \right] N_L \cos \theta_L \\ & - J \sqrt{N_L N_R} \cos \theta_R. \end{aligned} \quad (2.31)$$

multiplying Eq.(2.30) by $\cos \theta_L$ and Eq.(2.31) by $-\sin \theta_L$ and adding them to each other yields to,

$$\frac{dN_L}{dt} = -\frac{2J}{\hbar} \sqrt{N_L N_R} \sin \Phi. \quad (2.32)$$

Analogous calculations for the right time-dependent amplitude in Eq.(2.26b) results

$$\frac{dN_R}{dt} = \frac{2J}{\hbar} \sqrt{N_L N_R} \sin \Phi. \quad (2.33)$$

Comparing both equations (2.32) and (2.33) one can notice that

$$\frac{dN_L}{dt} = -\frac{dN_R}{dt}. \quad (2.34)$$

Therefore, using equations (2.32),(2.33) and (2.34), and by introducing a re-scaled dimensionless time $t \rightarrow \frac{2J}{\hbar} t$, the differential equation of the fractional population imbalance is

$$\frac{dZ(t)}{dt} = -\sqrt{1 - Z(t)^2} \sin \Phi. \quad (2.35)$$

It can be observed that the fractional population imbalance expression stays exactly the same whether the system consists of interacting or non-interacting atoms within the double-well potential trap.

Regarding the differential equations of the left and right phases, we multiply this time (for the left phase) the imaginary part in Eq.(2.30) by $\sin \theta_L$ and the real part

in Eq.(2.31) by $\cos \theta_L$ where adding them to each other gives us

$$\frac{d\theta_L}{dt} = -\frac{\mathcal{E}_L^0 + U_L N_L + (\eta_{L1} - \eta_{L3}) N_L}{\hbar} + \frac{J}{\hbar} \sqrt{\frac{N_R}{N_L}} \cos \Phi. \quad (2.36)$$

Similarly for the right time-dependent amplitude we find the differential equation of the right phase:

$$\frac{d\theta_R}{dt} = -\frac{\mathcal{E}_R^0 + U_R N_R + (\eta_{R1} - \eta_{R3}) N_R}{\hbar} + \frac{J}{\hbar} \sqrt{\frac{N_L}{N_R}} \cos \Phi. \quad (2.37)$$

Usually not the phase of the condensate but the relative phase between two overlapping condensates is measured. Therefore, as the relative phase is given by Eq.(2.28), we subtract Eq.(2.36) from Eq.(2.37) and we have

$$\begin{aligned} \frac{d\Phi(t)}{dt} &= \frac{\mathcal{E}_L^0 - \mathcal{E}_R^0}{2J} + \frac{(U_L - U_R)(N_L + N_R)}{4J} + \frac{(U_L + U_R)(N_L + N_R)}{4J} \frac{(N_L - N_R)}{(N_L + N_R)} \\ &+ \frac{\left[(\eta_{L1} + \eta_{R1}) - (\eta_{L3} + \eta_{R3}) \right] (N_L + N_R)}{4J} \frac{(N_L - N_R)}{(N_L + N_R)} \\ &+ \frac{\left[(\eta_{L1} - \eta_{R1}) - (\eta_{L3} - \eta_{R3}) \right] (N_L + N_R)}{4J} + \frac{(N_L - N_R)}{(N_L + N_R) \sqrt{\frac{4N_L N_R}{(N_L + N_R)^2}}} \cos \Phi. \end{aligned}$$

Introducing the following parameters:

$$\begin{aligned} \Delta \mathcal{E} &= \frac{\mathcal{E}_L^0 - \mathcal{E}_R^0}{2J} + \frac{(U_L - U_R)(N_L + N_R)}{4J} + \frac{\left[(\eta_{L1} - \eta_{R1}) - (\eta_{L3} - \eta_{R3}) \right] (N_L + N_R)}{4v} \\ \Lambda &= \frac{(U_L + U_R)(N_L + N_R)}{4J} \\ \Xi &= \frac{\left[(\eta_{L1} + \eta_{R1}) - (\eta_{L3} + \eta_{R3}) \right] (N_L + N_R)}{4J}, \end{aligned}$$

where, $\Delta \mathcal{E}$ is the trap asymmetry, Λ is the short-range interaction and Ξ is the long-range interaction. Therefore, the differential equation of the relative phase can be finally expressed by

$$\frac{d\Phi(t)}{dt} = \Delta\mathcal{E} + (\Lambda + \Xi)Z(t) + \frac{Z(t)}{\sqrt{1 - Z(t)^2}} \cos \Phi. \quad (2.38)$$

As a result, including the long-range interaction between atoms inside the double-well potential, the dynamics of N_T^{dw} interacting bosonic atoms are mainly described by the dynamical equations or the so-called *non-linear Josephson equations* Eq.(2.35) and Eq.(2.38). It is important to notice from Eq.(2.38) that both; short- Λ and long- Ξ range interactions contribute similarly to the atom's dynamics. Therefore, despite the presence of the long-range interaction term, Ξ , new physics does not occur, as it will be shown in subsection (2.1.6).

2.1.5.3. Symmetric double-well potential trap

For a symmetric double-well trap we have:

$$\left. \begin{aligned} \mathcal{E}_L^0 &= \mathcal{E}_R^0 \\ U_L &= U_R = U \\ \eta_{L1} &= \eta_{R1} = \eta_1 \\ \eta_{L3} &= \eta_{R3} = \eta_3 \end{aligned} \right\} \Longrightarrow \begin{aligned} \Delta\mathcal{E} &= 0 \\ \Lambda &= \frac{U}{2J} N_T^{\text{dw}} \\ \Xi &= \frac{(\eta_1 - \eta_3)}{2J} N_T^{\text{dw}} \end{aligned}.$$

Then we rewrite the differential equations in Eq.(2.35) and Eq.(2.38) as

$$\frac{dZ(t)}{dt} = \dot{Z}(t) = -\sqrt{1 - Z(t)^2} \sin \Phi \quad (2.39a)$$

$$\frac{d\Phi(t)}{dt} = \dot{\Phi}(t) = (\Lambda + \Xi) Z(t) + \frac{Z(t)}{\sqrt{1 - Z(t)^2}} \cos \Phi. \quad (2.39b)$$

These are two coupled first order differential equations that can be solved numerically. These equations can be cast into the canonical form [91]

$$\left\{ \begin{aligned} \dot{Z}(t) &= -\frac{\partial \hat{H}_{\text{symmetric}}}{\partial \Phi(t)} \\ \dot{\Phi}(t) &= \frac{\partial \hat{H}_{\text{symmetric}}}{\partial Z(t)} \end{aligned} \right\},$$

where both $Z(t)$ and $\Phi(t)$ are canonically conjugate variables as the Hamiltonian reads as

$$\hat{H}_{\text{symmetric}} = \frac{(\Lambda + \Xi)}{2} Z^2 - \sqrt{1 - Z^2} \cos \Phi. \quad (2.40)$$

In a simple mechanical analogy, $\hat{H}_{\text{symmetric}}$ describes a nonrigid pendulum, of tilt angle Φ and length proportional to $\sqrt{1 - Z^2}$, that decreases with the angular momentum Z [72].

2.1.6. Dynamical regimes

Josephson junctions depend strongly on the initial conditions which are defined by the population imbalance and relative phase at time $t = 0$, respectively $Z(0)$ and $\Phi(0)$. For the initial conditions $Z(0) = 0$ and $\Phi(0) = 2\pi j$ where $j \in \mathbb{N}$, the equations of motion vanish and the system is in the symmetric ground state at rest. In the case of $Z(0) = 0$ and $\Phi(0) = \pi(1 + 2j)$ with $j \in \mathbb{N}$, the system is at rest as well, but this state correspond to an anti-symmetric metastable state only. If one of the two variables is prepared to a different initial value, a particle flow will start through the barrier and compensate for imbalance. In our work here, we consider the case of a non-zero initial population imbalance and a zero initial phase, that is $Z(0) \neq 0$ and $\Phi(0) = 0$.

According to different values of the interaction and initial conditions for both the fractional population imbalance and relative phase, we consider three different types of regimes inside the double-well potential; Rabi, Josephson and Fock regimes.

2.1.6.1. Non-interacting limit (Rabi regime)

Rabi regime corresponds to the non-interacting limit where the system consists of N_T^{dw} non-interacting atoms. The coherence here is very high allowing for the definition of a relative phase between the matter-wave packets within the two wells [94].

For a symmetric well $\Delta\mathcal{E} = 0$, and negligible interactions $\Lambda \rightarrow 0$, $\Xi \rightarrow 0$, it is interesting to look back again at the time-dependant amplitudes expressed in Eqs.(2.26) where in the non-interacting limit are written as

$$i\hbar \frac{d\psi_L(t)}{dt} = -J\psi_R(t) \quad (2.41a)$$

$$i\hbar \frac{d\psi_R(t)}{dt} = -J\psi_L(t). \quad (2.41b)$$

Comparing with the Rabi oscillation equations in a two-level atom system coupled to a laser field in case of a zero detuning $\Delta = 0$ which are given by

$$i\hbar \frac{dA(t)}{dt} = \hbar \frac{\Omega}{2} B(t) \quad i\hbar \frac{dB(t)}{dt} = \hbar \frac{\Omega}{2} A(t),$$

where $A(t)$ and $B(t)$ are the complex time-dependant amplitudes for the ground and first excited states of the two-level atom, respectively, and Ω is the Rabi frequency. It can be concluded that in the absence of interactions, the time-dependent amplitude equations Eqs.(2.41) describe sinusoidal Rabi-like oscillations between the two wells with a frequency equals to $\omega_{\text{Ra}}^{\text{dw}} = 2J/\hbar$. These oscillations are equivalent to a single-atom dynamics (uncorrelated tunnelling [95]) rather than a Josephson effect arising from the interacting superfluid condensate [96]. Fig(2.9) illustrates the numerical solutions for both dynamical equations Eq.(2.39) where it shows Rabi-like oscillations between both wells where the fractional population imbalance $Z(t)$ and the relative phase $\Phi(t)$ are plotted as a function of the dimensionless time t .

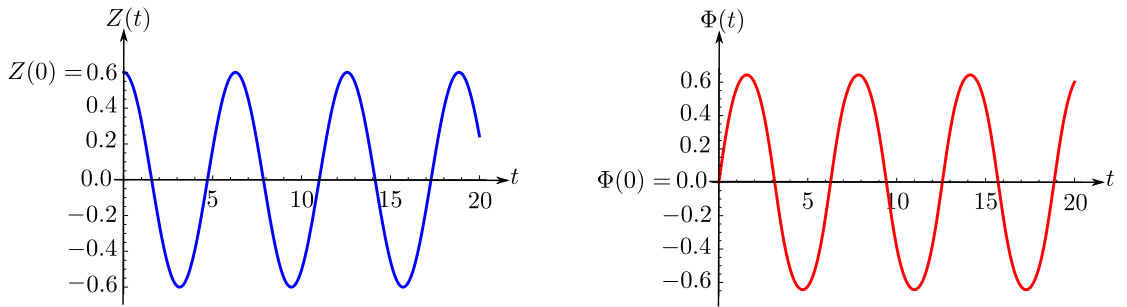


Figure 2.9.: Fractional population imbalance $Z(t)$ (left) and the relative phase $\Phi(t)$ (right) versus re-scaled time in the non-interacting regime (Rabi regime), with initial conditions for the fractional population imbalance $Z(0) = 0.6$ and for the relative phase $\Phi(0) = 0$.

2.1.6.2. Linear-interacting limit (Josephson regime)

The linear-interacting limit or as it refers to “Josephson oscillation regime”, occurs when we restrict to small values for relative phases $|\Phi(t)| \ll 1$ and small population imbalances $|Z(t)| \ll 1$. In the Josephson regime the fluctuation of the atom numbers are reduced but the coherence is high. Thus, also in this regime a relative phase can be defined, which has only a small quantum mechanical uncertainty [94]. To investigate the dynamics of the N_T^{dw} interacting atoms in the Josephson regime we need to linearise the non-linear differential equations in Eqs.(2.39) around an equilibrium point, i.e., $(Z(0), \Phi(0)) = (0, 0)$. In order to linearise our non-linear system, we will use the Taylor Series expansion by applying

$$\begin{aligned} \frac{dZ(t)}{dt} = f(Z(t), \Phi(t)) &\approx f(Z(0), \Phi(0)) + \frac{\partial f(Z(0), \Phi(0))}{\partial Z(t)}(Z - Z(0)) \\ &+ \frac{\partial f(Z(0), \Phi(0))}{\partial \Phi(t)}(\Phi - \Phi(0)), \end{aligned}$$

$$\begin{aligned} \frac{d\Phi(t)}{dt} = g(Z(t), \Phi(t)) &\approx g(Z(0), \Phi(0)) + \frac{\partial g(Z(0), \Phi(0))}{\partial Z(t)}(Z - Z(0)) \\ &+ \frac{\partial g(Z(0), \Phi(0))}{\partial \Phi(t)}(\Phi - \Phi(0)), \end{aligned}$$

which yields to the following linearised dynamical equations

$$\frac{dZ(t)}{dt} = \dot{Z}(t) = -\Phi(t) \quad (2.42a)$$

$$\frac{d\Phi(t)}{dt} = \dot{\Phi}(t) = (\Lambda + \Xi + 1) Z(t). \quad (2.42b)$$

The Josephson frequency $\omega_{\text{Jo}}^{\text{dw}}$, or the linear frequency, is determined by comparing these two linearised equations with the harmonic oscillator equations of motion⁷,

⁷The harmonic oscillator equation of motion is $\ddot{x} = -\omega_{\text{ho}}^2 x$ where $\omega_{\text{ho}} = \sqrt{k/m}$ is the harmonic oscillator frequency with k and m being a positive constant and the atom mass respectively. Changing the variable based on $y = \dot{x}$, would make the comparison easier to conclude the frequency of the linear regime where $\dot{y} = \ddot{x} = -\omega^2 x$.

then we find that the linear frequency is given by

$$\omega_{Jo}^{dw} = \sqrt{\Lambda + \Xi + 1} = \sqrt{2N_T^{dw}J(U + \eta_1 - \eta_3) + 4J^2}. \quad (2.43)$$

The Josephson oscillations are shown in Fig.(2.10) for different long-range interaction values and a fixed short-range interaction after solving numerically the differential equations Eqs.(2.42). It can be clearly observed that the oscillations of both $Z(t)$ and $\Phi(t)$ with a frequency ω_{Jo}^{dw} get faster as the long-range interaction gets stronger. Additionally, the oscillations of the relative phase $\Phi(t)$ not only get faster when increasing the long-range interaction strength, but also their amplitudes increase consequently.

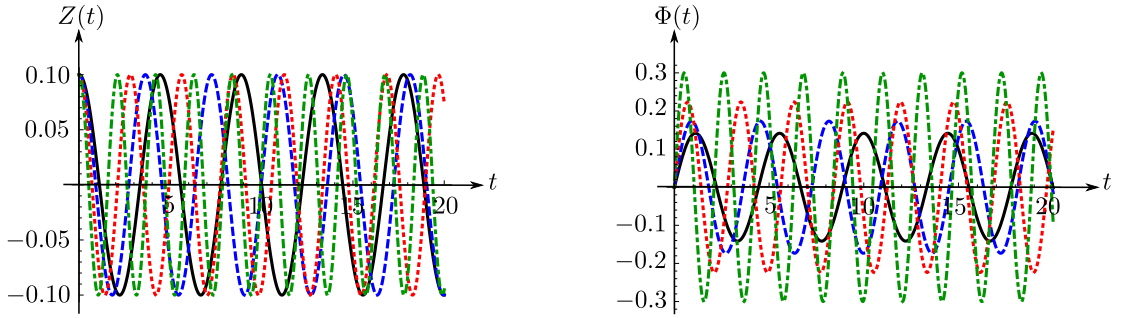


Figure 2.10.: Fractional population imbalance $Z(t)$ (left) and the relative phase $\Phi(t)$ (right) versus re-scaled time in the linear-interacting regime (Josephson regime) for different long-range interaction values Ξ and a fixed local interaction $\Lambda = 1$, with initial conditions for the fractional population imbalance $Z(0) = 0.1$ and for the relative phase $\Phi(0) = 0$, with the solid black line for $\Xi = 0$, the dashed blue line is for $\Xi = 1$, the dotted red line is for $\Xi = 3$ and the dotted-dashed green line is for $\Xi = 7$.

2.1.6.3. Non-linear interacting limit (Fock regime)

In the non-linear regime, or the Fock regime, the Josephson junction is dominated by the interaction energy, therefore the eigenstates have a well-defined atom number in each well and as the coherence vanishes, the phase is completely undefined. In this regime the ground state cannot be described by a single condensate, but corresponds to a fragmented state, where the single-particle density matrix has two macroscopic

eigenvalues⁸ [94]. A numerical solution of the dynamical equations Eqs.(2.39) yields to the most spectacular phenomenon in the non-linear regime when the interaction energy is greater than the coupling. The transfer of particles from one site to the other gives rise to a dynamical renormalisation of the energy in each site, resulting in non-sinusoidal oscillations, that are the anharmonic generalisation of the sinusoidal Josephson effects. If the interactions are strong enough, i.e., above a specific critical value, the self-induced energy renormalisation quenches the tunnelling, and most of the particles remain localised in one of the sites showing a highly asymmetric distribution. This out of equilibrium metastable regime is called *macroscopic quantum self-trapping* (MQST) [97] and has been observed in the lab recently [74]. Therefore, the self-trapping of an initial BEC population imbalance arises because of the inter-atomic interaction in the Bose gas (non-linear self-interaction in GPE). Hence, the self-trapping occurrence corresponds to dynamical modes, for which the population imbalance shows only small oscillations around a non-zero value and the atoms are trapped in one well where the phase winds up as its harmonic oscillations disappear and changes linearly with time.

There are different ways in which MQST state can be achieved, and all of them correspond to the condition (which we shall term the macroscopic quantum self-trapping condition):

$$H_0 = H[Z(0), \Phi(0)] = \frac{(\Lambda + \Xi)}{2} Z(0)^2 - \sqrt{1 - Z(0)^2} \cos \Phi(0) > 1. \quad (2.44)$$

Moreover, for a fixed short-range interaction Λ and under certain initial conditions $Z(0)$, $\Phi(0)$, MQST phenomenon depends on a critical long-range interaction value $\Xi_c = \Xi_c(Z(0), \Phi(0))$, and it can be explained as follows. The system's critical transition from Josephson oscillation to self-trapping happens if the interaction strength exceeds a critical value which can be easily found from the energy conservation constraint and the boundness of the tunnelling energy in Eq.(2.40) and Eq.(2.44) [72] which leads to

⁸The diagonal elements of the density matrix which correspond to the probabilities are defined and non-zero values, whereas the coherences which correspond to the off-diagonal ones are vanished.

$$\Xi_c = \frac{2}{Z(0)^2} \left[\sqrt{1 - Z(0)^2} \cos \Phi(0) - \frac{\Lambda}{2} Z(0)^2 + 1 \right]. \quad (2.45)$$

Consequently, for $\Xi < \Xi_c$, Josephson oscillations can be expected and the fractional population imbalance oscillates around zero value. However, the system enters the MQST regime if and only if $\Xi > \Xi_c$ leading to oscillations around a non-zero value. The dramatic changes of both the fractional population imbalance and the relative phase as a function of time for increasing long-range interaction strengths Ξ are shown in Fig.(2.11). The oscillations for both $Z(t)$ and $\Phi(t)$ tend to behave symmetrically and harmonically for $\Xi < \Xi_c$, as in Fig(2.11, a), until the symmetry and the periodicity⁹ are broken at a critical point $\Xi = \Xi_c$, as illustrated in Fig(2.11, b). Above this point $\Xi > \Xi_c$, Fig(2.11, c) shows that the fractional population imbalance oscillates asymmetrically and periodically around a non-zero value time averaged $\langle Z(t) \rangle \neq 0$, meaning that the atoms are self-trapped in only one well (in the left in our case). However, the relative phase changes linearly as a function of time. This clearly indicates the appearance of the macroscopic quantum self-trapping in the double-well potential trap.

In conclusion to this section, we have examined the dynamics of N_T^{dw} Rydberg-dressed atoms trapped in a double well potential in the presence of non-local interactions and have found that coupled non-linear Josephson equations for the relative population and phase difference between the two wells were derived by assuming the system to be described by a superposition of left and right localised condensates (two-mode model) governed by the one-dimensional time-dependant Gross pitaevskii equation. Such non-linear Josephson equations allow the study to be categorised into three distinct regimes where the tunnelling dynamics turn out to depend strongly on the initial conditions of both, the fractional population imbalance and the relative phase. In the non-interacting regime, where the coherence is very high and the atom number fluctuations are large, the atoms oscillate back and forth independently with a Rabi-like frequency $\omega_{\text{Ra}}^{\text{dw}}$ resembling a two-level atom in a coherent field. However,

⁹Despite the fact that the system is initially coherent at $t_0 = 0$, the possibility for the periodicity of the dynamics at a later time $t > t_0$ and for a certain strength of the non-linear long-range interaction $\Xi = \Xi_c$, to be disappeared is present due to the non-linear character of the interactions.

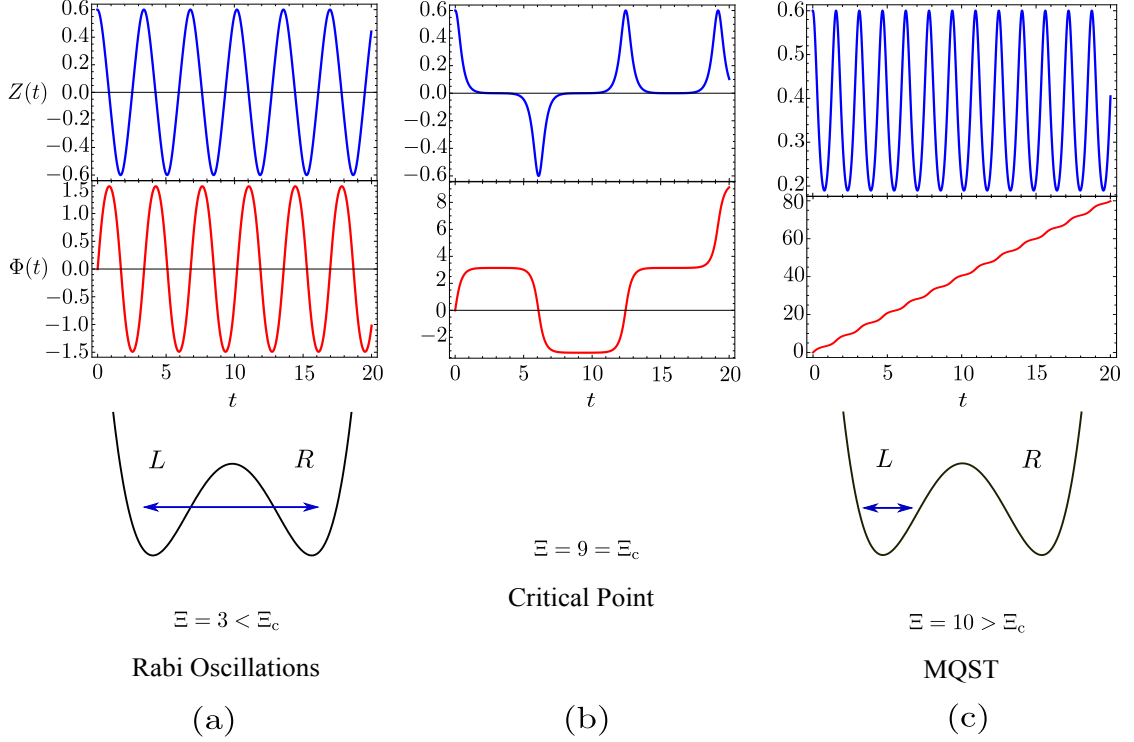


Figure 2.11.: Fractional population imbalance $Z(t)$ (up) and the relative phase $\Phi(t)$ (down) versus dimensionless time t in the non-linear-interacting regime (Fock regime) for different long-range interaction values Ξ and a fixed local interaction is to $\Lambda = 1$, with initial conditions for the fractional population imbalance $Z(0) = 0.6$ and for the relative phase $\Phi(0) = 0$.

in the linear-interacting regime, where the coherence is high and the atom number fluctuations are small, these equations admit solutions in the form of small periodic oscillations with a Josephson frequency (linear frequency) ω_{Jo}^{dw} , whose period is determined by the strength of the long-range interactions. When the non-linearity arising from the mean-field long-range interaction under certain initial conditions exceeds a critical value, the system may exhibit self-trapped solutions with the relative populations oscillating around a non-zero value where the atoms essentially occupy preferably one side of the trap during the experimental lifetime even though they repel each other. Therefore, within this regime, the coherence is low and the atom number fluctuations vanish. Comparing with the results presented in Ref [72], it is obvious that no new physics has occurred as a consequence of adding the long-range interaction and the dynamics are pretty similar to the case where only the short-range contact-interaction is involved.

2.2. Triple-well potential

If one wants to make an extension of the double-well system, the triple-well is the straightforward natural one [98]. Compared with the double-well system, the difference is essential both in mathematics and physics for the triple-well system, which has two distinguished characteristics. Firstly, it has a much richer structure and can support the simplest model for exhibiting the effect of the next-nearest neighbour coupling on quantum tunnelling. The quantum tunnelling may happen between several wells simultaneously, then the tunnelling dynamics in the triple-well will show more interesting behaviour. In addition, the study of the triple-well system will also provide a bridge between the simple double-well and the multi-well systems as a prototype of optical lattices, helping us provide a bottom-up understanding of mechanisms operating in the infinite optical lattice [78]. Considering these reasons, the dynamics of ultracold atomic clouds in triple-well potentials have attracted a substantial attention recently which has been practically realised and applied in atomic physics and Bose-Einstein condensates. Experimentally, the triple-well potential can be created by means of focused Gaussian laser beams of different frequencies [90].

The aim here is to apply the same methods in the proceeding section to study the influence of the long-range interaction on the quantum tunnelling of N_T^{tw} Rydberg-dressed atoms trapped in a quasi one-dimensional triple-well potential (composed of three wells around the origin) based on the dynamical equations of the fractional population imbalances (or the atom numbers) and relative phases that are obtained after describing the evolution of the Bose-Einstein wave-packet under the three-mode approximation.

As a start, we will briefly introduce some of the triple-well potential characteristics by firstly expressing its quasi one-dimensional form [99]:

$$V_{\text{tw}}(x) = Ax^2(x - B)^2(x + B)^2, \quad (2.46)$$

where $A \neq 0$. This potential has three wells among which two side wells are identical, and central well is rather broader as schematically shown in Fig.(2.12). As a result, there are two different trapping frequencies which are obtained analogously to the double-well potential, i.e., by quadratically expanding the triple-well poten-

tial expression around its minima $\pm B$ and 0, and then compare it with the harmonic oscillator formula which yields to

$$\omega_x^{L,R} = B^2 \sqrt{\frac{8A}{m}} \quad \omega_x^M = B^2 \sqrt{\frac{2A}{m}}, \quad (2.47)$$

where $\omega_x^{L,R}$ and ω_x^M are the trapping frequencies along the x axis for the left, right and middle wells, respectively.

2.2.1. Three-mode approximation for a single-atom tunnelling

Generally in the case of a triple-well potential, an energy level is split into three levels with slightly different energy values due to the quantum tunnelling through barriers [99]. If the energy difference between two of the first three energies, i.e., $\Delta\varepsilon_1$ or $\Delta\varepsilon_2$ as Fig.(2.12) shows, is much smaller than the difference to all energetically higher lying states, i.e., χ , thus the system is reduced to three mean field orbitals in which the atoms are located, this is the so-called *three-mode approximation*.

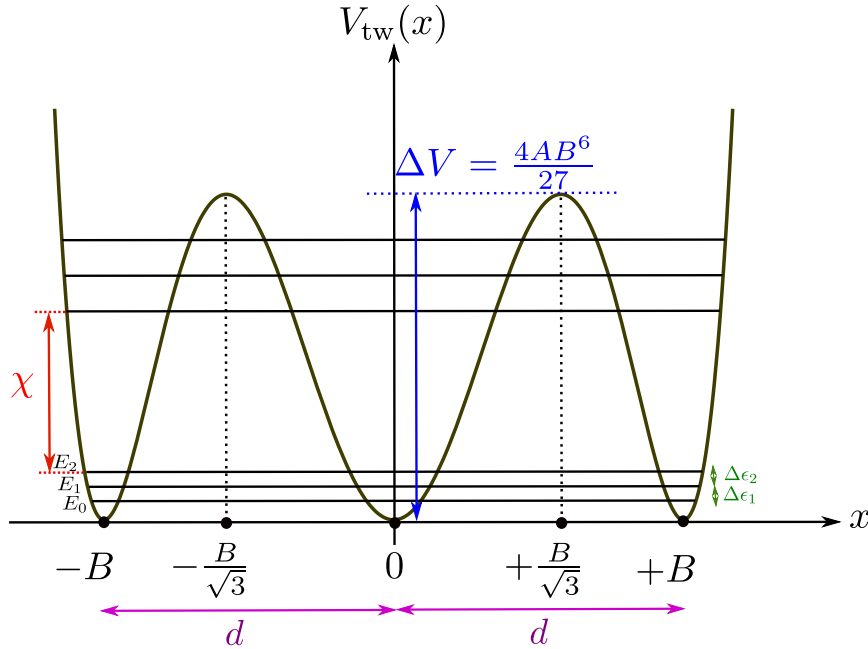


Figure 2.12.: A quasi one-dimensional triple-well potential $V_{tw}(x)$. The potential minima are $0, \pm B$. d and ΔV are the well separation between two neighbouring wells and the potential barrier height, respectively. Three-mode approximation condition is $\chi \gg \Delta\varepsilon_{1,2}$ where $\Delta\varepsilon_{1,2}$ are the energy differences between the first three eigenenergies $E_{0,1,2}$.

In the quasi one-dimensional triple-well potential expressed in Eq.(2.46) where both the right and left wells are symmetric, the tunnelling rate under the Gaussian approximation is given by:

$$J_{\text{tw}} = -\langle G_j(x) | \hat{H}(x) | G_{j+1}(x) \rangle = - \int_{-\infty}^{+\infty} G_j(x) \hat{H}(x) G_{j+1}(x) dx, \quad (2.48)$$

where $G_j(x), G_{j+1}(x)$ are the on-site wave functions of two neighbouring wells which are assumed to be fixed (localised), and they are taken as one-dimensional Gaussian functions, as illustrated in Fig(2.13):

$$\langle \vec{x} | G_j \rangle = G_j(\vec{x}) = \left(\frac{1}{\xi_j^2 \pi} \right)^{\frac{1}{4}} \exp \left[-\frac{(x - x_j)^2}{2\xi_j^2} \right],$$

where: $\xi_j = \sqrt{\hbar/m\omega_x^j}$ with $j = L, M, R$ are the Gaussian widths for the left, middle and right wave functions, respectively. We limit to the case where ξ_j is small enough with respect to the separation between two neighbouring wells d so that the sites are well defined with small spatial overlap.

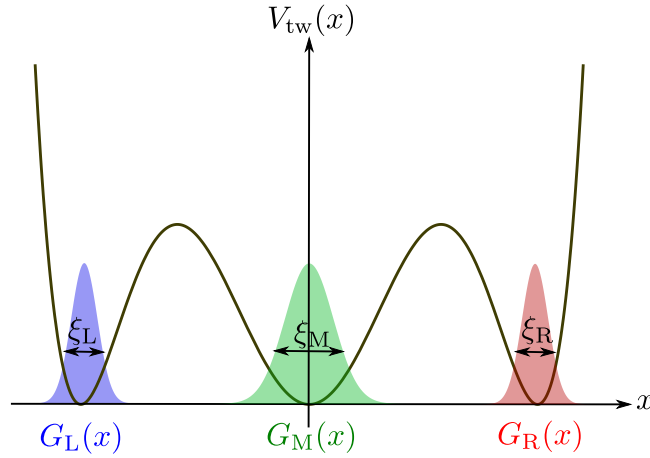


Figure 2.13.: Three localised left, middle and right Gaussian wave functions $G_{L,M,R}(x)$, respectively.

The Hamiltonian which describes one tunnelling atom in the triple-well potential is given by:

$$\hat{H}(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{\text{tw}}(x).$$

Similarly to subsection (2.1.4.2), in order to calculate the matrix element $\langle G_j(x)|\hat{H}(x)|G_{j+1}(x)\rangle$ we approximate this Hamiltonian in a way that it describes an atom tunnelling only between two adjacent wells. Therefore, the triple-well potential can be harmonically-approximated in the vicinity of either $x = +\frac{B}{\sqrt{3}}$ (if we want to study the right $\leftrightarrow$ middle tunnelling rate), or $x = -\frac{B}{\sqrt{3}}$ (if we want to study the left $\leftrightarrow$ middle tunnelling rate). Here, we investigate the tunnelling rate between the right and middle wells, thus according to Eq.(2.48) one gets:

$$J_{\text{tw}} = -\langle G_R(x)|\hat{H}(x)|G_M(x)\rangle = -\int_{-\infty}^{+\infty} G_R(x)\hat{H}(x)G_M(x)dx, \quad (2.49)$$

where the right and middle Gaussian wave functions are given by:

$$G_R(x) = \left(\frac{1}{\xi_R^2\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{(x-B)^2}{2\xi_R^2}\right] \quad G_M(x) = \left(\frac{1}{\xi_M^2\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{x^2}{2\xi_M^2}\right]. \quad (2.50)$$

Substituting Eqs.(2.50) in Eq.(2.49) we get

$$\begin{aligned} J_{\text{tw}} &= -\langle G_R(x)|\hat{H}(x)|G_M(x)\rangle = -\int_{-\infty}^{+\infty} G_R(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{\text{tw}}(x)\right)G_M(x)dx \\ &\approx -\left(\frac{1}{\pi\xi_R^2}\right)^{\frac{1}{4}}\left(\frac{1}{\pi\xi_M^2}\right)^{\frac{1}{4}}\int_{-\infty}^{+\infty} \exp\left[-\frac{(x-B)^2}{2\xi_R^2}\right]\exp\left[-\frac{x^2}{2\xi_M^2}\right] \\ &\quad \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{4}{3}AB^4x^2 + \frac{8}{3\sqrt{3}}AB^5x - \frac{4}{9}AB^6\right)dx. \end{aligned}$$

After a couple of analytical steps we find

$$\begin{aligned} J_{\text{tw}} &= -N\left[-\frac{\hbar^2}{2m}\frac{B^2 - (\xi_M^2 + \xi_R^2)}{(\xi_M^2 + \xi_R^2)^2} - \frac{4}{3}AB^4\frac{\xi_M^2(\xi_R^4 + \xi_M^2B^2 + \xi_M^2\xi_R^2)}{(\xi_M^2 + \xi_R^2)^2}\right. \\ &\quad \left. + \frac{8}{3\sqrt{3}}AB^6\frac{\xi_M^2}{(\xi_M^2 + \xi_R^2)} - \frac{4}{9}AB^6\right], \end{aligned} \quad (2.51)$$

where:

$$N = -\left(\frac{1}{\xi_R^2\pi}\right)^{\frac{1}{4}}\left(\frac{1}{\xi_M^2\pi}\right)^{\frac{1}{4}}\frac{\xi_M\xi_R\sqrt{2\pi}}{\sqrt{\xi_M^2 + \xi_R^2}}\exp\left[-\frac{B^2}{2(\xi_R^2 + \xi_M^2)}\right],$$

is a dimensionless number ¹⁰. Interestingly, when $\xi_R = \xi_M = \xi$, Eq.(2.51) is reduced to

$$J_{\text{tw}}^{\xi_R=\xi_M} = -\xi^2 \exp\left(-\frac{B^2}{4\xi^2}\right) \left[-\frac{\hbar^2}{2m} \frac{B^2 - 2\xi^2}{4\xi^6} - \frac{4}{3} AB^4 \frac{2\xi^2 + B^2}{4\xi^2} + \frac{1}{\xi^2} AB^6 \frac{12 - 4\sqrt{3}}{9\sqrt{3}} \right], \quad (2.52)$$

where the tunnelling rate:

1. is proportional to the square of the Gaussian widths $J_{\text{tw}}^{\xi_R=\xi_M} \propto \xi^2$, meaning that the tunnelling rate gets stronger as the Gaussian widths gets larger.
2. is inversely proportional to the mass of the atom as $J_{\text{tw}}^{\xi_R=\xi_M} \propto 1/m$.
3. decreases with increasing the separation between the minima of neighbouring wells as $d = 2|x_{\min}|$ and $J_{\text{tw}}^{\xi_R=\xi_M} \propto e^{-B^2}$.

Comparing with the double-well potential case in subsubsection (2.1.4.2), the tunnelling rate $J_{\text{tw}}^{\xi_R=\xi_M}$ has the same relations with ξ , $x_{\min}$ and m .

2.2.2. Mean-field description of three BECs in a triple-well potential

Being interested in the ground state of the quasi one-dimensional triple-well potential within the three-mode approximation, the wave function of the whole wave-packet inside the trap can be defined as a superposition of three wave functions describing the condensate in each trap, i.e,

$$\psi(x, t) = \psi_L(t)\phi_L(x) + \psi_M(t)\phi_M(x) + \psi_R(t)\phi_R(x), \quad (2.53)$$

where: $\psi_L(t)$, $\psi_M(t)$ and $\psi_R(t)$ are the time-dependent amplitudes, and $\phi_L(x)$, $\phi_M(x)$ and $\phi_R(x)$ are the localised wave functions for the left, middle and right wells, respectively.

¹⁰In order to know the units of both A and B , we approximate the triple-well potential as a harmonic oscillator around the minimum point $x_{\min} = 0$ where we find that the dimensions of $[AB^4] = [m\omega^2] = [\text{kg} \cdot \text{sec}^{-2}]$, then the tunnelling rate in Eq.(2.51) scales in the unit of energy $[J_{\text{tw}}] = [\text{Joule}]$.

2.2.2.1. Differential equations of the time-dependent amplitudes

Similarly to the double-well case, to get the equations of motion for the three condensates, i.e., the differential equations of the time-dependant amplitudes $\psi_L(t)$, $\psi_M(t)$ and $\psi_R(t)$, we insert the approximated wave function in Eq.(2.53) into the non-linear one-dimensional GP equation expressed in Eq.(2.21), and then we project the resulting equation onto the single well states $\phi_L(x)$, $\phi_M(x)$ and $\phi_R(x)$ by multiplying from the left with $\phi_L^*(x)$, $\phi_M^*(x)$ and $\phi_R^*(x)$ and integrate over the space x , bearing in mind that the normalisation and the orthogonality conditions have to be fulfilled. Consequently after a few analytical steps we write

$$\begin{aligned}
i\hbar \frac{d\psi_L(t)}{dt} = & \left[E_L^0 + U_L N_L + \eta_{L1} N_L + (\eta_{L4} + \eta_{L11}) N_M + (\eta_{L7} + \eta_{L15}) N_R \right] \psi_L(t) \\
& - \left[J_{L1} - (\eta_{L2} + \eta_{L10}) N_L - (\eta_{L8} + \eta_{L18}) N_R - \eta_{L5} N_M \right] \psi_M(t) \\
& - \left[J_{L2} - (\eta_{L3} + \eta_{L13}) N_L - (\eta_{L6} + \eta_{L17}) N_M - \eta_{L9} N_R \right] \psi_R(t) \\
& + \left[\eta_{L12} + \eta_{L14} + \eta_{L16} \right] \psi_L(t) \psi_R(t) \psi_M(t)
\end{aligned} \tag{2.54}$$

$$\begin{aligned}
i\hbar \frac{d\psi_R(t)}{dt} = & \left[E_R^0 + U_R N_R + \eta_{R1} N_R + (\eta_{R4} + \eta_{R11}) N_M + (\eta_{R7} + \eta_{R15}) N_L \right] \psi_R(t) \\
& - \left[J_{R1} - (\eta_{R2} + \eta_{R10}) N_R - (\eta_{R8} + \eta_{R18}) N_L - \eta_{R5} N_M \right] \psi_M(t) \\
& - \left[J_{R2} - (\eta_{R3} + \eta_{R13}) N_R - (\eta_{R6} + \eta_{R17}) N_M - \eta_{R9} N_L \right] \psi_L(t) \\
& + \left[\eta_{R12} + \eta_{R14} + \eta_{R16} \right] \psi_L(t) \psi_R(t) \psi_M(t)
\end{aligned} \tag{2.55}$$

$$\begin{aligned}
i\hbar \frac{d\psi_M(t)}{dt} = & \left[E_M^0 + U_M N_M + \eta_{M1} N_M + (\eta_{M4} + \eta_{M11}) N_L + (\eta_{M7} + \eta_{M15}) N_R \right] \psi_M(t) \\
& - \left[J_{M1} - (\eta_{M2} + \eta_{M10}) N_M - (\eta_{M8} + \eta_{M18}) N_R - \eta_{M5} N_L \right] \psi_L(t) \\
& - \left[J_{M2} - (\eta_{M3} + \eta_{M13}) N_M - (\eta_{M6} + \eta_{M17}) N_L - \eta_{M9} N_R \right] \psi_R(t) \\
& + \left[\eta_{M12} + \eta_{M14} + \eta_{M16} \right] \psi_L(t) \psi_R(t) \psi_M(t),
\end{aligned} \tag{2.56}$$

where we have denoted

$$\begin{aligned}
E_{L,R,M}^0 &= \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2}{2m} |\nabla \phi_{L,R,M}(x)|^2 + V_{\text{tw}}(x) |\phi_{L,R,M}(x)|^2 \right] \\
J_{L1,R1,M1} &= - \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2}{2m} \nabla \phi_{L,R,M}(x) \nabla \phi_{M,M,L}(x) + V_{\text{tw}}(x) \phi_{L,R,M}(x) \phi_{M,M,L}(x) \right] \\
J_{L2,R2,M2} &= - \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2}{2m} \nabla \phi_{L,R,M}(x) \nabla \phi_{R,L,R}(x) + V_{\text{tw}}(x) \phi_{L,R,M}(x) \phi_{R,L,R}(x) \right] \\
U_{L,R,M} &= g_{1D} \int_{-\infty}^{+\infty} dx |\phi_{L,R,M}(x)|^4,
\end{aligned}$$

where $E_{L,R,M}^0$ are the zero-point energies in each well, $U_{L,R,M}$ are proportional to the atomic self-interaction energies and $J_{L1,R1,M1}$, $J_{L2,R2,M2}$ are the coupling matrix elements. $|\psi_{L,R,M}(t)|^2 = N_{L,R,M}$ are the number of atoms localised in the left, right and middle wells, respectively, where the total number of atoms $N_T^{\text{tw}} = N_L + N_R + N_M$ is assumed to be constant. Here and henceforth, we associate N_L , N_R and N_M with the number of atoms in the wells, left, right and middle, respectively. Analogously to the double-well case, $E_{L,R,M}^0$, $J_{L1,R1,M1}$, $J_{L2,R2,M2}$ correspond to one-atom dynamic in the triple-well potential, while $U_{L,R,M}$ relate to the short-range contact-interaction between the atoms. However, additional matrix elements, which are a consequence of including the long-range interaction, also appear where¹¹ for the left, right and middle wells where the non-negligible ones are given by

$$\begin{aligned}
\eta_{L1,R1,M1} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R,M}(x')|^2 |\phi_{L,R,M}(x)|^2 \\
\eta_{L4,R3,M4} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{M,M,L}(x')|^2 |\phi_{L,R,M}(x)|^2 \\
\eta_{L7,R7,M7} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{R,L,R}(x')|^2 |\phi_{L,R,M}(x)|^2.
\end{aligned} \tag{2.57}$$

Fig.(2.14) shows how the previous matrix elements $\eta_{Li,Ri,Mi}/\zeta$ with $i = 1, 2, \dots, 18$ change as a function of the soft-core interaction radius R_{SC} . In the local interaction regime, i.e., for small R_{SC} , the integrals $\eta_{L1,R1,M1}/\zeta$ are the dominant terms. However, in the near-local interaction regime, i.e., for slightly larger values of R_{SC} , the integrals $\eta_{L4,R4,M4,M7}/\zeta$ begin to be involved in the dynamics and start to increase with increasing R_{SC} . Moreover, in the non-local interaction regime, i.e., for large values

¹¹The entire matrix elements are found in the Appendix E

of R_{SC} , the integrals $\eta_{L7,R7}/\zeta$ with all the preceding ones become on the same order of magnitude. The rest of the integrals $\eta_{Lj,Rj,Mj}/\zeta$ with $j = 2, 3, 5, 6, 8, \dots, 18$ remain negligible for any value of R_{SC} . Therefore, we retain only $\eta_{L1,R1,M1}/\zeta$, $\eta_{L4,R4,M4,M7}/\zeta$ and $\eta_{L7,R7}/\zeta$ for the case of large R_{SC} leading to the simplified time-dependent amplitudes differential equations that can be re-written as

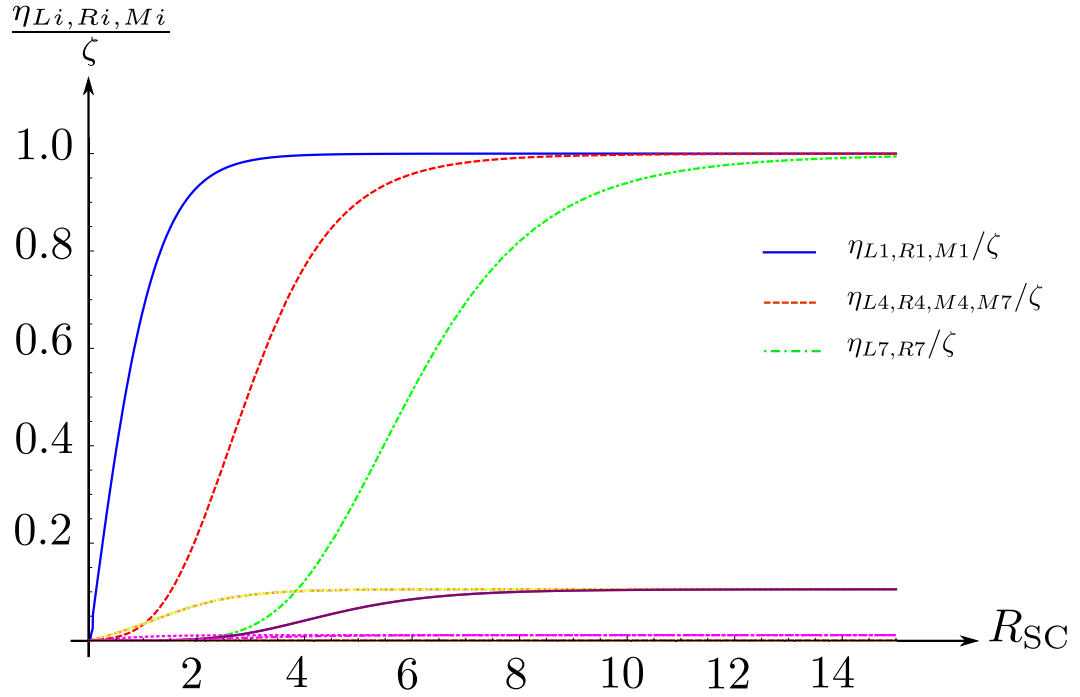


Figure 2.14.: The matrix elements $\eta_{Li,Ri,Mi}/\zeta$ where $i = 1, 2, \dots, 18$ for the triple-well potential trap are shown as a function of the soft-core interaction radius R_{SC} where the triple-well potential minima are taken to be equal to $B = \pm 3, 0$.

$$i\hbar \frac{d\psi_L(t)}{dt} = [E_L^0 + U_L N_L + \eta_{L1} N_L + \eta_{L4} N_M + \eta_{L7} N_R] \psi_L(t) - J_1 \psi_M(t) - J_3 \psi_R(t) \quad (2.58)$$

$$i\hbar \frac{d\psi_R(t)}{dt} = [E_R^0 + U_R N_R + \eta_{R1} N_R + \eta_{R4} N_M + \eta_{R7} N_L] \psi_R(t) - J_2 \psi_M(t) - J_3 \psi_L(t) \quad (2.59)$$

$$i\hbar \frac{d\psi_M(t)}{dt} = [E_M^0 + U_M N_M + \eta_{M1} N_M + \eta_{M4} N_L + \eta_{L7} N_R] \psi_M(t) - J_1 \psi_L(t) - J_2 \psi_R(t), \quad (2.60)$$

where we have put $J_{L1} = J_{M1} = J_1$, $J_{R1} = J_{M2} = J_2$ and $J_{L2} = J_{R2} = J_3$. It is worth noting that $\eta_{L1,R1,M1}$ represent the “local” long-range interaction between atoms in the same well, whereas, $\eta_{L4,R4,M4,M7}$ refer to the “nearest neighbour” long-range interaction, i.e., the interaction between atoms via adjacent wells. However, $\eta_{L7,R7}$ represent the “next-nearest neighbour” long-range interaction, i.e., the interaction between atoms residing in the outermost wells. It is important to note, when comparing Eqs.(2.58,2.59,2.60) with Eqs.(2.26), that there are two additional terms in each differential equation of the time-dependent amplitudes in the triple-well potential case, which can be considered as a sign for new dynamics and different from the double-well study, as we shall see later on.

2.2.2.2. Tunnelling dynamics

In the triple-well potential case, we will analyse the tunnelling dynamics in terms of four canonical variables; two fractional population imbalances $Z_1(t) = (N_L - N_M)/N_T^{\text{tw}}$, $Z_2(t) = (N_L - N_R)/N_T^{\text{tw}}$ and two relative phases $\Phi_1(t) = \theta_M(t) - \theta_L(t)$, $\Phi_2(t) = \theta_R(t) - \theta_L(t)$. To start with the differential equations of both $Z_1(t)$, $Z_2(t)$, we obtain, as a first step, the differential equations of the atom numbers N_L, N_R, N_M by employing the Madelung representation on the time-dependent amplitudes Eqs.(2.58,2.59,2.60), and redo similar calculations as were done in the subsubsection (2.1.5.2), as well as considering the dimensionless time as $t \rightarrow 2J_1 t/\hbar$, then we can write

$$\frac{dN_L(t)}{dt} = -\sqrt{N_L N_M} \sin \Phi_1 - \frac{J_3}{J_1} \sqrt{N_L N_R} \sin (\Phi_1 - \Phi_2) \quad (2.61)$$

$$\frac{dN_R(t)}{dt} = -\frac{J_2}{J_1} \sqrt{N_R N_M} \sin \Phi_2 + \frac{J_3}{J_1} \sqrt{N_L N_R} \sin (\Phi_1 - \Phi_2) \quad (2.62)$$

$$\frac{dN_M(t)}{dt} = \sqrt{N_M N_L} \sin \Phi_1 + \frac{J_2}{J_1} \sqrt{N_M N_R} \sin \Phi_2. \quad (2.63)$$

Comparing these equations with each other allows us to note that

$$\frac{dN_L(t)}{dt} = - \left(\frac{\partial N_R(t)}{\partial t} + \frac{\partial N_M(t)}{\partial t} \right). \quad (2.64)$$

Therefore, since the atoms number $N_{L,M,R}$ are related to both fractional population imbalances $Z_{1,2}(t)$ via the following

$$N_L = \frac{(Z_1 + Z_2 + 1)}{3} N_T \quad N_M = \frac{(Z_2 - 2Z_1 + 1)}{3} N_T \quad N_R = \frac{(Z_1 - 2Z_2 + 1)}{3} N_T,$$

thus, the differential equations of both fractional population imbalances are analytically calculated as

$$\begin{aligned} \frac{dZ_1(t)}{dt} = & -\frac{2}{3} \sqrt{(Z_1 + Z_2 + 1)(Z_2 - 2Z_1 + 1)} \sin \Phi_1 \\ & - \frac{J_3}{3J_1} \sqrt{(Z_1 + Z_2 + 1)(Z_1 - 2Z_2 + 1)} \sin \Phi_2 \\ & - \frac{J_2}{3J_1} \sqrt{(Z_1 - 2Z_2 + 1)(Z_2 - 2Z_1 + 1)} \sin(\Phi_1 - \Phi_2) \end{aligned} \quad (2.65)$$

$$\begin{aligned} \frac{dZ_2(t)}{dt} = & -\frac{1}{3} \sqrt{(Z_1 + Z_2 + 1)(Z_2 - 2Z_1 + 1)} \sin \Phi_1 \\ & - \frac{2J_3}{3J_1} \sqrt{(Z_1 + Z_2 + 1)(Z_1 - 2Z_2 + 1)} \sin \Phi_2 \\ & + \frac{J_2}{3J_1} \sqrt{(Z_1 - 2Z_1 + 1)(Z_1 - 2Z_2 + 1)} \sin(\Phi_1 - \Phi_2). \end{aligned} \quad (2.66)$$

Regarding the relative phases, and repeating the same calculation steps as in the double-well potential, we write the left, right and middle phases as

$$\begin{aligned} \frac{d\theta_L(t)}{dt} = & -\frac{E_L^0 + U_L N_L + \eta_{L1} N_L + \eta_{L4} N_M + \eta_{L7} N_R}{2K_1} + \frac{1}{2} \sqrt{\frac{N_M}{N_L}} \cos \Phi_1 \\ & + \frac{J_3}{2J_1} \sqrt{\frac{N_R}{N_L}} \cos \Phi_2 \end{aligned} \quad (2.67)$$

$$\begin{aligned} \frac{d\theta_R(t)}{dt} = & -\frac{E_R^0 + U_R N_R + \eta_{R1} N_R + \eta_{R4} N_M + \eta_{R7} N_L}{\hbar} + \frac{J_2}{2J_1} \sqrt{\frac{N_M}{N_R}} \cos(\Phi_1 - \Phi_2) \\ & + \frac{J_3}{2J_1} \sqrt{\frac{N_L}{N_R}} \cos \Phi_2 \end{aligned} \quad (2.68)$$

$$\begin{aligned} \frac{d\theta_M(t)}{dt} = & -\frac{E_M^0 + U_M N_M + \eta_{M1} N_M + \eta_{M4} N_R + \eta_{M7} N_L}{\hbar} + \frac{1}{2} \sqrt{\frac{N_L}{N_M}} \cos \Phi_1 \\ & + \frac{J_2}{2J_1} \sqrt{\frac{N_R}{N_M}} \cos(\Phi_1 - \Phi_2). \end{aligned} \quad (2.69)$$

Owing to the assumption that the first relative phase is $\Phi_1(t) = \theta_M(t) - \theta_L(t)$ we can write

$$\begin{aligned} \frac{d\Phi_1(t)}{dt} = & \Delta E_{LM} + (\Xi_{LM1} - \Lambda_{LM1}) \frac{N_M - N_L}{N_T^{\text{tw}}} + (\Xi_{LM2} - \Lambda_{LM2}) \frac{N_R}{N_T^{\text{tw}}} + \frac{N_L - N_M}{2\sqrt{N_M N_L}} \cos \Phi_1 \\ & + \frac{J_2}{2J_1} \sqrt{\frac{N_R}{N_M}} \cos(\Phi_1 - \Phi_2) - \frac{J_3}{2J_1} \sqrt{\frac{N_R}{N_L}} \cos \Phi_2, \end{aligned} \quad (2.70)$$

or as a function of both fractional population imbalances $Z_1(t), Z_2(t)$ we formulate the first relative phase as

$$\begin{aligned} \frac{d\Phi_1(t)}{dt} = & \Delta E_{LM} - (\Xi_{LM1} - \Lambda_{LM1}) Z_1(t) + (\Xi_{LM2} - \Lambda_{LM2}) \left(\frac{Z_1 - 2Z_2 + 1}{3} \right) \\ & + \frac{3}{2} \frac{Z_1(t)}{\sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)}} \cos \Phi_1 \\ & + \frac{J_2}{2J_1} \sqrt{\frac{Z_1(t) - 2Z_2(t) + 1}{Z_2(t) - 2Z_1(t) + 1}} \cos(\Phi_1 - \Phi_2) - \frac{J_3}{2J_1} \sqrt{\frac{Z_1(t) - 2Z_2(t) + 1}{Z_1(t) + Z_2(t) + 1}} \cos \Phi_2, \end{aligned} \quad (2.71)$$

where the energy parameters read:

$$\begin{aligned}
\Delta E_{LM} &= \frac{E_L^0 - E_M^0}{2J_1} + \frac{(U_L - U_M)}{4J_1} N_T^{\text{tw}} + \left[\frac{(\eta_{L1} - \eta_{M1}) + (\eta_{L4} - \eta_{M4})}{4J_1} \right] N_T^{\text{tw}} \\
\Lambda_{LM1} &= \frac{(U_L + U_M)}{4J_1} N_T^{\text{tw}} \\
\Lambda_{LM2} &= \frac{(U_L - U_M)}{4J_1} N_T^{\text{tw}} \\
\Xi_{LM1} &= \left[\frac{(\eta_{L4} + \eta_{M4}) - (\eta_{L1} + \eta_{M1})}{4J_1} \right] N_T^{\text{tw}} \\
\Xi_{LM2} &= \left[\frac{2(\eta_{L7} - \eta_{M7}) - (\eta_{L1} - \eta_{M1}) - (\eta_{L4} - \eta_{M4})}{4J_1} \right] N_T^{\text{tw}}.
\end{aligned}$$

With the same manner, we get the second relative phase $\Phi_2(t) = \theta_R(t) - \theta_L(t)$ as:

$$\begin{aligned}
\frac{d\Phi_2(t)}{dt} &= \Delta E_{LR} + (\Xi_{LR1} - \Lambda_{LR1}) \frac{N_L - N_R}{N_T^{\text{tw}}} + (\Xi_{LR2} - \Lambda_{LR2}) \frac{N_M}{N_T^{\text{tw}}} + \frac{J_2}{2J_1} \sqrt{\frac{N_M}{N_R}} \cos(\Phi_1 - \Phi_2) \\
&\quad - \frac{1}{2} \sqrt{\frac{N_M}{N_L}} \cos \Phi_1 + \frac{J_3}{2J_1} \frac{N_L - N_R}{\sqrt{N_L N_R}} \cos \Phi_2.
\end{aligned} \tag{2.72}$$

The differential equation of $\Phi_2(t)$ as a function of $Z_1(t), Z_2(t)$ takes the form of

$$\begin{aligned}
\frac{d\Phi_2(t)}{dt} &= \Delta E_{LR} + (\Xi_{LR1} - \Lambda_{LR1}) Z_2(t) + (\Xi_{LR2} - \Lambda_{LR2}) \left(\frac{Z_2(t) - 2Z_1(t) + 1}{3} \right) \\
&\quad + \frac{1}{2} \sqrt{\frac{Z_2(t) - 2Z_2(t) + 1}{Z_1 - 2Z_2(t) + 1}} \cos(\Phi_1 - \Phi_2) - \frac{1}{2} \sqrt{\frac{Z_2(t) - 2Z_1(t) + 1}{Z_1(t) + Z_2(t) + 1}} \cos \Phi_1 \\
&\quad + \frac{3J_3}{2J_1} \frac{Z_2(t)}{\sqrt{(Z_1(t) + Z_2(t) + 1)(Z_1(t) - 2Z_2(t) + 1)}} \cos \Phi_2,
\end{aligned} \tag{2.73}$$

where:

$$\begin{aligned}
\Delta E_{LR} &= \frac{E_L^0 - E_R^0}{2J_1} + \frac{(U_L - U_R)}{4J_1} N_T^{\text{tw}} + \left[\frac{(\eta_{L1} - \eta_{R1}) + (\eta_{L7} - \eta_{R7})}{4J_1} \right] N_T^{\text{tw}} \\
\Lambda_{LR1} &= \frac{(U_L + U_R)}{4J_1} N_T^{\text{tw}} \\
\Lambda_{LR2} &= \frac{(U_L - U_R)}{4J_1} N_T^{\text{tw}} \\
\Xi_{LR1} &= \left[\frac{(\eta_{L1} + \eta_{R1}) - (\eta_{L7} + \eta_{R7})}{4J_1} \right] N_T^{\text{tw}} \\
\Xi_{LR2} &= \left[\frac{2(\eta_{L4} - \eta_{R4}) - (\eta_{L1} - \eta_{R1}) - (\eta_{L7} - \eta_{R7})}{4J_1} \right] N_T^{\text{tw}}.
\end{aligned}$$

As a consequence, the dynamics of N_T^{tw} interacting Rydberg-dressed atoms trapped in a quasi one-dimensional triple-well potential are governed by

- i. three differential equations of atom number and two for the relative phases which are formulated in Eqs.(2.61,2.62,2.63,2.70,2.72)
- ii. or, two differential equations of fractional population imbalances and two relative phases that are expressed in Eqs.(2.65, 2.66, 2.71, 2.73).

2.2.2.3. Symmetric triple-well potential trap

For simplicity, we will assume that all the three wells are symmetric where their localised wave functions have the same widths $\xi_L = \xi_R = \xi_M$, therefore,

$$\left. \begin{aligned}
E_L^0 &= E_R^0 = E_M^0 \\
U_L &= U_R = U_M \\
\eta_{L1} &= \eta_{R1} = \eta_{M1} = \eta_L \\
\eta_{L4} &= \eta_{R4} = \eta_{M4} = \eta_{M7} = \eta_{NN} \\
\eta_{L7} &= \eta_{R7} = \eta_{NNN}
\end{aligned} \right\} \implies \begin{aligned}
\Delta E_{LM} &= \Delta E_{LR} = 0 \\
\Lambda_{LM1} &= \Lambda_{LR1} = \Lambda = \frac{U}{2J_1} N_T^{\text{tw}} \\
\Lambda_{LM2} &= \Lambda_{LR2} = 0 \\
\Xi_{LM1} &= \Xi_1 = \frac{(\eta_{NN} - \eta_L)}{2J_1} N_T^{\text{tw}} \\
\Xi_{LM2} &= \Xi_2 = \frac{(\eta_{NNN} - \eta_{NN})}{2J_1} N_T^{\text{tw}} \\
\Xi_{LR1} &= \Xi' = \frac{(\eta_L - \eta_{NNN})}{2J_1} N_T^{\text{tw}} \\
\Xi_{LR2} &= 0
\end{aligned}$$

where the η_L , η_{NN} and η_{NNN} represent the local, nearest and next-nearest neighbour

long-range interactions, respectively. Moreover, On account of the fact that the wave functions of the three wells are localised and independent of each other, it can be assumed that the tunnelling matrix element between the left $\leftrightarrow$ right wells is negligible, i.e., $J_3 \approx 0$. In addition, the coupling matrix elements between right $\leftrightarrow$ middle and left $\leftrightarrow$ middle wells are presumed to be on the same order of magnitude, i.e., $J_1 \approx J_2$. Furthermore, based on the above assumptions, a simple relation $\Xi_2 = -(\Xi_1 + \Xi')$ allows us to keep only Ξ_1 and Ξ' in the dynamical differential equations expressions. For these simplified cases, we rewrite the dynamical differential equations Eqs.(2.61, 2.62, 2.63, 2.70, 2.72) as following

$$\frac{dN_L(t)}{dt} = -\sqrt{N_L N_M} \sin \Phi_1 \quad (2.74a)$$

$$\frac{dN_R(t)}{dt} = -\sqrt{N_R N_M} \sin (\Phi_1 - \Phi_2) \quad (2.74b)$$

$$\frac{dN_M(t)}{dt} = \sqrt{N_M N_L} \sin \Phi_1 + \sqrt{N_M N_R} \sin (\Phi_1 - \Phi_2) \quad (2.74c)$$

$$\frac{d\Phi_1(t)}{dt} = (\Xi_1 - \Lambda) \frac{N_M - N_L}{N_T^{\text{tw}}} - (\Xi_1 + \Xi') \frac{N_R}{N_T^{\text{tw}}} + \frac{N_L - N_M}{2\sqrt{N_M N_L}} \cos \Phi_1 + \frac{1}{2} \sqrt{\frac{N_R}{N_M}} \cos (\Phi_1 - \Phi_2) \quad (2.74d)$$

$$\frac{d\Phi_2(t)}{dt} = (\Xi' + \Lambda) \frac{N_L - N_R}{N_T^{\text{tw}}} + \frac{1}{2} \sqrt{\frac{N_M}{N_R}} \cos (\Phi_1 - \Phi_2) - \frac{1}{2} \sqrt{\frac{N_M}{N_L}} \cos \Phi_1, \quad (2.74e)$$

and likewise for Eqs.(2.65, 2.66, 2.71, 2.73) we find

$$\begin{aligned} \frac{dZ_1(t)}{\partial t} = & -\frac{2}{3} \sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)} \sin \Phi_1 \\ & - \frac{1}{3} \sqrt{(Z_1(t) - 2Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)} \sin (\Phi_1 - \Phi_2) \end{aligned} \quad (2.75a)$$

$$\begin{aligned} \frac{dZ_2(t)}{\partial t} = & -\frac{1}{3} \sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)} \sin \Phi_1 \\ & + \frac{1}{3} \sqrt{(Z_2(t) - 2Z_1(t) + 1)(Z_1(t) - 2Z_2(t) + 1)} \sin (\Phi_1 - \Phi_2) \end{aligned} \quad (2.75b)$$

$$\begin{aligned} \frac{d\Phi_1(t)}{dt} = & -(\Xi_1 - \Lambda) Z_1(t) - (\Xi_1 + \Xi') \left(\frac{Z_1(t) - 2Z_2(t) + 1}{3} \right) \\ & + \frac{1}{2} \sqrt{\frac{Z_1(t) - 2Z_2(t) + 1}{Z_2(t) - 2Z_1(t) + 1}} \cos (\Phi_1 - \Phi_2) \end{aligned}$$

$$+ \frac{3}{2} \frac{Z_1(t)}{\sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)}} \cos \Phi_1 \quad (2.75c)$$

$$\begin{aligned} \frac{d\Phi_2(t)}{dt} = & (\Xi' + \Lambda)Z_2(t) + \frac{1}{2} \sqrt{\frac{Z_2(t) - 2Z_1(t) + 1}{Z_1(t) - 2Z_2(t) + 1}} \cos(\Phi_1 - \Phi_2) \\ & - \frac{1}{2} \sqrt{\frac{Z_2(t) - 2Z_1(t) + 1}{Z_1(t) + Z_2(t) + 1}} \cos \Phi_1. \end{aligned} \quad (2.75d)$$

In the following, we will investigate the dynamics of N_T^{tw} atoms in three interacting limits; non-interacting (Rabi), linear interacting (Josephson) and non-linear interacting (Fock) limits.

2.2.3. Dynamical regimes

The dynamics of N_T^{tw} atoms trapped in a quasi one-dimensional triple-well potential depend on the initial conditions of both fractional population imbalances and both relative phases at $t = 0$, i.e., $Z_{1,2}(0)$, $\Phi_{1,2}(0)$, respectively (or $N_{L,M,R}(0)$, $\Phi_{1,2}(0)$). Here, we consider the case of $Z_{1,2}(0) \neq 0$ ($N_{L,R,M}(0) \neq 0$) with different populations in three wells and $\Phi_{1,2}(0) = 0$. Analogously to the double-well analysis, the dynamics of Rydberg-dressed atoms in the triple-well trap will be studied in three distinct regimes; Rabi, Josephson and Fock regimes, based on different interactions strengths and initial conditions.

2.2.3.1. Non-interacting limit (Rabi regime)

For symmetric wells $\Delta E_{\text{LM}} = \Delta E_{\text{LR}} = 0$ and the absent of any interactions $\Lambda \rightarrow 0$, $\Xi_1 \approx \Xi_2 \approx \Xi' \rightarrow 0$, the differential equations of the time-dependant amplitudes in Eqs.(2.58,2.59,2.60) are similar to the time-dependent amplitudes of Λ -type three-level atom coupled to two laser fields with zero detuning $\Delta = 0$. Therefore, it can be said that the atoms inside the triple-well potential Rabi-like oscillate with a frequency equal to $\omega_{\text{Ra}}^{\text{tw}} = 2J_1/\hbar$. Thus, the dynamical equations Eqs.(2.75) are brought down in the Rabi regime to

$$\frac{dZ_1(t)}{dt} = -\frac{2}{3} \sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)} \sin \Phi_1$$

$$-\frac{1}{3}\sqrt{(Z_1(t) - 2Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)}\sin(\Phi_1 - \Phi_2) \quad (2.76a)$$

$$\begin{aligned} \frac{dZ_2(t)}{dt} = & -\frac{1}{3}\sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)}\sin\Phi_1 \\ & + \frac{1}{3}\sqrt{(Z_2(t) - 2Z_1(t) + 1)(Z_1(t) - 2Z_2(t) + 1)}\sin(\Phi_1 - \Phi_2) \end{aligned} \quad (2.76b)$$

$$\begin{aligned} \frac{d\Phi_1(t)}{dt} = & \frac{3}{2}\frac{Z_1(t)}{\sqrt{(Z_1(t) + Z_2(t) + 1)(Z_2(t) - 2Z_1(t) + 1)}}\cos\Phi_1 \\ & + \frac{1}{2}\sqrt{\frac{Z_1(t) - 2Z_2(t) + 1}{Z_2(t) - 2Z_1(t) + 1}}\cos(\Phi_1 - \Phi_2) \end{aligned} \quad (2.76c)$$

$$\frac{d\Phi_2(t)}{dt} = \frac{1}{2}\sqrt{\frac{Z_2(t) - 2Z_1(t) + 1}{Z_1(t) - 2Z_2(t) + 1}}\cos(\Phi_1 - \Phi_2) - \frac{1}{2}\sqrt{\frac{Z_2(t) - 2Z_1(t) + 1}{Z_1(t) + Z_2(t) + 1}}\cos\Phi_1, \quad (2.76d)$$

and likewise for Eqs.(2.74) we find

$$\frac{dN_L(t)}{dt} = -\sqrt{N_L N_M}\sin\Phi_1 \quad (2.77a)$$

$$\frac{dN_R(t)}{dt} = -\sqrt{N_R N_M}\sin\Phi_2 \quad (2.77b)$$

$$\frac{dN_M(t)}{dt} = \sqrt{N_L N_M}\sin\Phi_1 + \sqrt{N_R N_M}\sin\Phi_2 \quad (2.77c)$$

$$\frac{d\Phi_1(t)}{dt} = \frac{N_L - N_M}{2\sqrt{N_L N_M}}\cos\Phi_1 + \frac{1}{2}\sqrt{\frac{N_R}{N_M}}\cos\Phi_2 \quad (2.77d)$$

$$\frac{d\Phi_2(t)}{dt} = \frac{N_R - N_M}{2\sqrt{N_R N_M}}\cos\Phi_2 + \frac{1}{2}\sqrt{\frac{N_L}{N_M}}\cos\Phi_1. \quad (2.77e)$$

The dynamics of three condensates could be visualised by solving numerically Eqs.(2.76) and then plotting both fractional population imbalances $Z_1(t), Z_2(t)$ and relative phases $\Phi_1(t), \Phi_2(t)$ as a function of time t for specific initial conditions as shown in Fig.(2.15) where the initial conditions are taken to be non-zero for both imbalances $Z_1(0) = 0.2, Z_2(0) = 0.4$ and zero initial relative phases $\Phi_1(0) = \Phi_2(0) = 0$. It is clearly perceived in Fig.(2.15,a) that $Z_1(t)$ oscillates asymmetrically around a non-zero value which is completely different from the double-well potential case, and that is due to the presence of the third well. However, in Fig.(2.15,b) both relative phases

oscillate symmetrically around the zero point. It is interesting to note that $Z_{1,2}(t)$ and $\Phi_{1,2}(t)$ are canonically conjugate variables and their dynamical behaviours in $Z_1 - \Phi_1$ and $Z_2 - \Phi_2$ phase diagrams are also shown in Fig.(2.15, c, d), respectively, where each point $(Z_i(t), \Phi_i(t))$ corresponds to a specific state of the system. It can be seen that both trajectories are closed with non-circular curves.

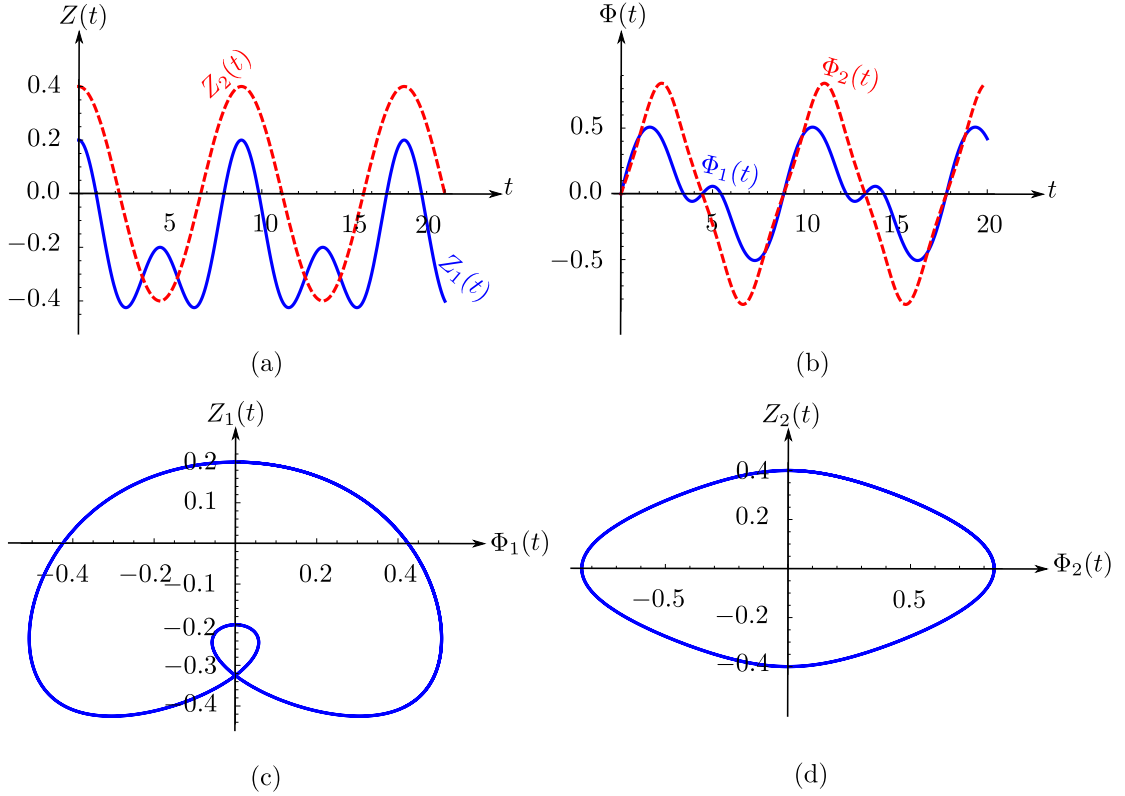


Figure 2.15.: The time evolution of both fractional population imbalances $Z_1(t), Z_2(t)$ in (a) and both relative phases $\Phi_1(t), \Phi_2(t)$ in (b). The $Z_1 - \Phi_1$ phase diagram is shown in (c) as well as $Z_2 - \Phi_2$ phase diagram in (d) where we have taken the initial conditions to be equal for the imbalances to $Z_1(0) = 0.2, Z_2(0) = 0.4$ and for the relative phases $\Phi_1(0) = \Phi_2(0) = 0$.

More precisely, the time-evolution of the non-interacting atoms in each well can be also observed by solving numerically Eqs.(2.77) as Fig.(2.16) exhibits, where we have taken two initial conditions for the atom numbers¹². Firstly, when $N_L(0) = N_M(0) = 1, N_R(0) = 16$, Fig.(2.16, a) exhibits coherent and independent oscillations of the atom numbers N_L, N_M and N_R through the potential barriers where the atoms swing

¹²It is important to mention that the state $|N_{L,M,R}(0) = 0\rangle$ is not possible in our case as Eqs.(2.77) show. Alternatively, the differential equations of the time-dependent amplitudes in Eqs.(2.58, 2.60, 2.59) allow one to consider a zero initial condition for one of the atom number.

back and forth starting from the right to the nearest neighbouring middle and then to the next-nearest neighbouring left wells and vice versa. However, both relative phases $\Phi_1(t)$, $\Phi_2(t)$ keep oscillating symmetrically around zero value as Fig.(2.16, b) shows. On the other hand, when the initial conditions are taken to be equal to $N_L(0) = N_R(0) = 1, N_M(0) = 16$, Fig.(2.16, c) shows an equal number of atoms (seven bosons) oscillating back and forth between middle $\leftrightarrow$ right and middle $\leftrightarrow$ left wells. Moreover, in Fig.(2.16, d), the relative phase $\Phi_1(t)$ in this case has harmonic and symmetric behaviours around a zero value, whereas $\Phi_2(t)$ has a zero change as a function of time. This can be explained since the atom number oscillations occur only between neighbouring wells (middle $\leftrightarrow$ right and middle $\leftrightarrow$ left) where the outermost wells (left $\leftrightarrow$ right) are completely isolated and do not see each other during the experiment time leading to a "no-change" behaviour for the $\Phi_2(t) = \theta_R - \theta_L$ as a function of time.

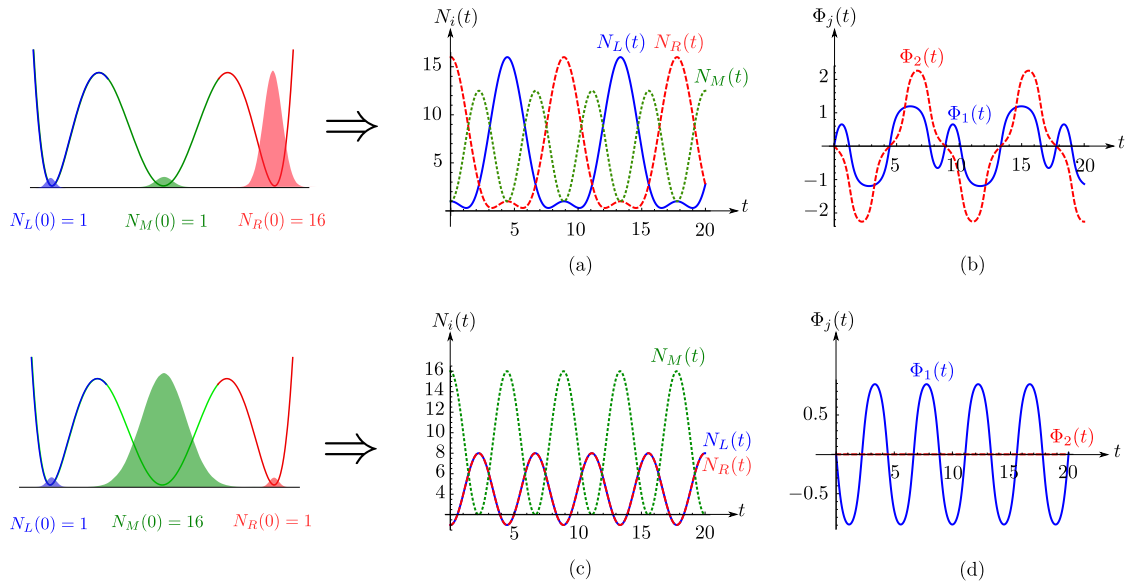


Figure 2.16.: Atom numbers $N_i(t)$ with $i = L, R, M$ and relative phases $\Phi_j(t)$ with $j = 1, 2$ time evolution in two cases for the initial conditions $N_L(0) = N_M(0) = 1, N_R(0) = 16$ (up) and $N_L(0) = N_R(0) = 1, N_M(0) = 16$ (down), and for initial relative phases $\Phi_1(0) = \Phi_2(0) = 0$ as $N_T^{\text{tw}} = 18$.

2.2.3.2. Linear-interacting limit (Josephson regime)

As was explained in subsubsection (2.1.6.2), the fluctuations of the atom number in the Josephson regime are reduced but the coherence is high. For that matter,

to observe the Josephson dynamics of N_T^{tw} interacting atoms trapped in the triple-well potential we need to linearise the non-linear dynamical equations expressed in Eqs.(2.75) around an equilibrium point, i.e., $(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0)) = (0, 0, 0, 0)$ by applying the Taylor expansion, i.e.,

$$\begin{aligned} \frac{dZ_{1,2}(t)}{dt} &= f_{1,2}(Z_1(t), Z_2(t), \Phi_1(t), \Phi_2(t)) \approx f_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0)) \\ &+ \frac{\partial f_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial Z_1(t)} (Z_1 - Z_1(0)) \\ &+ \frac{\partial f_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial Z_2(t)} (Z_2 - Z_2(0)) \\ &+ \frac{\partial f_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial \Phi_1(t)} (\Phi_1 - \Phi_1(0)) \\ &+ \frac{\partial f_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial \Phi_2(t)} (\Phi_2 - \Phi_2(0)) \end{aligned}$$

$$\begin{aligned} \frac{d\Phi_{1,2}(t)}{dt} &= g_{1,2}(Z_1(t), Z_2(t), \Phi_1(t), \Phi_2(t)) \approx g_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0)) \\ &+ \frac{\partial g_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial Z_1(t)} (Z_1 - Z_1(0)) \\ &+ \frac{\partial g_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial Z_2(t)} (Z_2 - Z_2(0)) \\ &+ \frac{\partial g_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial \Phi_1(t)} (\Phi_1 - \Phi_1(0)) \\ &+ \frac{\partial g_{1,2}(Z_1(0), Z_2(0), \Phi_1(0), \Phi_2(0))}{\partial \Phi_2(t)} (\Phi_2 - \Phi_2(0)), \end{aligned}$$

which yields to the following linearised differential and dynamical equations

$$\frac{dZ_1(t)}{dt} \approx -\Phi_1(t) + \frac{1}{3}\Phi_2(t) \quad (2.78a)$$

$$\frac{dZ_2(t)}{dt} \approx -\frac{1}{3}\Phi_2(t) \quad (2.78b)$$

$$\frac{d\Phi_1(t)}{dt} \approx \left(\frac{-(\Xi_1 + \Xi')}{3} + \frac{1}{2} \right) + \left(\Lambda - \Xi_1 - \frac{(\Xi_1 + \Xi')}{3} + \frac{9}{4} \right) Z_1(t) - \left(\frac{3}{4} - \frac{2}{3}(\Xi_1 + \Xi') \right) Z_2(t) \quad (2.78c)$$

$$\frac{d\Phi_2(t)}{dt} \approx \left(\Xi' + \Lambda + \frac{3}{4} \right) Z_2(t). \quad (2.78d)$$

A numerical solution for these linearised differential equations is reported in Fig.(2.17) where the time-evolution of both relative population imbalances $Z_{1,2}(t)$ and phase differences $\Phi_{1,2}(t)$ is studied for each long-range interaction independently with a fixed short-range interaction $\Lambda = 1$. It is clearly noticeable that $Z_2(t)$ and $\Phi_2(t)$ in the dashed red lines share a common feature between both cases where their time-evolution shows harmonic, periodic, symmetric and complete oscillations. Specifically speaking, when $\Xi_1 > \Xi'$, Fig.(2.17, a) shows that $Z_1(t)$ and $\Phi_1(t)$ have symmetric oscillations with the same “collective” period with $Z_2(t)$ and $\Phi_2(t)$, respectively. However, when $\Xi' > \Xi_1$, as Fig(2.17, b) illustrates, the time-evolution symmetry around a zero value remains for $Z_1(t)$ and $\Phi_1(t)$ but with different collective periods with both $Z_2(t)$ and $\Phi_2(t)$, respectively.

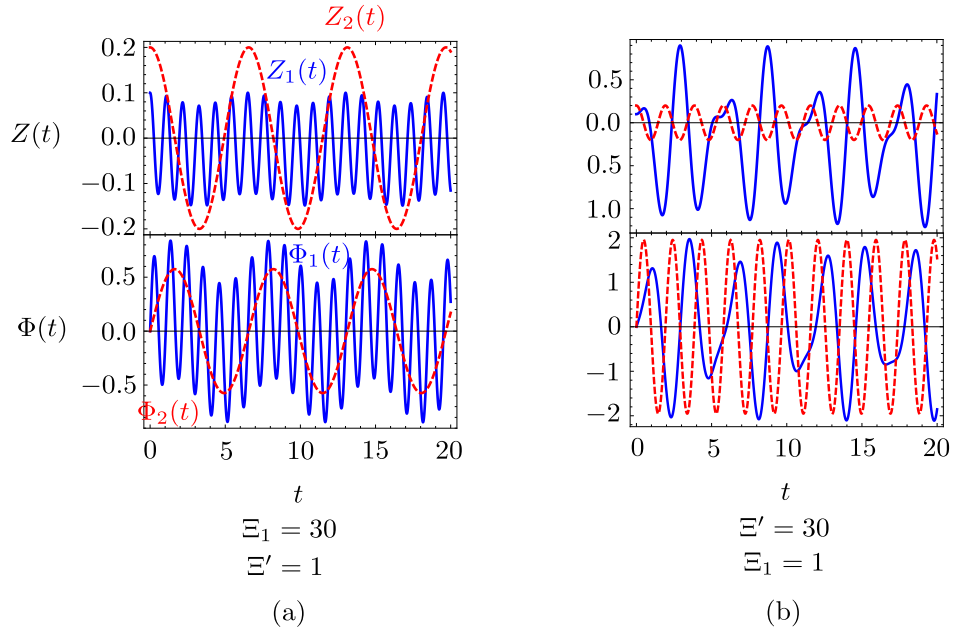


Figure 2.17.: Time evolution dynamics of the fractional population imbalances $Z_{1,2}(t)$ (up) and relative phases $\Phi_{1,2}(t)$ (down) in the linear interacting limit for different long-range interaction strengths and a fixed short-range interaction $\Lambda = 1$, bearing in mind that the initial conditions for the system are taken to be equal to $Z_1(0) = 0.1$, $Z_2(0) = 0.2$ and $\Phi_1(0) = \Phi_2(0) = 0$.

2.2.3.3. Non-linear interacting limit (Fock regime)

As was previously indicated in subsubsection (2.1.6.3), in the non-linear interacting limit, or Fock regime, the potential trap is dominated by the interaction energy and the tunnelling is suppressed. To investigate the non-linear behaviour of three condensates, a numerical solution for Eqs.(2.75) is obtained after considering the following initial conditions: non-zero imbalances $Z_1(0) = 0.2 \neq 0$, $Z_2(0) = 0.4 \neq 0$, zero relative phases $\Phi_{1,2}(0) = 0$ and a fixed short-range interaction strength $\Lambda \neq 0$. The resulting effects of the dynamics arising from reaching the long-range interactions critical values, i.e., Ξ_1^c and Ξ'_c , are studied independently.

Beginning with changing $\Xi_1 \propto \eta_{NN} - \eta_L$ and fixing $\Xi' \neq 0$, it is clear from Fig.(2.18, a) that both fractional population imbalances $Z_{1,2}(t)$ behave asymmetrically around a non-zero value with the same collective oscillation period. At this critical point, both imbalances exhibit the phenomenon of the macroscopic quantum self-trapping (MQST) in the triple-potential trap. However, it is worth noting that both imbalances at this value overlay with each other referring to a possible tunnelling among wells leading to a “non-pure” MQST phenomenon between the three condensates which is different from the double-well potential case. This overlaying can be explained as follows. When the overlapping occurs between both imbalances, this means that there is a point at time t where:

$$Z_1 = Z_2 \implies N_L - N_M = N_L - N_R \implies N_M = N_R,$$

which is a pretty good sign of tunnelling since the initial conditions of the atom numbers in these both wells at $t = 0$ are different. On the other hand, at the critical value $\Xi_1 \geq \Xi_1^c$, $\Phi_1(t)$ increases linearly toward the negative values of Φ_1 , whereas $\Phi_2(t)$ does not change with time. This can be readily understood as follows. Since Ξ_1 is proportional to the interaction between neighbouring atoms, i.e., between M and L or M and R , and the interaction between atoms located in the outermost wells remains unchanged as it composed of fixed interactions Λ and Ξ' , therefore, the only changing relative phase would be the one which depends on adjacent wells, i.e., $\Phi_1(t) = \theta_M - \theta_L$, and as the second relative phase $\Phi_2(t)$ depends on the phases of the outermost wells, $\Phi_2(t) = \theta_R - \theta_L$, then it remains unvaried with time.

Roughly similar dynamics occur when changing $\Xi' \propto \eta_L - \eta_{\text{NNN}}$ as Fig.(2.18, b) manifests. At $\Xi' \geq \Xi'_c$, a similar non-pure self-trapping behaviour between condensates appears as both imbalances $Z_{1,2}(t)$ have asymmetric oscillations with the same collective period and a sign of possible tunnelling between the three condensates due to the overlaying between both imbalances. The first relative phase $\Phi_1(t)$ does not vary with time and the second one $\Phi_2(t)$ increases linearly with time. This is because the long-range interaction Ξ' acts on atoms which are located in the outermost wells, then it is explainable that $\Phi_2(t)$ changes linearly as it depends on the phases of these wells, whereas $\Phi_1(t)$ remains with zero change over time.

Consequently, this critical behaviour depends on $\Xi_1 = \Xi_1^c(Z_{1,2}(0), \Phi_{1,2}(0))$ and $\Xi' = \Xi'_c(Z_{1,2}(0), \Phi_{1,2}(0))$ which are the critical values of the long-range interactions Ξ_1 and Ξ' , respectively. Both imbalances take periodic, regular and asymmetric oscillations with an obvious sign of possible tunnelling due to some overlaying between both imbalances. Additionally, according to the nature of the varied long-range interaction, i.e., whether it is nearest or next-nearest neighbour interaction, one of the relative phases increases linearly whereas the other one has no change with time.

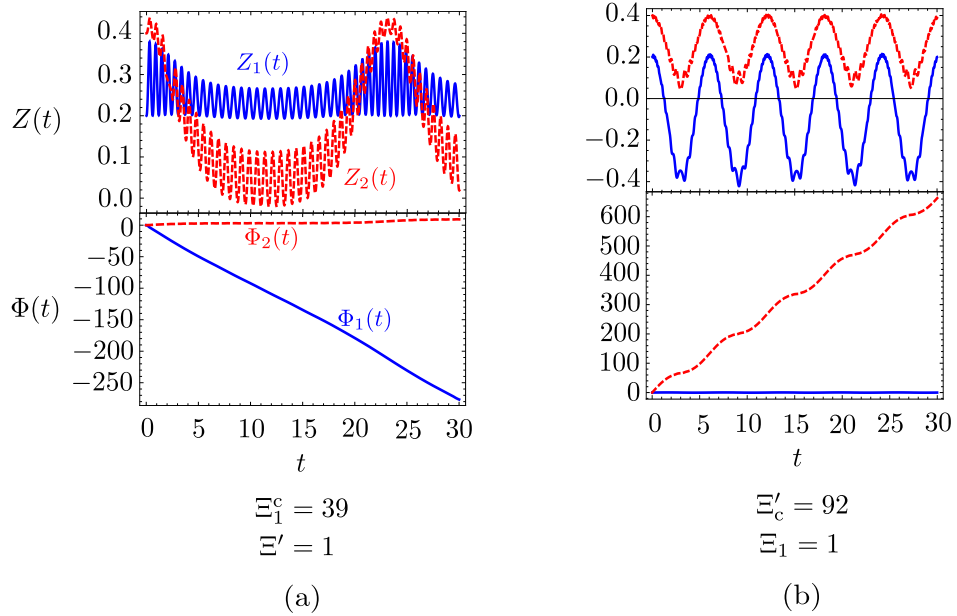


Figure 2.18.: Time evolution dynamics of the fractional population imbalances $Z_{1,2}(t)$ (up) and relative phases $\Phi_{1,2}(t)$ (down) as the long-range interactions Ξ_1 and Ξ' reach their critical strengths, i.e., $\Xi_1^{(c)}$ and $\Xi'_{(c)}$, in (a) and (b), respectively, bearing in mind that the initial conditions for the system are taken to be equal to $Z_1(0) = 0.2$, $Z_2(0) = 0.4$ and $\Phi_1(0) = \Phi_2(0) = 0$.

Apart from the non-sinusoidal oscillations and self-trapped effects, we find another novel phenomenon between the three trapped BECs. With some initial conditions ($Z_1(0), Z_2(0) \neq 0, \Phi_1(0) = \Phi_2(0) = 0$) and fixed interaction strengths $\Xi_1, \Lambda \neq 0$, the trajectory of the $Z_1 - \Phi_1$ phase-diagram is not closed for any value of Ξ' within the interval $0 < \Xi' < \Xi'_c$ as Fig.(2.19) illustrates. As was perviously shown in Fig.(2.15, c), in case of zero interaction, i.e., $\Lambda = \Xi_1 = \Xi' = 0$, the trajectory of $Z_1 - \Phi_1$ phase-diagram is closed indicating that the system is in a stable equilibrium state. However, when the interactions are switched on, this trajectory becomes opened where the system enters the unstable equilibrium state. When Ξ' reaches its critical value, i.e., $\Xi' \geq \Xi'_c$, the phase-diagram's constant energy curve is closed again which shows that the system returns to its stable equilibrium state. These phase trajectories exhibit transition from closed in the non-interacting limit, to open when Ξ' is at any value above zero and below the critical value, to closed trajectories once more at the critical value or above. Only a special value of Ξ' can make $Z_1 - \Phi_1$ phase-diagram closed. This property can be used to determine the value of Ξ' in experiments [100]. On the other hand, we have seen as Fig(2.15, d) showed that $Z_2 - \Phi_2$ phase diagram has a closed trajectory for the non-interacting case. This trajectory becomes open too but with no change in $Z_2(t)$ as a function of $\Phi_2(t)$ when the interactions are switched on as shown in Fig(2.20), and this behaviour keeps occurring even when Ξ' reaches its critical value. It is noteworthy to point out that the phase diagrams $Z_{1,2} - \Phi_{1,2}$ when Ξ_1 is switched on with a fixed Ξ' and Λ :

1. have open trajectories at all times.
2. both imbalances $Z_{1,2}(t)$ have no change as a function of $\Phi_{1,2}(t)$ no matter how we vary the strength of Ξ_1 .

Specifically speaking, solving numerically Eqs.(2.74) shows the time-evolution of the atom numbers $N_{L,R,M}(t)$ and the relative phases $\Phi_{1,2}(t)$ for each condensate. Fig.(2.21) displays the MQST phenomenon at specific critical values for each long-range interactions where they are taken under zero initial values for both relative phases $\Phi_{1,2}(0) = 0$ and two different initial conditions for the atom numbers: $N_L(0), N_M(0) = 1, N_R(0) = 16$ as it shown in Fig.(2.21, a), and $N_L(0), N_R(0) =$

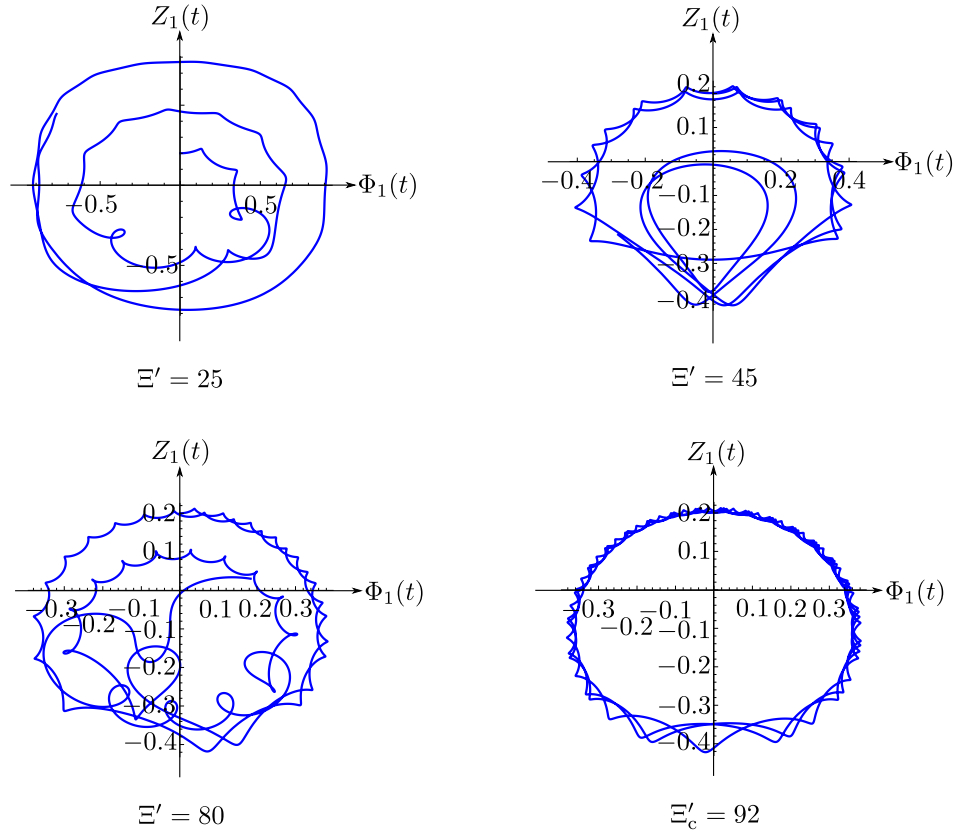


Figure 2.19.: $Z_1 - \Phi_1$ phase-diagram for increasing long-range interaction Ξ' strengths.

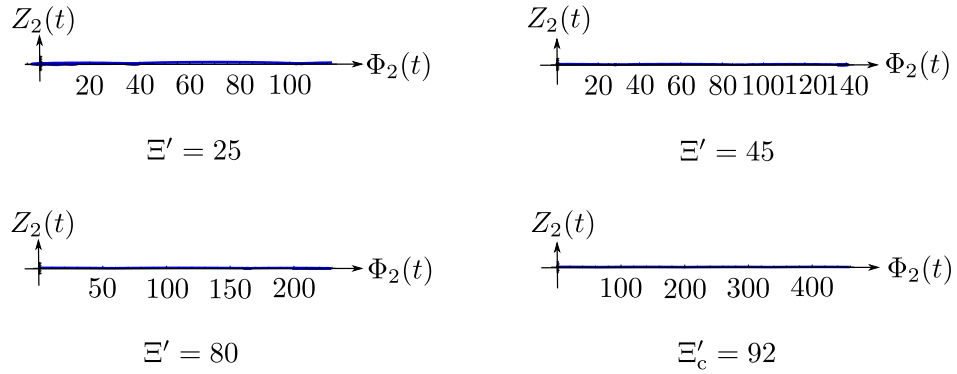


Figure 2.20.: $Z_2 - \Phi_2$ phase-diagram for increasing long-range interaction Ξ' strengths.

1, $N_M(0) = 16$ as in Fig.(2.21, b). Interestingly, and proving the above discussion, in the strong interaction regime, the population of the atoms in both cases does not exhibit a complete MQST phenomenon when the long-range interactions reach their critical values $\Xi_1, \Xi' = \Xi_1^c, \Xi'_c$, respectively. There are a few atoms tunnel from the wells in which the atoms were initially located toward the neighbouring two wells,

whereas, the rest of the atoms remain trapped in their initial wells. However, both or one of the relative phases change linearly when the long-range interactions reach their critical strengths. What is striking, though, is that when the atom numbers are $N_L(0), N_R(0) = 1, N_M(0) = 16$, no matter how Ξ' is increased, the system does not reach the MQST state where the time-evolution of the atom numbers and the relative phases remain unaffected as if there is no increasing Ξ' , as Fig(2.21, b, 3) illustrates.

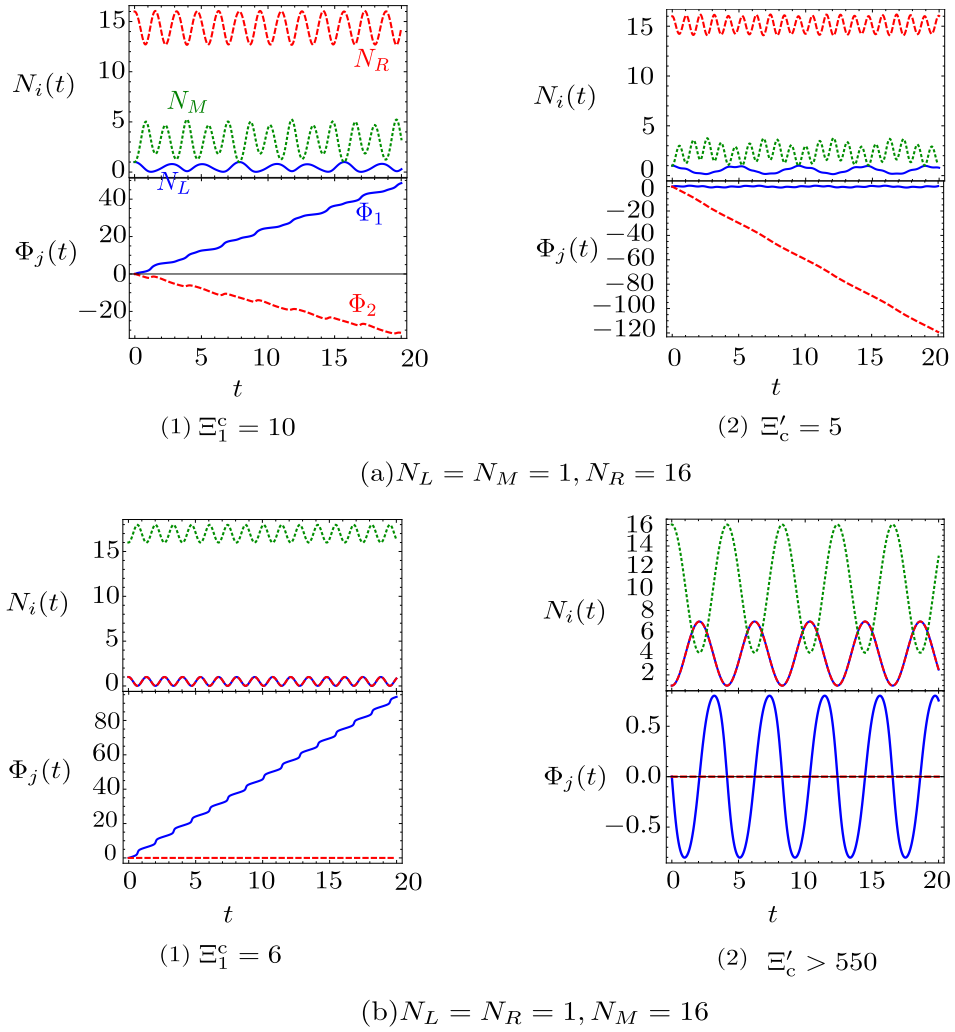


Figure 2.21.: Atom number $N_{L,R,M}(t)$ and relative phases $\Phi_{1,2}(t)$ time-evolution at critical strengths for long-range interactions Ξ_1^c and Ξ'_c where $N_T^{\text{tw}} = 18$ and under zero initial relative phases $\Phi_{1,2}(0) = 0$ and two different initial atom number conditions: (a) $N_L(0), N_M(0) = 1, N_R(0) = 16$, (b) $N_L(0), N_R(0) = 1, N_M(0) = 16$.

Summarizing to this section, this analysis studied the properties of N_T^{tw} Rydberg-

dressed atoms loaded into a quasi one-dimensional triple-well potential. It has been demonstrated from using the numerical solutions of the non-local Gross-Pitaevskii equation via the three-mode approximation that adjusting the interaction can give rise to richer behaviour. The results indicate that the feature of the tunnelling strongly depends on the initial conditions of the fractional population imbalances (or the atom numbers) and the relative phases, in addition to the long-range interactions strengths. In the Rabi regime, the atoms oscillate back and forth independently with a Rabi-like frequency $\omega_{\text{Ra}}^{\text{tw}}$ resembling a Λ -type three level atom in two coherent fields with zero detunings. In the Josephson regime, the solutions of the linearised differential equations show harmonic, periodic and symmetric oscillations for $Z_2(t)$ and $\Phi_2(t)$. Whereas for $Z_1(t)$ and $\Phi_1(t)$, the oscillations change according to the nature of the applied long range interaction. However, in the Fock regime, when one of the long-range interaction strengths Ξ_1, Ξ' goes beyond a certain critical value, the macroscopic quantum self-trapping occurs once more, similarly to the double-well case, where the self-trapping is achievable just by tuning the interaction strength. That being said, the self-trapping behaviour is non-pure in the triple-well potential where a sign of tunnelling between atoms among the condensates appears both in the time-evolution of the fractional imbalances and the atom numbers, leading to a state where some of the atoms are trapped and the other can tunnel between two adjacent wells. Another interesting feature, the Z_1 - Φ_1 phase-diagrams are not closed in general cases, but for some special conditions, i.e., when $\Xi' = 0$ or $\Xi' \geq \Xi'_c$, the phase diagrams are closed which can be used to determine the interaction parameter between atoms of BEC in experiments [100].

2.3. Quadruple-well potential

An interesting extension to our study would be a similar analysis in a higher dimensional setting: this would refer to N_T^{qw} interacting Rydberg-dressed atoms confined in a quadruple-well potential trap. It is expected that any generalisation to this study would increase the difficulty significantly. The reward is that more complex non-linearity and the more parameters in the basic equations would bring richer dynamics into the model [100]. The two-dimensional quadruple-well configuration

can be created, according to Ref [101], as the combination of an isotropic parabolic magnetic trap, or a similar optical dipole trap, and a cosinusoidal two-dimensional optical lattice in Bose-Einstein condensates, in a wide range of parameters (the trapping frequency and lattice strength). In our study we consider a symmetric set of four wells; two double-well potentials each of which lies along two different axes. Therefore, based on Eq.(2.8) we write the quadruple-well potential trap as

$$V_{\text{qw}}(x, y) = \alpha_x + \alpha_y - (\beta_x x^2 + \beta_y y^2) + (\gamma_x x^4 + \gamma_y y^4).$$

As our study is restricted to four symmetric wells, then $\alpha_x = \alpha_y$, $\beta_x = \beta_y$ and $\gamma_x = \gamma_y$ and as a result, the two-dimensional quadruple-well potential as shown in Fig.(2.22) becomes

$$V_{\text{qw}}(x, y) = 2\alpha - \beta(x^2 + y^2) + \gamma(x^4 + y^4). \quad (2.79)$$

It is worth mentioning that this expression produces a quadruple-well potential with four minima $(\pm x_{\min}, \pm y_{\min}) = (\pm \sqrt{\frac{\beta}{2\gamma}}, \pm \sqrt{\frac{\beta}{2\gamma}})$ if $\beta, \gamma > 0$.

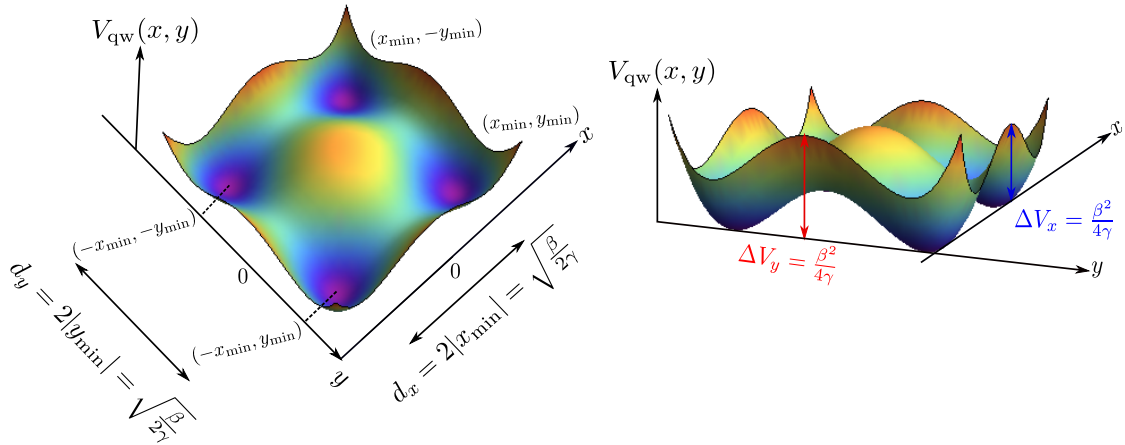


Figure 2.22.: Quadruple-well potential with its minima $(\pm x_{\min}, \pm y_{\min})$, well separations d_x, d_y and the potential barriers $\Delta V_x, \Delta V_y$.

2.3.1. Mean-field description of four BECs in a quadruple-well potential

We consider N_T^{qw} interacting Rydberg-dressed bosonic atoms trapped in a symmetric quadruple-well potential. The dynamical properties of this system are governed by the two-dimensional non-linear Gross-Pitaevskii equation which is expressed as

$$i\hbar \frac{\partial \Psi(x, y, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(x, y, t) + [V_{\text{qw}}(x, y) + g_{2D} |\Psi(x, y, t)|^2 + \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dy' |\Psi(x', y', t)|^2 V_{\text{SC}}(x, y, x', y')] \Psi(x, y, t), \quad (2.80)$$

where $V_{\text{SC}}(x, y, x', y') = \frac{\zeta R_{\text{SC}}^6}{|(x-x')+(y-y')|^6 + R_{\text{SC}}^6}$ and g_{2D} are the two-dimensional soft-core potential and coupling constant for the contact-interaction, respectively. Similarly to the double-well potential trap, if the energy difference between the first two single atom mean field states -in both axes- is much smaller than the difference to all energetically higher lying states, then the system is reduced to four mean field orbitals in which the atoms are located, and this is the *four-mode approximation*, where the condensate wave function reads

$$\Psi(x, y, t) = \psi_0(t)\phi_0(x, y) + \psi_1(t)\phi_1(x, y) + \psi_2(t)\phi_2(x, y) + \psi_3(t)\phi_3(x, y), \quad (2.81)$$

where: $\psi_i(t)$ are the time-dependent amplitudes and $\phi_i(x, y)$ are the on-site wave functions of the i th site with two nearest and one next-nearest neighbours where $i = 0, 1, 2, 3$ as Fig(2.23) shows, and they are taken as two-dimensional Gaussian wave functions:

$$\begin{aligned} \phi_i(x, y) &= \left(\frac{1}{\xi_x^2 \pi} \right)^{\frac{1}{4}} \left(\frac{1}{\xi_y^2 \pi} \right)^{\frac{1}{4}} \exp \left[- \left(\frac{(x \pm x_{\min})^2}{2\xi_x^2} + \frac{(y \pm y_{\min})^2}{2\xi_y^2} \right) \right] \\ &= \left(\frac{1}{\xi^2 \pi} \right)^{\frac{1}{2}} \exp \left[- \frac{(x \pm x_{\min})^2 + (y \pm y_{\min})^2}{2\xi^2} \right], \quad \text{As : } \xi_x = \xi_y = \xi = \sqrt{\frac{\hbar}{m\omega}}. \end{aligned}$$

We consider the same limitation as before where ξ is small enough with respect to

the distance between two neighbouring wells d , so that the sites are well defined.

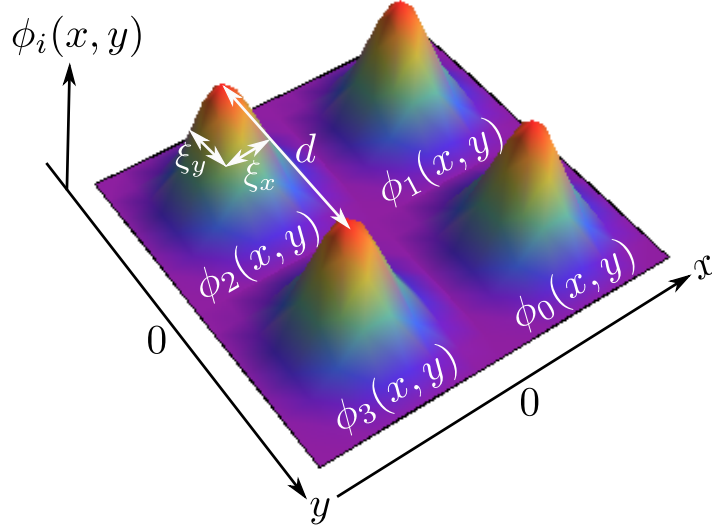


Figure 2.23.: Four localised Gaussian wave functions in the quadruple-well potential $\phi_i(x, y) = \phi_{0,1,2,3}(x, y)$ where $\xi_x = \xi_y = \xi$ is their width and d is the separation between two neighbouring wells.

2.3.1.1. Differential equations of the time-dependent amplitudes

Four differential equations of the time-dependant amplitudes are obtained by inserting the approximated wave function in Eq.(2.81) into the two-dimensional GP equation in Eq.(2.80) and then project it onto the single well states $\phi_0(x, y)$, $\phi_1(x, y)$, $\phi_2(x, y)$ and $\phi_3(x, y)$ as was implemented in the previous sections¹³. As a result we write them as following

$$i\hbar \frac{\partial \psi_0(t)}{\partial t} = [E_0 + U_0 N_0 + \eta_{0,0} N_0 + \eta_{0,1} N_1 + \eta_{0,2} N_2 + \eta_{0,3} N_3] \psi_0(t) - J_{0 \leftrightarrow 1} \psi_1(t) - J_{0 \leftrightarrow 2} \psi_2(t) - J_{0 \leftrightarrow 3} \psi_3(t) \quad (2.82a)$$

$$i\hbar \frac{\partial \psi_1(t)}{\partial t} = [E_1 + U_1 N_1 + \eta_{1,1} N_1 + \eta_{1,0} N_0 + \eta_{1,2} N_2 + \eta_{1,3} N_3] \psi_1(t) - J_{1 \leftrightarrow 2} \psi_2(t) - J_{1 \leftrightarrow 3} \psi_3(t) - J_{1 \leftrightarrow 0} \psi_0(t) \quad (2.82b)$$

$$i\hbar \frac{\partial \psi_2(t)}{\partial t} = [E_2 + U_2 N_2 + \eta_{2,2} N_2 + \eta_{2,0} N_0 + \eta_{2,1} N_1 + \eta_{2,3} N_3] \psi_2(t)$$

¹³Bearing in mind that the normalisation condition is $\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \phi_i(x, y) \phi_i(x, y) dx dy \approx 1$ and the orthogonal condition is $\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \phi_i(x, y) \phi_j(x, y) dx dy \approx 0$ with $i \neq j$.

$$- J_{2\leftrightarrow 1}\psi_1(t) - J_{2\leftrightarrow 3}\psi_3(t) - J_{2\leftrightarrow 0}\psi_0(t) \quad (2.82c)$$

$$\begin{aligned} i\hbar \frac{\partial \psi_3(t)}{\partial t} = & [E_3 + U_3 N_3 + \eta_{3,3} N_3 + \eta_{3,0} N_0 + \eta_{3,1} N_1 + \eta_{3,2} N_2] \psi_3(t) \\ & - J_{3\leftrightarrow 2}\psi_2(t) - J_{3\leftrightarrow 1}\psi_1(t) - J_{3\leftrightarrow 0}\psi_0(t), \end{aligned} \quad (2.82d)$$

where we have denoted that

$$\begin{aligned} E_i &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dxdy \left[\frac{\hbar^2}{2m} |\nabla \phi_i(x, y)|^2 + V_{\text{qw}}(x, y) |\phi_i(x, y)|^2 \right] \\ J_{i\leftrightarrow j} &= - \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dxdy \left[\frac{\hbar^2}{2m} \nabla \phi_i(x, y) \nabla \phi_j(x, y) + V_{\text{qw}}(x, y) \phi_i(x, y) \phi_j(x, y) \right] \quad i \neq j \\ U_i &= g_{2D} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dxdy |\phi_i(x, y)|^4 \\ N_i &= |\psi_i(t)|^2, \end{aligned}$$

where $i, j = 0, 1, 2, 3$. Additionally, the non-negligible matrix elements¹⁴ resulting from the long-range interaction can be summarized as

$$\eta_{i,j} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dxdydx'dy' V_{\text{SC}}(x, y, x', y') |\phi_i(x, y)|^2 |\phi_j(x', y')|^2. \quad (2.83)$$

Fig(2.24) displays the non-negligible matrix elements $\eta_{i,j}/\zeta$ as a function of an increasing soft-core radius R_{SC} . When $i = j$ then Eq.(2.83) refers to a local (on-site) interaction regime, i.e., for small R_{SC} , and therefore the integrals in the blue solid line $\eta_{i,i}/\zeta$ are the dominant terms. However, when $i \neq j$ there are two distinct regimes; the nearest neighbour interaction regime $\eta_{i,j}/\zeta$, i.e., for relatively large R_{SC} as the dashed red and dotted green lines show (since there are two nearest neighbours for each well) and they become non-trivial comparing to $\eta_{i,i}/\zeta$. Also, there is the next-nearest neighbour interaction regime, i.e., for very large values of R_{SC} as the dot-dashed magenta line illustrates where all integrals turn to be roughly on the same magnitude.

¹⁴There are 40 matrix elements "for each site", 4 of them are significantly important and the rest 36 contribute insignificantly with respect to the soft-core interaction radius R_{SC} .

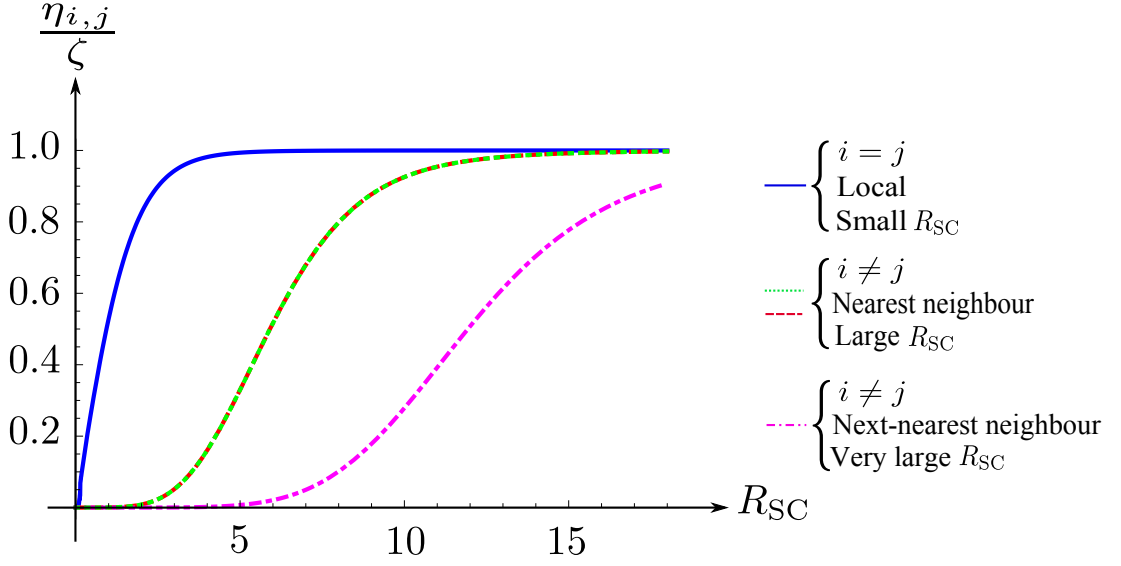


Figure 2.24.: The matrix elements $\eta_{i,j}/\zeta$ with $i, j = 0, 1, 2, 3$ for the quadruple-well potential trap as a function of the soft-core interaction radius R_{SC} . when $i = j$ the integrals represents the local behaviour of the interaction (the solid blue line). when $i \neq j$ two interactions are being significant, nearest neighbour (the dashed red and the dotted green lines), and the next-nearest neighbour (the dotted-dashed magenta line).

2.3.1.2. Tunnelling dynamics

At this time, the quantum dynamics of the four condensates are described in terms of six canonical variables, three fractional population imbalances $Z_1(t) = (N_2 - N_1)/N_T^{\text{qw}}$, $Z_2(t) = (N_2 - N_3)/N_T^{\text{qw}}$ and $Z_3(t) = (N_2 - N_0)/N_T^{\text{qw}}$, in addition to three relative phases $\Phi_1 = \theta_2 - \theta_1$, $\Phi_2 = \theta_2 - \theta_3$ and $\Phi_3 = \theta_2 - \theta_0$. Similarly to previous sections, the differential equations of these variables are analytically derived. Assuming that $J_{2\leftrightarrow 3} = J_{3\leftrightarrow 2} = J_i$, $J_{1\leftrightarrow 2} = J_{2\leftrightarrow 1} = J_j$, $J_{0\leftrightarrow 2} = J_{2\leftrightarrow 0} = J_k$, $J_{3\leftrightarrow 1} = J_{1\leftrightarrow 3} = J_l$, $J_{3\leftrightarrow 0} = J_{0\leftrightarrow 3} = J_m$ and $J_{0\leftrightarrow 1} = J_{1\leftrightarrow 0} = J_n$, then, to simplify the problem, and as the on-site wave functions are assumed to be localised, we consider the tunnelling amplitudes between each two nearest neighbouring wells are equal, i.e., $J_i \approx J_j \approx J_m \approx J_n$, whereas the tunnelling amplitudes between two next-nearest neighbouring wells are insignificant, i.e., $J_k \approx J_l \approx 0$. Additionally, as the potential trap setup is taken to be composed of four symmetric wells, hence it is legit to introduce the following interaction parameters

$$\Lambda = \frac{UN_T^{\text{qw}}}{2J_i}$$

$$\left. \begin{array}{l} \eta_{0,0} = \eta_{1,1} = \eta_{2,2} = \eta_{3,3} = \eta_L \\ \eta_{0,1} = \eta_{1,2} = \eta_{2,3} = \eta_{3,0} \\ \eta_{1,0} = \eta_{2,1} = \eta_{3,2} = \eta_{0,3} \\ \eta_{1,3} = \eta_{0,2} = \eta_{\text{NNN}} \end{array} \right\} = \eta_{\text{NN}} \left\{ \begin{array}{l} \Xi = \frac{(\eta_L - \eta_{\text{NNN}})}{2J_i} N_T^{\text{qw}} \\ \Xi' = \frac{(\eta_{\text{NNN}} - \eta_{\text{NN}})}{2J_i} N_T^{\text{qw}} \\ \Xi'' = \frac{(\eta_L - \eta_{\text{NN}})}{2J_i} N_T^{\text{qw}}. \end{array} \right. \rightarrow$$

Based on the above assumptions, a simple relation $\Xi'' = \Xi + \Xi'$ allows us to keep only Ξ and Ξ' in the dynamical differential equations. Considering all of the above simplifications, the differential equations for atom numbers are given by

$$\begin{aligned} \frac{\partial N_0(t)}{\partial t} &= \sqrt{N_0 N_3} \sin(\Phi_2 - \Phi_3) - \sqrt{N_0 N_1} \sin(\Phi_3 - \Phi_1) \\ \frac{\partial N_1(t)}{\partial t} &= -\sqrt{N_1 N_2} \sin \Phi_1 + \sqrt{N_1 N_0} \sin(\Phi_3 - \Phi_1) \\ \frac{\partial N_2(t)}{\partial t} &= \sqrt{N_2 N_3} \sin \Phi_2 + \sqrt{N_2 N_1} \sin \Phi_1 \\ \frac{\partial N_3(t)}{\partial t} &= -\sqrt{N_3 N_2} \sin \Phi_2 - \sqrt{N_3 N_0} \sin(\Phi_2 - \Phi_3) \end{aligned} \quad (2.84)$$

and the differential equations of the relative phases as a function of atom numbers

$$\begin{aligned} \frac{\partial \Phi_1(t)}{\partial t} &= (\Xi + \Xi' + \Lambda) \frac{N_3 - N_2}{N_T^{\text{qw}}} + \Xi' \frac{N_1 - N_0}{N_T^{\text{qw}}} + \frac{N_3 - N_2}{2\sqrt{N_3 N_2}} \cos \Phi_2 + \frac{1}{2} \sqrt{\frac{N_1}{N_2}} \cos \Phi_1 \\ &\quad - \frac{1}{2} \sqrt{\frac{N_0}{N_3}} \cos(\Phi_2 - \Phi_3) \\ \frac{\partial \Phi_2(t)}{\partial t} &= (\Xi + \Xi' + \Lambda) \frac{N_1 - N_2}{N_T^{\text{qw}}} + \Xi' \frac{N_3 - N_0}{N_T^{\text{qw}}} + \frac{N_1 - N_2}{2\sqrt{N_1 N_2}} \cos \Phi_1 + \frac{1}{2} \sqrt{\frac{N_3}{N_2}} \cos \Phi_2 \\ &\quad - \frac{1}{2} \sqrt{\frac{N_0}{N_1}} \cos(\Phi_3 - \Phi_1) \\ \frac{\partial \Phi_3(t)}{\partial t} &= (\Xi + \Lambda) \frac{N_0 - N_2}{N_T^{\text{qw}}} + \frac{1}{2} \sqrt{\frac{N_3}{N_2}} \cos \Phi_2 + \frac{1}{2} \sqrt{\frac{N_1}{N_2}} \cos \Phi_1 - \frac{1}{2} \sqrt{\frac{N_3}{N_0}} \cos(\Phi_2 - \Phi_3) \\ &\quad - \frac{1}{2} \sqrt{\frac{N_1}{N_0}} \cos(\Phi_3 - \Phi_1). \end{aligned} \quad (2.85)$$

However, the fractional population imbalances are formulated as

$$\begin{aligned} \frac{\partial Z_1(t)}{\partial t} = & \frac{1}{2} \sqrt{(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)} \sin \Phi_1 \\ & + \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) + Z_3(t) + 1)(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)} \sin \Phi_2 \\ & - \frac{1}{4} \sqrt{(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)(Z_1(t) + Z_2(t) - 3Z_3(t) + 1)} \sin (\Phi_3 - \Phi_1) \end{aligned} \quad (2.86)$$

$$\begin{aligned} \frac{\partial Z_2(t)}{\partial t} = & \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) + Z_3(t) + 1)(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)} \sin \Phi_1 \\ & + \frac{1}{2} \sqrt{(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)} \sin \Phi_2 \\ & + \frac{1}{4} \sqrt{(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)(Z_1(t) + Z_2(t) - 3Z_3(t) + 1)} \sin (\Phi_2 - \Phi_3) \end{aligned} \quad (2.87)$$

$$\begin{aligned} \frac{\partial Z_3(t)}{\partial t} = & \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) + Z_3(t) + 1)(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)} \sin \Phi_1 \\ & + \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) + Z_3(t) + 1)(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)} \sin \Phi_2 \\ & - \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) - 3Z_3(t) + 1)(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)} \sin (\Phi_2 - \Phi_3) \\ & + \frac{1}{4} \sqrt{(Z_1(t) + Z_2(t) - 3Z_3(t) + 1)(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)} \sin (\Phi_3 - \Phi_1), \end{aligned} \quad (2.88)$$

and the three differential equations of the relative phases as a function of imbalances are

$$\begin{aligned}
\frac{\partial \Phi_1(t)}{\partial t} = & -(\Xi + \Xi' + \Lambda) Z_2(t) + \Xi' (Z_3(t) - Z_1(t)) \\
& + \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_1 \\
& - \frac{2Z_2(t)}{\sqrt{(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)}} \cos \Phi_2 \\
& - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}} \cos (\Phi_2 - \Phi_3)
\end{aligned} \tag{2.89}$$

$$\begin{aligned}
\frac{\partial \Phi_2(t)}{\partial t} = & -(\Xi + \Xi' + \Lambda) Z_1(t) + \Xi' (Z_3(t) - Z_2(t)) \\
& + \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_2 \\
& - \frac{2Z_1(t)}{\sqrt{(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)}} \cos \Phi_1 \\
& - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}} \cos (\Phi_3 - \Phi_1)
\end{aligned} \tag{2.90}$$

$$\begin{aligned}
\frac{\partial \Phi_3(t)}{\partial t} = & -(\Xi + \Lambda) Z_3(t) + \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_2 \\
& + \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_1 \\
& - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}} \cos (\Phi_2 - \Phi_3) \\
& - \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}} \cos (\Phi_3 - \Phi_1).
\end{aligned} \tag{2.91}$$

In the following, we focus on these simplified differential equations, i.e., Eq.(2.84, 2.85) and Eq.(2.86, 2.87, 2.88, 2.89, 2.90, 2.91) to study the behaviour of N_T^{qw} atoms trapped in a symmetric two-dimensional quadruple-well potential trap in different dynamical regimes.

2.3.2. Dynamical regimes

Here, we investigate the quantum dynamical behaviour of an ensemble of N_T^{qw} interacting bosonic Rydberg-dressed atoms confined in the two-dimensional quadruple-well potential within three dynamical regimes; Rabi, Josephson and Fock, where we consider the case of non-zero initial populations $N_{0,1,2,3}(0) \neq 0$ and zero initial relative phases $\Phi_{1,2,3}(0) = 0$.

2.3.2.1. Non-interacting limit (Rabi regime)

Without considering the interactions, i.e., $\Lambda \rightarrow 0$ and $\Xi = \Xi' \rightarrow 0$, the time-dependant amplitudes in Eqs.(2.82) resemble the time-dependent amplitudes for the four-level atom which is coupled to four coherent fields. Therefore, and similarly to previous studies, one can say that in the absence of interactions, the trapped atoms oscillate inside the quadruple-well potential with a Rabi-like frequency which is equivalent to $\omega_{\text{Ra}}^{\text{qw}} = 2J_{i,j,m,n}/\hbar = 2J/\hbar$, as the tunnelling amplitudes between neighbouring wells are assumed to be identical. Consequently, the dynamical equations of the relative phases in Eqs.(2.85) are reduced to

$$\frac{\partial \Phi_1(t)}{\partial t} = \frac{N_3 - N_2}{2\sqrt{N_3 N_2}} \cos \Phi_2 + \frac{1}{2} \sqrt{\frac{N_1}{N_2}} \cos \Phi_1 - \frac{1}{2} \sqrt{\frac{N_0}{N_3}} \cos (\Phi_2 - \Phi_3) \quad (2.92a)$$

$$\frac{\partial \Phi_2(t)}{\partial t} = \frac{N_1 - N_2}{2\sqrt{N_1 N_2}} \cos \Phi_1 + \frac{1}{2} \sqrt{\frac{N_3}{N_2}} \cos \Phi_2 - \frac{1}{2} \sqrt{\frac{N_0}{N_1}} \cos (\Phi_3 - \Phi_1) \quad (2.92b)$$

$$\frac{\partial \Phi_3(t)}{\partial t} = \frac{1}{2} \sqrt{\frac{N_3}{N_2}} \cos \Phi_2 + \frac{1}{2} \sqrt{\frac{N_1}{N_2}} \cos \Phi_1 - \frac{1}{2} \sqrt{\frac{N_3}{N_0}} \cos (\Phi_2 - \Phi_3) - \frac{1}{2} \sqrt{\frac{N_1}{N_0}} \cos (\Phi_3 - \Phi_1). \quad (2.92c)$$

Similarly for Eqs.(2.89, 2.90, 2.91) we get

$$\begin{aligned} \frac{\partial \Phi_1(t)}{\partial t} = & \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_1 \\ & - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}} \cos (\Phi_2 - \Phi_3) \end{aligned}$$

$$- \frac{2Z_2(t)}{\sqrt{(Z_1(t) + Z_3(t) - 3Z_2(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)}} \cos \Phi_2 \quad (2.93a)$$

$$\begin{aligned} \frac{\partial \Phi_2(t)}{\partial t} = & \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_2 \\ & - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}} \cos(\Phi_3 - \Phi_1) \\ & - \frac{2Z_1(t)}{\sqrt{(Z_2(t) + Z_3(t) - 3Z_1(t) + 1)(Z_1(t) + Z_2(t) + Z_3(t) + 1)}} \cos \Phi_1 \quad (2.93b) \\ \frac{\partial \Phi_3(t)}{\partial t} = & \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_2 + \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) + Z_3(t) + 1}} \cos \Phi_1 \\ & - \frac{1}{2} \sqrt{\frac{Z_1(t) + Z_3(t) - 3Z_2(t) + 1}{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}} \cos(\Phi_2 - \Phi_3) \\ & - \frac{1}{2} \sqrt{\frac{Z_2(t) + Z_3(t) - 3Z_1(t) + 1}{Z_1(t) + Z_2(t) - 3Z_3(t) + 1}} \cos(\Phi_3 - \Phi_1). \quad (2.93c) \end{aligned}$$

The dynamical behaviour for the four condensates is investigated by solving numerically the differential equations in Eqs.(2.84, 2.92) or in Eqs.(2.86, 2.87, 2.88, 2.93). Plotting the fractional population imbalances $Z_{1,2,3}(t)$ and relative phases $\Phi_{1,2,3}(t)$ as a function of dimensionless time $t \rightarrow 2Jt/\hbar$ for certain initial conditions, as seen in Fig(2.25, a, b), respectively, shows that all imbalances and relative phases oscillate symmetrically around a zero value, which is analogous to the double-well potential case. The phase diagrams for the six canonical conjugates are illustrated in Fig(2.25, c, d, e), where they show a similar behaviour to the triple-well potential since their trajectories are all closed.

Specifically speaking, the time-evolution of the atom numbers in each well are also investigated via solving the differential equations in Eqs.(2.84, 2.92) as Fig(2.26) shows, where two distinct initial conditions for the atom number have been taken. When $N_0(0) = 17, N_1(0) = N_2(0) = N_3(0) = 1$, Fig(2.26, a) illustrates the behaviour of the atom number as they oscillate back and forth starting from the well 0 then to both wells of 1 and 3, and finally to well 2, and vice versa. However, all the relative phases $\Phi_{1,2,3}(t)$, as seen in Fig(2.26, b), oscillate symmetrically around a zero value. Furthermore, if the initial conditions for the atom number are taken as

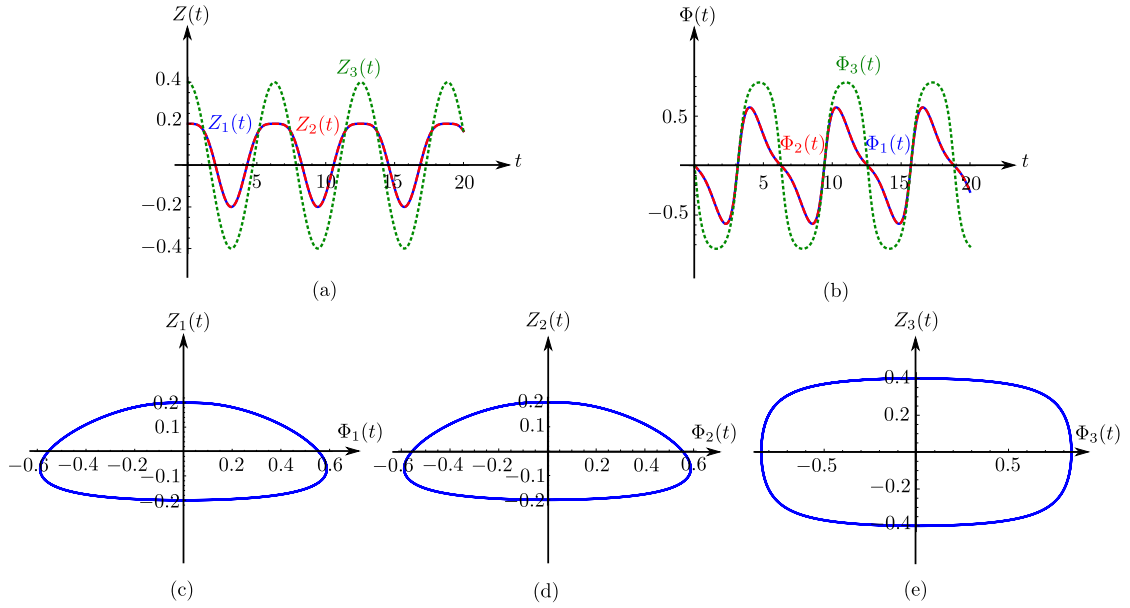


Figure 2.25.: The time evolution of the three fractional population imbalances $Z_{1,2,3}(t)$ in (a) and three relative phases $\Phi_{1,2,3}(t)$ in (b). The $Z_{1,2,3} - \Phi_{1,2,3}$ phase diagrams are shown in (c),(d) and (e), respectively. The initial conditions are taken to be equal for the imbalances to $Z_1(0) = Z_2(0) = 0.2, Z_3(0) = 0.4$ and for the relative phases $\Phi_{1,2,3}(0) = 0$.

$N_0(0) = 2, N_1(0) = N_2(0) = N_3(0) = 6$, it can be noticed from Fig(2.26, c) the same back-and-forth behaviour but this time it starts from well 2 to both 1 and 3 and ends at 0, and vice versa. Similar behaviour for the relative phases as it is shown in Fig(2.26, d).

2.3.2.2. Linear-interacting limit (Josephson regime)

The Josephson oscillations for N_T^{qw} atoms in a quadruple-well potential when their fluctuations are reduced can be observed by, similarly to previous, linearising our differential equations, expressed in Eqs.(2.86, 2.87, 2.88, 2.89, 2.90, 2.91) by applying the Taylor expansion on both the fractional population imbalances $Z_{1,2,3}(t)$ and relative phases $\Phi_{1,2,3}(t)$ where we obtain

$$\frac{dZ_1(t)}{dt} \approx \frac{3}{4}\Phi_1(t) + \frac{1}{4}\Phi_2(t) - \frac{1}{4}\Phi_3(t) \quad (2.94a)$$

$$\frac{dZ_2(t)}{dt} \approx \frac{1}{4}\Phi_1(t) + \frac{3}{4}\Phi_2(t) - \frac{1}{4}\Phi_3(t) \quad (2.94b)$$

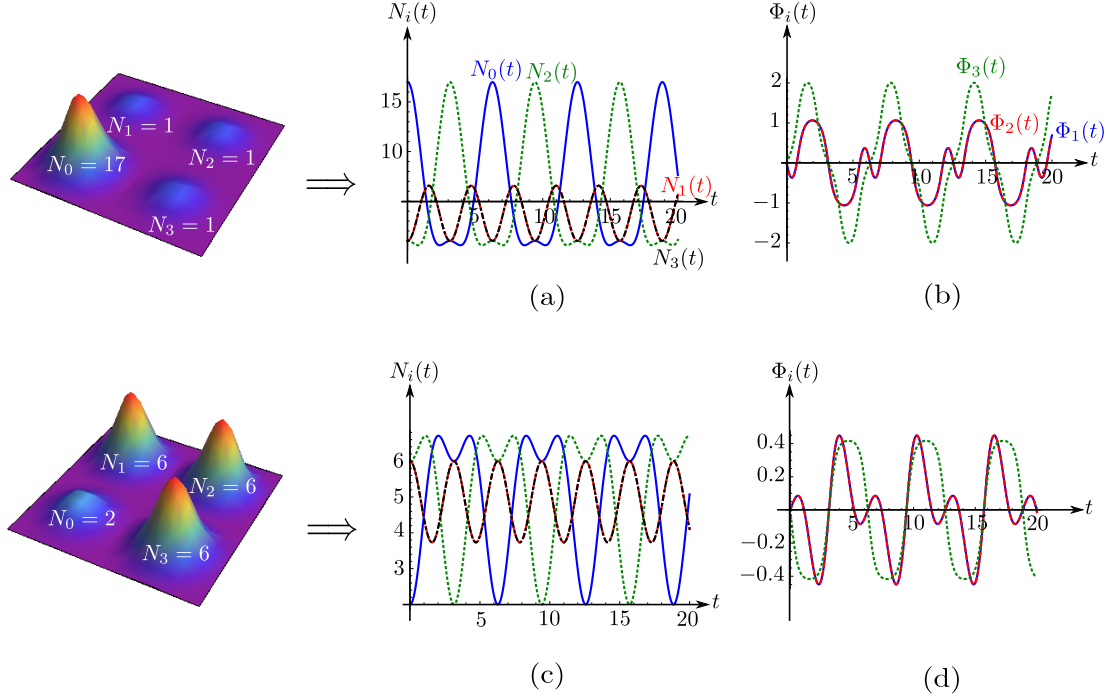


Figure 2.26.: The time evolution of the four atom numbers that correspond to the four condensates in each well in the quadruple-well potential, i.e., $N_i(t)$, in addition to the relative phases $\Phi_i(t)$, with $i = 0, 1, 2, 3$. (a) and (b) represent the initial conditions of $N_0(0) = 17, N_1(0) = N_2(0) = N_3(0) = 1$ and $\Phi_{1,2,3}(0) = 0$. However, (c) and (d) the initial conditions have been taken to be equal to $N_0(0) = 2, N_1(0) = N_2(0) = N_3(0) = 6$ and $\Phi_{1,2,3}(0) = 0$.

$$\frac{dZ_3(t)}{dt} \approx \frac{1}{2} \Phi_3(t) \quad (2.94c)$$

$$\frac{d\Phi_1(t)}{dt} \approx -(\Xi' + 1) Z_1(t) - (\Lambda + \Xi + \Xi' + 3) Z_2(t) + (\Xi' + 1) Z_3(t) \quad (2.94d)$$

$$\frac{d\Phi_2(t)}{dt} \approx -(\Lambda + \Xi + \Xi' + 3) Z_1(t) - (\Xi' + 1) Z_2(t) + (\Xi' + 1) Z_3(t) \quad (2.94e)$$

$$\frac{d\Phi_3(t)}{dt} \approx -(\Lambda + \Xi + 2) Z_3(t). \quad (2.94f)$$

A numerical solution for these linear differential equations is illustrated in Fig(2.27). When increasing $\Xi \propto \eta_L - \eta_{\text{NNN}}$ and fixing both Ξ' and Λ , Fig(2.27, a, b, c) show a similar behaviour to the double-well potential case where the period of the fractional population imbalances oscillations is decreased when increasing the next-nearest long-range interaction strength. Additionally, the relative phases, analogous the

double-well potential case too, not only their oscillations get faster with increasing Ξ , but also their amplitudes are slightly increased. Interestingly, $\Xi' \propto \eta_{\text{NNN}} - \eta_{\text{NN}}$ has no role in the linear dynamics in the quadruple-well potential since the oscillation period of all the fractional population imbalances $Z_{1,2,3}(t)$ and relative phases $\Phi_{1,2,3}(t)$ do not change with increasing Ξ' and fixing both Ξ and Λ , as illustrated in Fig(2.27, d, e).

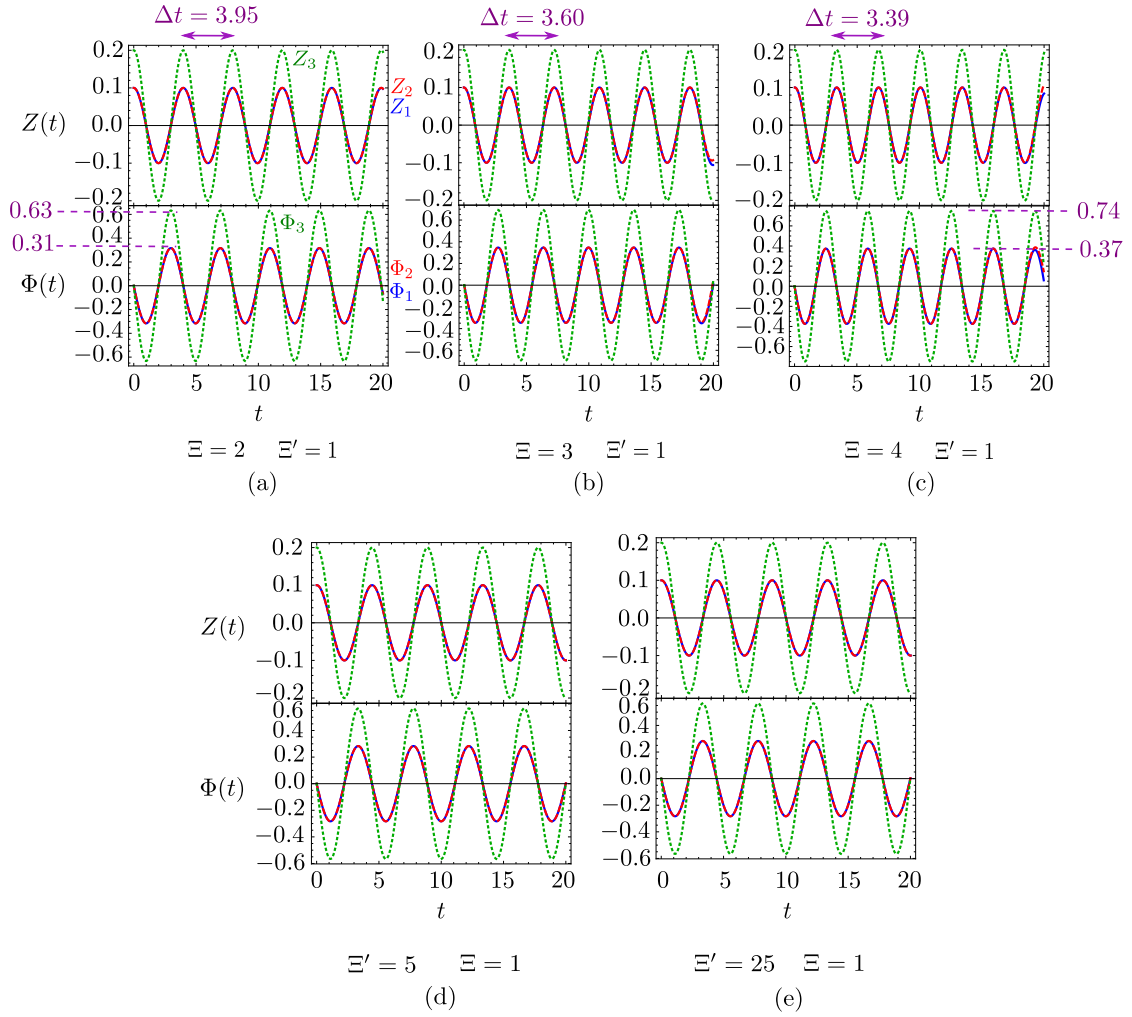


Figure 2.27.: The time evolution of the three fractional population imbalances $Z_{1,2,3}(t)$ in and three relative phases $\Phi_{1,2,3}(t)$ in the quadruple-well potential within the linear interacting limit, the so-called, Josephson regime. The initial conditions are taken to be equal for the imbalances to $Z_1(0) = Z_2(0) = 0.1, Z_3(0) = 0.2$ and for the relative phases $\Phi_{1,2,3}(0) = 0$, and the contact-interaction is $\Lambda = 1$.

2.3.2.3. Non-linear interacting limit (Fock regime)

Finally, we investigate the behaviour of the N_T^{qw} interacting Rydberg dressed atoms in the non-linear interacting limit. To do that, and similarly to the triple-well potential case, we analyse the following cases:

1. The time-evolution of the fractional population imbalances $Z_{1,2,3}(t)$ and the relative phases $\Phi_{1,2,3}(t)$ in Fig(2.28)

A numerical solution for the differential equations Eqs.(2.86, 2.87, 2.88, 2.89, 2.90, 2.91) is obtained as Fig(2.28) shows. At the critical value of $\Xi \propto \eta_L - \eta_{\text{NNN}}$, as in Fig(2.28, a), all fractional population imbalances show a non-pure macroscopic quantum self-trapping (MQST) phenomenon with an obvious possibility of tunnelling between condensates due to the overlaying between the correspondent three solutions. However, the relative phases $\Phi_{1,2}(t)$ do not change with time, whereas Φ_3 increases linearly in the negative values of $\Phi(t)$. This can be easily explained as both relative phases $\Phi_{1,2}(t)$ relate to nearest neighbouring sites, whereas $\Phi_3(t)$ relates to a next-nearest neighbouring site, and since the increasing long-range interaction corresponds to the interaction between the site and its next-nearest neighbour, then it is plausible that $\Phi_{1,2}(t)$ stay without varying. On the other hand, no matter how we increase the strength of $\Xi' \propto \eta_{\text{NNN}} - \eta_{\text{NN}}$, the behaviour of both $Z_{1,2,3}(t)$ and $\Phi_{1,2,3}(t)$ stays the same without changing, i.e., no occurrence of MQST, as it is shown in Fig(2.28, b).

2. The phase-diagrams $Z_{1,2,3} - \Phi_{1,2,3}$ in Fig(2.29)

The trajectories of both phase diagrams of $Z_{1,2} - \Phi_{1,2}$ are closed at the critical value of Ξ_c , which is similar to what we have obtained in the triple-well potential case. However, $Z_3 - \Phi_3$ phase-diagram shows no change of $Z_3(t)$ as a function of $\Phi_3(t)$. The trajectories of all the phase-diagrams are closed for any value of Ξ' which means that Ξ' has no change in the phase diagram.

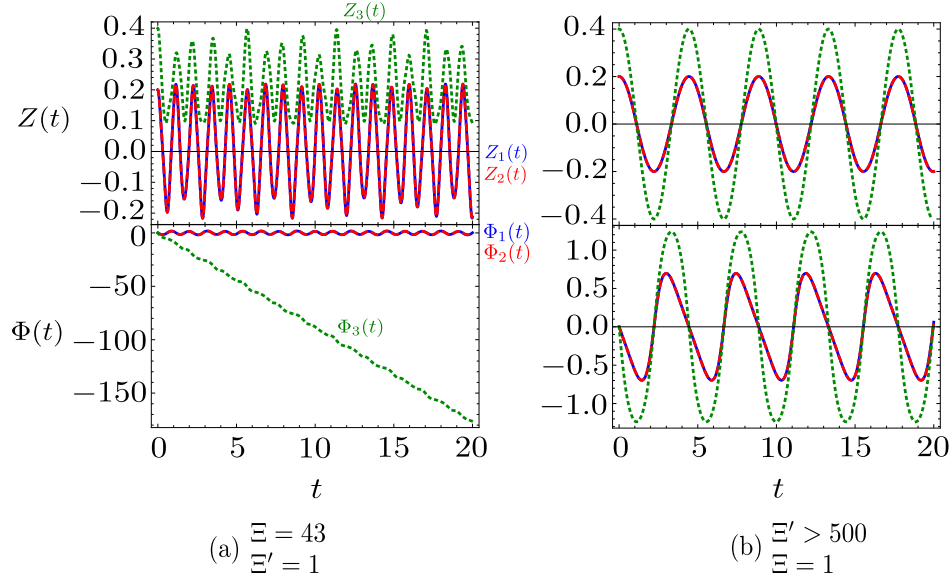


Figure 2.28.: The time-evolution for the fractional population imbalances $Z_{1,2,3}(t)$ and the relative phases $\Phi_{1,2,3}(t)$ at a critical value for Ξ_c with a fixed $\Xi' = 1$ in (a), and a very large value of $\Xi' > 500$ with a fixed $\Xi = 1$ in (b), with the initial conditions are being take as $Z_{1,2,3}(0) = 0.2, 0.2, 0.4$, respectively, and $\Phi_{1,2,3}(0) = 0$.

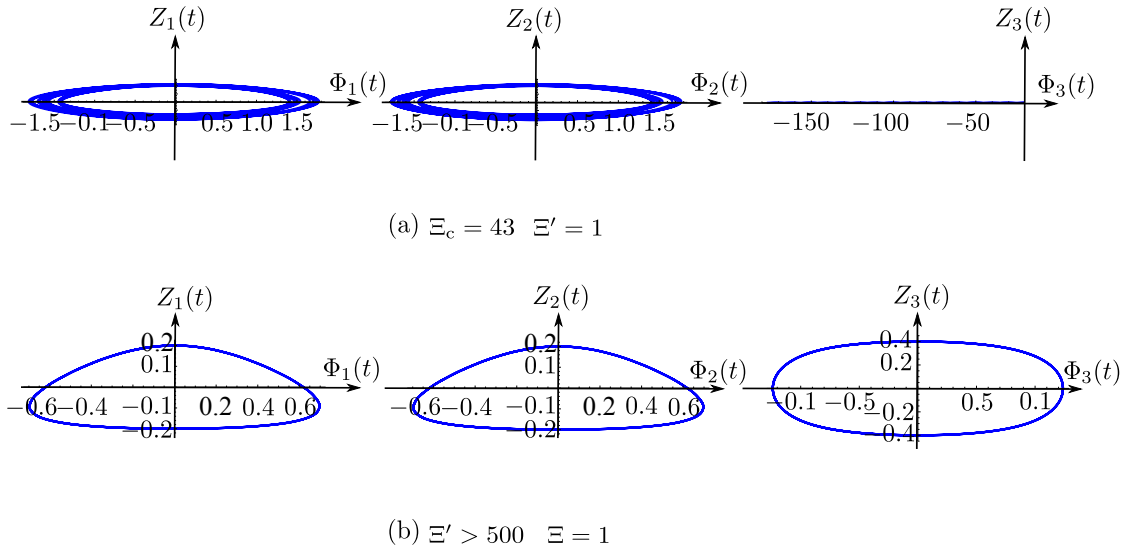


Figure 2.29.: The phase-diagrams of the canonical conjugates $Z_1 - \Phi_1$, $Z_2 - \Phi_2$ and $Z_3 - \Phi_3$, at a critical value for Ξ_c in (a) , and a very large value of Ξ' in (b).

3. The time-evolution of the atom numbers of each condensate $N_{0,1,2,3}(t)$ and the relative phases $\Phi_{1,2,3}$ in Fig(2.30)

The numerical solution for Eqs.(2.84, 2.85) is illustrated in Fig(2.30) and Fig(2.31). Different initial conditions for the atom-number and relative phases are considered in order to investigate the effect of long-range interactions on their time-evolution.

- i. $N_0(0) = 17, N_1(0) = N_2(0) = N_3(0) = 1$ and $\Phi_{1,2,3}(0) = 0$ in Fig(2.30, a): at a critical value of Ξ_c as shown in Fig(2.30, a, 1), the behaviour of the atom numbers confirms the non-pure MQST phenomenon where a few atoms are being tunnelling between the four wells, whereas the rest are self-trapped in their initial wells. Both relative phases $\Phi_{1,2}(t)$ show no change as a function of time, whereas $\Phi_3(t)$ increases linearly. Moreover, at the critical strength of Ξ'_c as illustrated in Fig(2.30, a, 2), the same physics occurs in the time-evolution of the atom-number. However, all relative phases increase linearly, either in the positive values of $\Phi(t)$, as in the case of $\Phi_3(t)$, or negatively as for $\Phi_{1,2}(t)$.
- ii. $N_0(0) = 2, N_1(0) = N_2(0) = N_3(0) = 6$ and $\Phi_{1,2,3}(0) = 0$ in Fig(2.30, b): at Ξ_c , not only a partial MQST is occurred, but also a similar collective oscillation frequency between $N_{1,2,3}(t)$ is shown, which is illustrated in Fig(2.30, b, (3)). In this case, $\Phi_3(t)$ increases linearly in the negative values of $\Phi(t)$. Additionally in Fig(2.30, b, (4)), at a critical value of Ξ'_c , the asymmetric oscillations of $N_{0,2}(t)$ show the same collective oscillation frequency, however, $N_{1,3}(t)$ exhibit harmonic oscillations. Furthermore, all relative phases in this case have oscillatory appearance with symmetric behaviours and a same collective frequency which implies that no MQST happens in this case.
- iii. $N_0(0) = 7, N_1(0) = 4, N_2(0) = 6, N_3(0) = 3$ in Fig(2.31): in this case, where the four sites are loaded with different numbers of atoms, three different initial conditions for relative phases have been taken into account; $\Phi_{1,2,3}(0) = 0$ in Fig(2.31, a), $\Phi_{1,2,3}(0) = \frac{\pi}{2}$ in Fig(2.31, b) and $\Phi_{1,2,3}(0) = \pi$ in Fig(2.31, c). It is clearly shown from Fig(2.31, (a,1), (b,1), (c,1)) that a common feature appears in the time-evolution of both the atom-number and relative phases when reaching the critical values of the long-range interaction Ξ_c with a fixed Ξ' . A nearly pure MQST occurs between the four sites which is pretty similar to what we have obtained in the double-well potential case. Additionally, both relative phases $\Phi_{1,2}(t)$ decrease linearly with time whereas $\Phi_3(t)$ increases accordingly.

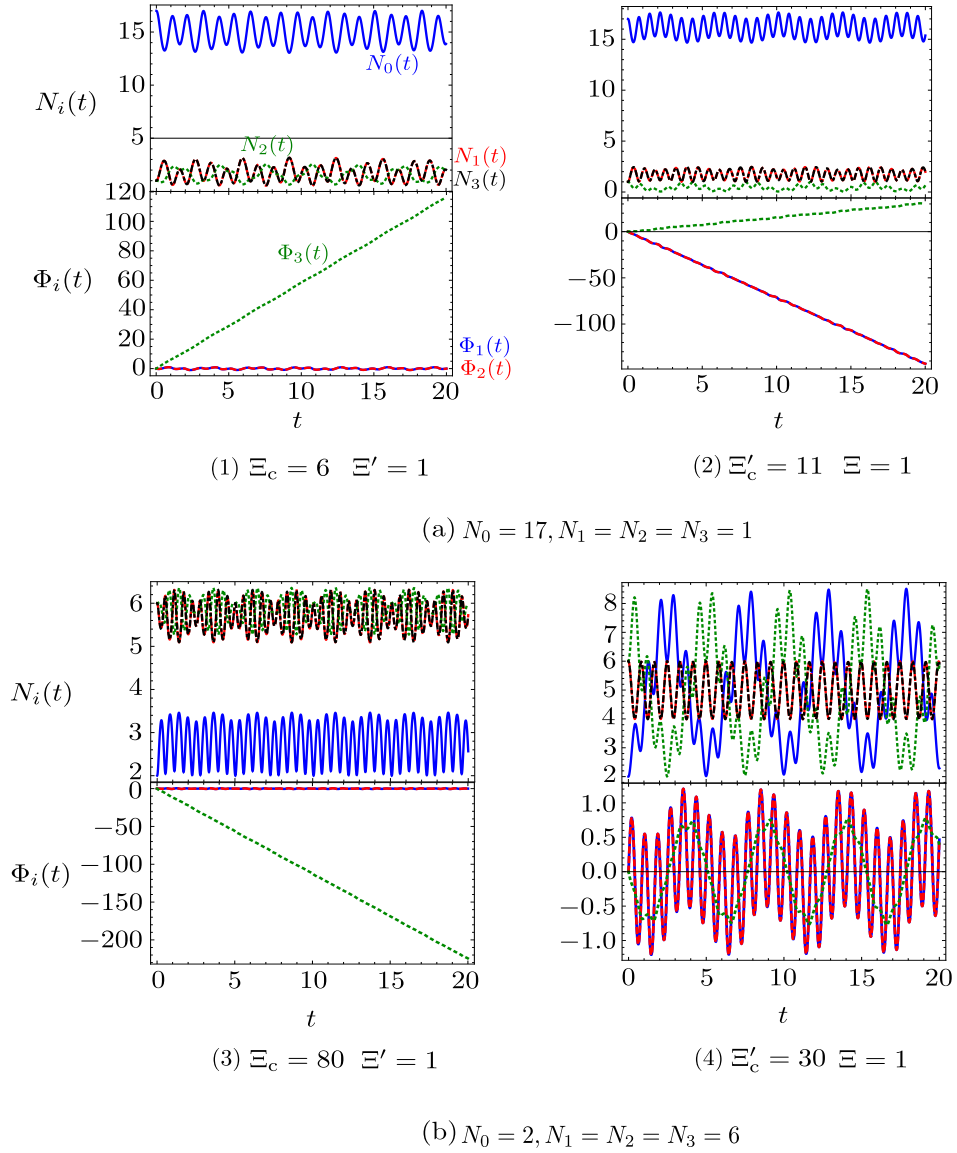


Figure 2.30.: The time-evolution of the atom-number for each condensate $N_{0,1,2,3}(t)$ and the correspondent relative phase $\Phi_{1,2,3}(t)$ in two distinct cases; in (a) $N_0(0) = 17, N_1 = N_2 = N_3 = 1$ and in (b) $N_0(0) = 2, N_1(0) = N_2(0) = N_3(0) = 6$, and the resulting behaviour at the critical values for both long-range interactions Ξ and Ξ' .

At the critical value Ξ'_c with a fixed Ξ in Fig(2.31, (a,2), (b,2), (c,2)), another common behaviour shows up where the atom-number time-evolution illustrates a non-pure MQST and both relative phases $\Phi_{1,2}(t)$ decrease linearly with time and no change according to $\Phi_3(t)$.

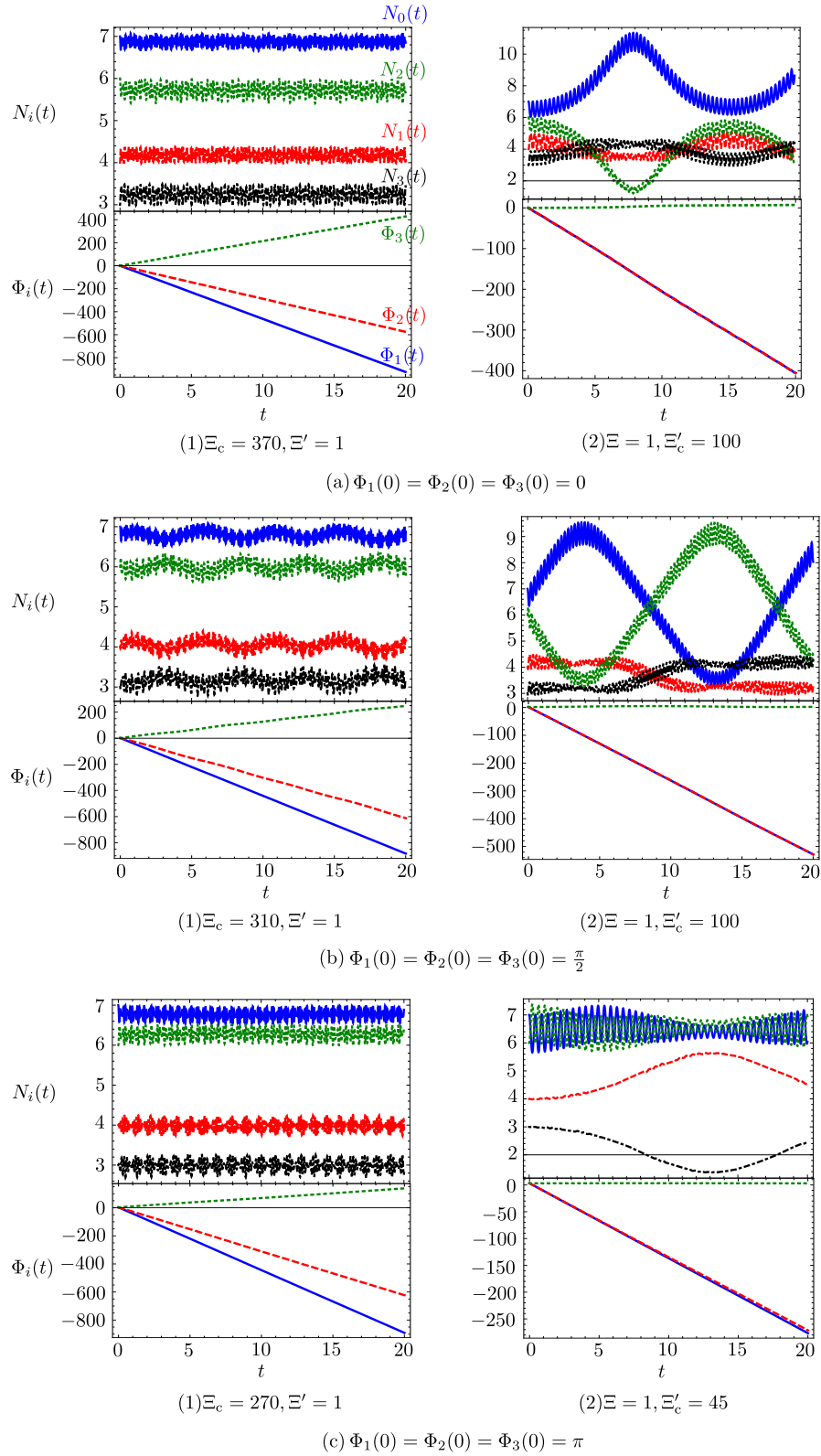


Figure 2.31.: The time-evolution of the atom-number for each condensate $N_{0,1,2,3}(t)$ and the relative phases $\Phi_{1,2,3}(t)$ when reaching the critical long-range interaction value. The initial conditions for the atom-number are: $N_0(0) = 7$, $N_1(0) = 4$, $N_2(0) = 6$ and $N_3(0) = 3$, and different initial values for the relative phases as shown in (a), (b) and (c).

As a summary to this section, we have studied the behaviour of N_T^{qw} Rydberg-dressed atoms trapped in a symmetric two-dimensional quadruple-well potential trap. Similarly to the previous sections, three main variables were investigated; fractional population imbalances, relative phases and atom numbers. Three dynamical regimes were analysed; Rabi, Josephson and Fock in order to study the response of these atoms to the applied long-range interaction. In the non-interacting limit, the atoms oscillate back and forth in the quadruple-well potential with a Rabi-like frequency $\omega_{\text{Ra}}^{\text{qw}}$ resembling a four-level atom in four coherent fields with zero detunings. However, in the linear interacting limit, the behaviour of both, fractional population imbalances and relative phases, is pretty similar to the double-well potential case when varying $\Xi \propto \eta_L - \eta_{NN}$. In the non-linear interacting limit, the fractional population imbalances show a non-pure macroscopic quantum self-trapping phenomenon with a tunnelling possibility between the four condensates which is similar to the triple-well potential case. However, when the four sites have different initial atom-number values, their time-evolution shows a pure MQST when reaching the critical long-range interaction Ξ_c . Additionally, the phase-diagrams of $Z_{1,2} - \Phi_{1,2}$ have an open trajectories when switching on the interaction Ξ and they turned to be closed at the interaction's critical strength Ξ_c which is also analogous to the triple-well potential case.

2.4. Conclusion

In conclusion, we have used mean-field theory (MFT) to overview the quantum dynamics of a BEC of N Rydberg-dressed atoms in a variety of shapes of multi-well potential traps. It has been shown that Rydberg-dressed atoms are strongly influenced not only by the geometry of different confinements, but also by the strength of interactions. Our analysis has started with studying N Rydberg-dressed atoms in one-dimensional trapping potentials where we have taken double- and triple-well traps. Then, we have extended the investigation to study a two-dimensional trapping potential where we have used the configuration of a quadruple-well trap. Basically, the dynamics of the multiple BECs have been analysed and interpreted by the numerical results obtained via solving the dynamical differential equations

that describe both, fractional population imbalances and relative phases between condensates. Three distinct dynamical regimes have been chosen to study the behaviour of these atoms based on the strength of the long-range interaction since the value of the contact-interaction has been put as fixed. In the non-interacting limit, i.e, Rabi regime, the behaviour of non-interacting Rydberg-dressed atoms does not differ conceptually according to the geometry of the trapping potential where the atoms have an intense tendency to Rabi-like oscillate with a Rabi frequency ω_{Ra} between multiple-condensates independently over time. However, in the linear interacting limit, i.e., Josephson regime, the numerical solutions of the linearised dynamical differential equations show a similar behaviour between condensates in both; one-dimensional double-well and two-dimensional quadruple-well traps where the oscillations of fractional population imbalances and relative phases are symmetric, harmonic and periodic over time. On the other hand, in the one-dimensional triple-well potential, the linear dynamics of the condensates depend on the nature of the applied long-range interaction. Moreover, in the non-linear interacting limit, i.e., Fock regime, the phenomenon of macroscopic quantum self-trapping (MQST) is generally occurred where it is a common sense that tunnelling in the multi-well trap is suppressed. Principally, self-trapping of Rydberg-dressed atoms is achievable just by tuning the long-range interaction strength to reach a certain critical value. A “pure” MQST, i.e., all the atoms are self-trapped and the tunnelling is completely suppressed, has been exhibited in the one-dimensional double-well potential trap. It has also been observed in the two-dimensional quadruple-well potential trap only in the case when the initial conditions of the atom-number in the four condensates are completely different. However, a “non-pure” MQST, i.e, most of the atoms are self-trapped in their initial wells forming a “suppressed-tunnelling background” with a tunnelling possibility related to the rest of the atoms, has been observed in both; one-dimensional triple-well and two-dimensional quadruple-well potential traps. All in all, this chapter has shown that different shapes of potential traps confinements means richer dynamics when studying Rydberg-dressed atoms. This analysis is a bridge toward gaining a plentiful information about interacting Rydberg-dressed atoms when confined in a finite optical lattice potential as we shall see in the next chapter.

CHAPTER 3

Probing the interaction between Rydberg-dressed atoms
through interference in optical lattices

In Chapter 2 we have studied the dynamics of an ensemble of strongly interacting Bose-Einstein condensates (BEC) in multiple trapping potentials within the mean-field theory. In this chapter we go one step ahead and describe the dynamics of the BEC in an optical lattice using the extended Bose-Hubbard model.

The systems we have studied so far can be regarded as building blocks toward large lattices. For systems of repulsively interacting ultracold bosonic atoms trapped in an optical lattice potential, the dynamics is described by the standard Bose-Hubbard (BH) model [102], which can be considered as a generalisation for the two-, three and four-mode approximations that have been analysed previously. The BH model includes the main physics that describe strongly interacting bosons, which is the competition between kinetic and interaction energy, and in which bosonic atoms undergo the superfluid-Mott insulator quantum phase transition. Recently, there is a growing interest in the study of extended BH models, in which the two-body interaction is long-ranged in the sense that it extends over several lattice sites. Extended BH models exhibit a host of quantum phases, including supersolid and checkerboard phases [103, 104]. Many studies employ dipolar atoms [105] or polar molecules [106] to establish many-body quantum systems with long-range interactions. A review about recent progress along this direction can be found in Ref [104].

In this chapter we will investigate the effect of the Rydberg induced interaction on a lattice gas of ground state atoms that is prepared in a superfluid state. In particular we are interested in studying the collapse and revival dynamics of the interference pattern that emerges upon the release of the atoms from the lattice. It has been demonstrated that collapses and revivals of a superfluid state released from an optical lattice provide important information on two-body interactions [107, 108]. For example, complete and periodic revivals are expected if atoms interact through short-range interactions [107]. In this work, we find that the peculiar shape of the interaction potential between Rydberg-dressed atoms gives rise to characteristic features in the collapse and revival dynamics of the interference pattern which originate from the competition of short-range and long-range parts of the interaction. Interference experiments therefore provide a way to probe the presence and to characterize the effective interaction between Rydberg-dressed atoms.

The chapter is organised as following. In section (3.1) we derive an effective BH model that governs the dynamics of Rydberg dressed atoms in an optical lattice. In section (3.2) we study the evolution of a superfluid state under the influence of the dressing, using the superfluid order parameter for a one-, two- and three-dimensional optical lattice. In section (3.3) we analyse the interference pattern of dressed atoms released from a one- and two-dimensional optical lattice. We conclude and provide experimental parameters in section (3.4).

3.1. Extended Bose-Hubbard Model of interacting bosonic atoms in an optical lattice

The system we consider here consists of N bosonic atoms distributed over L^D lattice sites, where D is the spatial dimension. The ensemble of N bosons are Rydberg-dressed atoms where a far off-resonant laser dresses the electronic ground state $|g\rangle$ with a Rydberg $|nS\rangle$ state, where n is the principal quantum number and S corresponds to the electronic angular momentum quantum number $l = 0$. The laser excitation is achieved by a two-photon process, as illustrated in Fig.(3.1, a). In our treatment, the Hamiltonian of the dressed ground state atoms is obtained in two steps. First, we calculate the Born-Oppenheimer many-body interaction potential by a perturbative diagonalisation of the electronic Hamiltonian. With this interaction potential, we then derive an extended BH Hamiltonian that governs the external dynamics of the dressed ground state atoms in the optical lattice.

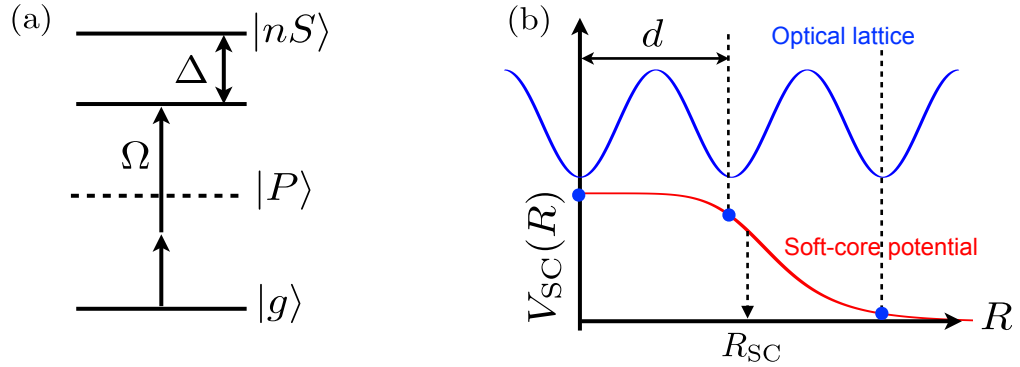


Figure 3.1.: (a) Schematics of the two-photon coupling between ground state and Rydberg state. The laser which couples the state $|g\rangle$ to the intermediate $|P\rangle$ -state is far detuned from resonance such that the ground state $|g\rangle$ and the Rydberg $|nS\rangle$ state form an effective two-level system. Here Ω is the effective Rabi frequency and Δ the (two-photon) detuning of the excitation laser frequencies with respect to the atomic transition. (b) Effective interaction potential between dressed atoms $V_{SC}(R)$ and its length scales in relation to the optical lattice with d is the lattice spacing. At short distances ($R \ll R_{SC}$) the interaction potential is constant and at large distances ($R \gg R_{SC}$) it is of van-der Waals type.

3.1.1. The electronic Hamiltonian

The internal level structure of the atoms is modeled by two states, the electronic ground state $|g\rangle$ and the Rydberg $|nS\rangle$ state. These two electronic states are coupled by a two-photon transition with an effective Rabi frequency $\Omega = \sqrt{N}\Omega_0$ where Ω_0 is the single-atom Rabi frequency as shown in Fig.(3.1, a) and discussed in subsection (1.3.6). The Hamiltonian for the internal (electronic) degrees of freedom of the atomic ensemble is given by (using $\hbar = 1$ and the rotating-wave-approximation)

$$\hat{H}_e = \sum_j^L \hat{H}_j + \frac{1}{2} \sum_{j \neq k}^L V_{\text{vdW}}(\mathbf{r}_j, \mathbf{r}_k) |nS\rangle_j \langle nS| \otimes |nS\rangle_k \langle nS|,$$

where $\hat{H}_j = \Omega(|g\rangle_j \langle nS| + \text{h.c.}) + \Delta |nS\rangle_j \langle nS|$ is the single-atom Hamiltonian where we assume that there is one atom per site. Here $V_{\text{vdW}}(\mathbf{r}_j, \mathbf{r}_k) = C_6/|\mathbf{r}_j - \mathbf{r}_k|^6$ is the vdW interaction that is present between two Rydberg atoms at positions $\mathbf{r}_j$ and $\mathbf{r}_k$, C_6 is the dispersion coefficient. We do not consider the two-body contact-interaction between ground state atoms. This interaction can be switched off for instance by a Feshbach resonance[109].

In our system, the electronic dynamics (Rydberg excitation and van-der-Waals interaction) takes place on a timescale ($\sim \mu\text{s}$) that is orders of magnitude faster than the typical timescales (related to interaction strength, tunnelling rate or phase-evolution) encountered in ultracold atomic experiments ($\sim \text{ms}$). The huge difference of these time scales permits the use of the Born-Oppenheimer approximation for treating the electronic parts of the Hamiltonian. In subsection (1.3.6) we obtained the effective Hamiltonian in Eq.(1.89) by applying the fourth order perturbation theory, which also called Born-Oppenheimer potential surface V_{BO} , that describes the dynamics of two ground state dressed Rydberg atoms in the regime where the effective Rabi frequency Ω is much smaller than the detuning Δ , i.e., $|\Omega/\Delta| \ll 1$. The analysis for N Rydberg-dressed atoms is exactly the same where the Born-Oppenheimer surface is written as a constant plus a sum of two-body interactions, i.e.,

$$V_{\text{BO}} = N \left(\frac{\Omega^4}{\Delta^3} - \frac{\Omega^2}{\Delta} \right) + \frac{1}{2} \sum_{j \neq k}^L V_{\text{SC}}(\mathbf{r}_j, \mathbf{r}_k), \quad (3.1)$$

with

$$V_{\text{SC}}(\mathbf{r}_j, \mathbf{r}_k) = \frac{\zeta R_{\text{SC}}^6}{|\mathbf{r}_j - \mathbf{r}_k|^6 + R_{\text{SC}}^6},$$

is the long-range soft-core interaction where $\zeta = 2\Omega^4/\Delta^3$ and $R_{\text{SC}} = (C_6/2\Delta)^{1/6}$ is the soft-core radius. In the following, we neglect the constant terms in Eq.(3.1) which correspond to the second and fourth order light shift.

3.1.2. The Hamiltonian of the external degrees of freedom

Let us now turn to the discussion of the external (motional) degrees of freedom. The Rydberg-dressed atoms are loaded into a D -dimensional optical lattice potential $V_{\text{L}}(\mathbf{r}) = V_0 \sin^2(\mathbf{k}\mathbf{r})$ (lattice spacing d). For $D < 3$ we assume that there is a tight transverse confining potential with respect to which the atoms are in the motional ground state. The different effective trapping frequencies due to varying AC-polarisabilities of the two states can lead to dephasing effect. However, as the Rydberg population is negligible, this allows us to neglect the dephasing. Such dephasing of the motional degrees of freedom can be minimised by choosing a particular frequency of the standing wave light field that produces the optical potential in conjunction with an appropriate choice of the Rydberg state [110]. With these approximations the second quantised Hamiltonian for the external motion of the dressed atoms reads

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{L}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') V_{\text{SC}}(\mathbf{r}, \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}), \quad (3.2)$$

where $\hat{\Psi}(\mathbf{r})$, $\hat{\Psi}^\dagger(\mathbf{r})$ are the annihilation and creation bosonic field operators of the dressed atoms, respectively. For a periodic potential and atom-atom interactions it is favorable to work in the Wannier basis of wave functions which are a set of orthogonal normalised wave functions localised at the lattice sites [21]. Therefore, We expand the field operator $\hat{\Psi}(\mathbf{r})$ in terms of Wannier states $w(\mathbf{r})$ in the lowest Bloch band of $V_{\text{L}}(\mathbf{r})$ such that

$$\hat{\Psi}(\mathbf{r}) = \sum_j \hat{b}_j w(\mathbf{r} - \mathbf{r}_j), \quad (3.3)$$

where $\hat{b}_j$ is the annihilation operator of a dressed atom at site j and $\mathbf{r}_j$ is the spatial position around which the Wannier states are centred. Therefore, $\hat{b}_j$ and the corresponding creation operator $\hat{b}_j^\dagger$ describe the annihilation and creation of a boson on the j th lattice site respectively. These operators obey the canonical commutation relations $[\hat{b}_j, \hat{b}_k^\dagger] = \delta_{jk}$ (and $[\hat{b}_j, \hat{b}_k] = [\hat{b}_j^\dagger, \hat{b}_k^\dagger] = 0$). We consider the case of a deep optical lattice where these Wannier states are strongly localised on a single lattice site, i.e. the variance (width) of the Wannier wave function is much smaller than the lattice spacing d . In this case Wannier state is given by a Gaussian function where in one-dimensional case we write

$$w(x - x_j) = \frac{1}{\sqrt{\xi}\sqrt{\pi}} \exp\left[-\frac{(x - jd)^2}{2\xi^2}\right], \quad (3.4)$$

with $\xi = \sqrt{\hbar/m\omega}$ is the harmonic oscillator length¹ (Wannier function width) as it shown in Fig.(3.2).

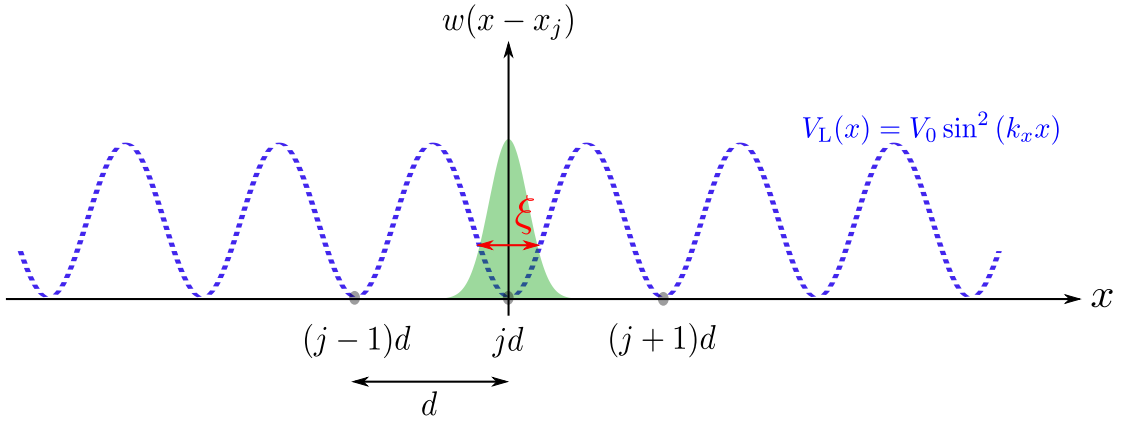


Figure 3.2.: Wannier function $w(x - x_j)$ (green Gaussian area) for an one-dimensional optical lattice $V_L(x)$ (blue dotted curves), where ξ , j and d are the Wannier function width, the lattice site and the lattice spacing, respectively.

¹The ratio between the width of the Gaussian ξ and the lattice spacing d can be calculated easily, which is, $\frac{\xi}{d} = \frac{1}{\pi} \left(\frac{V_0}{E_r} \right)^{-1/4}$, with V_0 being the barrier height and E_r is the recoil energy due to absorption of photon that is given by $E_r = \frac{\hbar^2 k^2}{2m}$. In our case, we take $V_0 \gg E_r$ in order to have deep lattice sites.

The Gaussian approximation is good when calculating the two-body interaction, but poor when calculating the tunnelling factor J . This is because the Gaussian ansatz neglects the small oscillations characteristic in the tail of the Wannier function, the tunnelling matrix element J is then underestimated by almost an order of magnitude [43] (see subsection (2.1.4.2)). As a result of using the expansion, the Hamiltonian becomes that of an extended BH model

$$\hat{\mathcal{H}}_{\text{EBH}} = -J \sum_{\langle j,k \rangle} b_j^\dagger b_k + \frac{\zeta}{2} \sum_j n_j (n_j - 1) + \frac{1}{2} \sum_{j \neq k} \gamma(j-k) n_j n_k, \quad (3.5)$$

with $\langle j, k \rangle$ indicating the summation over neighbouring lattice sites and $n_j = b_j^\dagger b_j$ counts the number of bosons on the j th lattice site. The Hamiltonian $\hat{\mathcal{H}}_{\text{EBH}}$ consists of three terms:

1. The first term is the hopping term that describes the tunnelling of bosons between neighbouring potential wells, j and k . The strength of the tunnelling coupling is characterised by the tunnelling matrix element $J = -\int d\mathbf{r} w(\mathbf{r} - \mathbf{r}_j) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_L(\mathbf{r}) \right] w(\mathbf{r} - \mathbf{r}_k)$, which is a generalised tunnelling matrix element for few-well setups discussed in the previous chapter.
2. The second term describes the on-site interaction on site j where the interaction constant reads $\zeta = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' |w(\mathbf{r} - \mathbf{r}_j)|^2 |w(\mathbf{r}' - \mathbf{r}_j)|^2$. This term is non-zero if two or more atoms are in the same Wannier state.
3. The third term characterises the long-range interaction among atoms located in distant sites j and k where

$$\gamma(j-k) = \gamma(m) = \frac{\zeta R_{\text{SC}}^6}{|m|^6 d^6 + R_{\text{SC}}^6}.$$

Note that in general the index j is a vector for $D > 1$. For example, $j = (j_x, j_y, j_z)$ in a three-dimensional optical lattice.

3.2. Collapse and revival of the superfluid order parameter

In this section, we study the effect that the Rydberg dressing has on the coherence properties of the atoms. The situation we have in mind is depicted in Fig.(3.3). At first, in Fig.(3.3, a), one prepares - in the absence of the dressing laser - a superfluid state which is the ground state of Hamiltonian Eq.(3.5). In the second step, in Fig.(3.3, b), one applies the dressing laser for a time t . Here we consider a regime in which the parameters are chosen such that $|J| \ll |\xi|, |\gamma(m)|$, i.e. the atomic tunnelling can be neglected during the time the dressing laser is switched on as the tunnelling is assumed to be very slow comparing to the duration of the dressing laser. The system then evolves approximately under the Hamiltonian Eq.(3.5) with $J = 0$. We are interested in the coherence properties of the superfluid state after this procedure. To this end, we will study the superfluid order parameter in this section, while in the next section the probing of the coherence properties via an interference experiment as in Fig.(3.3, c) is discussed.

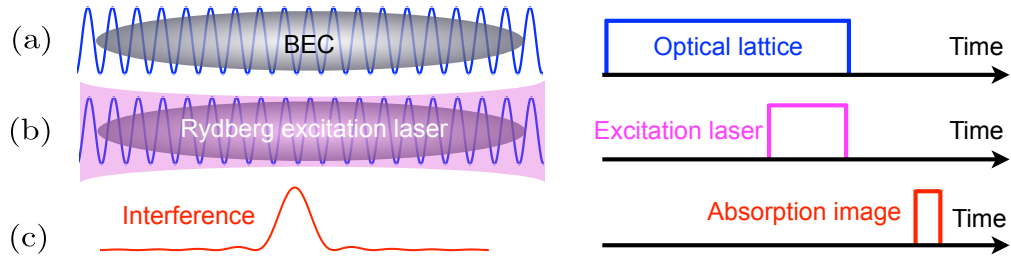


Figure 3.3.: The experimental sequence and timings. Firstly (a), a BEC is prepared in an optical lattice. Secondly (b), an off-resonant laser coupling the ground state to the Rydberg state is applied for a certain time. After the excitation laser pulse, the optical lattice is switched off immediately and the dressed ground state atoms expand freely. Finally (c), interference patterns are recorded by taking absorption images of the expanded atomic cloud.

3.2.1. Superfluid ground state

The initial many-body ground state of our system is a perfect superfluid state. In the superfluid system, the single-particle wave functions of N atoms are spread out, i.e., delocalised, over the entire lattice with L lattice sites. Neglecting the interactions,

the many-body ground state for a homogenous² system is then given by [111]

$$|\text{SF}\rangle = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{L}} \sum_j^L \hat{b}_j^\dagger \right]^N |0, 0, \dots\rangle, \quad (3.6)$$

where $|0, 0, \dots\rangle$ is the product of vacuum states (no-atom state) of sites $j = 1, 2, \dots, L$. An important feature of this state is that the probability distribution for the local occupation of atoms on a single lattice site $\hat{n}_j = \hat{b}_j^\dagger \hat{b}_j$ is Poissonian [111], that is, the variance given by average number of atoms on this lattice site, i.e., the expectation value of the on-site atom number $\text{Var}(n_j) = \langle \hat{n}_j \rangle$, is given by³

$$\langle n_j \rangle = \langle \hat{b}_j^\dagger \hat{b}_j \rangle = \langle \text{SF} | \hat{b}_j^\dagger \hat{b}_j | \text{SF} \rangle = \underbrace{\sum_k^N \binom{N}{k} \left(1 - \frac{1}{L}\right)^{N-k} \left(\frac{1}{L}\right)^k}_\text{Poisson distribution} k. \quad (3.7)$$

At the thermodynamic limit (for $N \gg 1$), Eq.(3.6) becomes indistinguishable to a product of coherent states where we can replace it by [112]

$$|\text{SF}\rangle \approx \prod_j^L |\alpha_j\rangle, \quad (3.8)$$

with $|\alpha_j\rangle$ being a coherent state of atoms in a single lattice site and it is by definition the eigenstate of the annihilation operator $\hat{b}_j$ and it is given by

$$|\alpha_j\rangle = e^{-\frac{|\alpha_j|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha_j^n}{\sqrt{n!}} |n\rangle, \quad (3.9)$$

with $\langle \hat{n}_j \rangle = |\alpha_j|^2$ being the average on-site occupation particle number. We will use this representation as an initial state for the following calculations. Moreover, we will exclusively consider a homogeneous system where the average atom number in each lattice site is constant, i.e., $\alpha_j = \alpha$ with $|\alpha_j|^2 = |\alpha|^2 = N/L$.

3.2.2. Superfluid order parameter

When the Rydberg excitation laser is applied, the dynamical evolution of the superfluid state can be investigated according to the order parameter. The order

²Homogeneous system means in our treatment that the lattice constant and the potential depth for all lattice sites are the same.

³The analytical proof can be found in the Appendix F.

parameter is a complex quantity characterised by

$$\phi^{(D)}(t) = \langle \hat{b}_j \rangle = \langle \text{SF}(t) | \hat{b}_j | \text{SF}(t) \rangle, \quad (3.10)$$

where

$$|\text{SF}(t)\rangle = \exp[-i\hat{\mathcal{H}}_{\text{EBH}}t] |\text{SF}(t=0)\rangle, \quad (3.11)$$

with $|\text{SF}(t=0)\rangle$ being the coherent wave function of the BEC at $t=0$ expressed in Eq.(3.8), and $\exp[-i\hat{\mathcal{H}}_{\text{EBH}}t]$ is the phase which plays a major role in characterizing the coherence and the superfluid phenomena [113]. Therefore, Eq.(3.10) can be written as

$$\phi_j^{(D)}(t) = \langle \hat{b}_j \rangle = \langle \text{SF}(t=0) | e^{i\hat{\mathcal{H}}_{\text{EBH}}t} \hat{b}_j | e^{-i\hat{\mathcal{H}}_{\text{EBH}}t} \text{SF}(t=0) \rangle = \alpha \exp[|\alpha|^2 F_D(t)].$$

where $F_D(t)$ is the phase factor. Here, we will discuss the effect of the dressing on the time-evolution of the superfluid order parameter, hence we consider D -dimensional optical lattices with linear ($D=1$), square ($D=2$) and cubic ($D=3$) geometry. We will focus our analysis on the phase factor $F_D(t)$ as it encodes the full dynamics of the order parameter $\phi^{(D)}(t)$ and has the advantage that it is independent of the particle density. For the following discussion we will furthermore consider a parameter regime in which the interactions between distant atoms, i.e., atoms whose position labels obey $|j-k| > 2$, is negligible. This is the situation depicted in Fig.(3.1, b). Let us now study $F_D(t)$ for lattices with different spatial dimension D .

3.2.2.1. One-dimensional lattice

Taking into account the on-site $j=1$, nearest-neighbour $j=2,4$ with interaction $\gamma(1)$ and next-nearest-neighbour $j=3,5$ with $\gamma(2)$ interaction, then the order parameter can be written as

$$\phi^{(1)}(t) = \left\langle \prod_{j=1}^5 \langle \alpha_j^* | e^{i\hat{\mathcal{H}}_{\text{EBH}}^\dagger t} | b_1 | e^{-i\hat{\mathcal{H}}_{\text{EBH}} t} \prod_{j=1}^5 | \alpha_j \rangle \right\rangle,$$

as the coherent state is given by Eq.(3.9), then we write

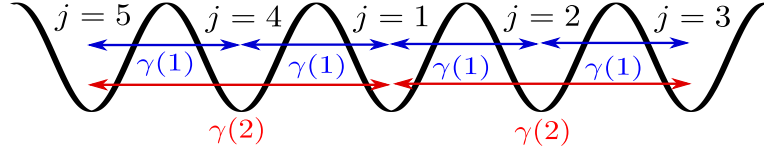


Figure 3.4.: One-dimensional optical lattice with five lattice sites, i.e., $j = 1, 2, \dots, 5$.

$$\begin{aligned}
\phi^{(1)}(t) &= e^{\sum_{j=1}^5 -|\alpha_i|^2} \sum_{\substack{m_1, m_2, m_3, m_4, m_5 \\ n_1, n_2, n_3, n_4, n_5}} \times \frac{\alpha_1^{*m_1} \alpha_1^{n_1}}{\sqrt{m_1! n_1!}} \sqrt{n} \langle m_1 | n_1 - 1 \rangle \frac{\alpha_2^{*m_2} \alpha_2^{n_2}}{\sqrt{m_2! n_2!}} \langle m_2 | n_2 \rangle \\
&\times \frac{\alpha_3^{*m_3} \alpha_3^{n_3}}{\sqrt{m_3! n_3!}} \langle m_3 | n_3 \rangle \frac{\alpha_4^{*m_4} \alpha_4^{n_4}}{\sqrt{m_4! n_4!}} \langle m_4 | n_4 \rangle \frac{\alpha_5^{*m_5} \alpha_5^{n_5}}{\sqrt{m_5! n_5!}} \langle m_5 | n_5 \rangle \\
&\times e^{it \left\{ \frac{\zeta}{2} \sum_{j=1}^5 [m_j(m_j-1) - n_j(n_j-1)] + \sum_{j \neq k} \left[\frac{\gamma(1)}{2} [(m_j m_k - n_j n_k) + \frac{\gamma(2)}{2} [(m_j m_k - n_j n_k)]] \right] \right\}} \\
&= \alpha_1 e^{\sum_{j=1}^5 -|\alpha_i|^2} \left[\sum_{n_1}^{\infty} e^{-i\zeta(n_1-1)t} \frac{|\alpha_1|^{2(n_1-1)}}{(n_1-1)!} \right] \left[\sum_{n_2}^{\infty} e^{-i\frac{\gamma(1)}{2} n_2 t} \frac{|\alpha_2|^{2n_2}}{n_2!} \right] \left[\sum_{n_3}^{\infty} e^{-i\frac{\gamma(2)}{2} n_3 t} \frac{|\alpha_3|^{2n_3}}{n_3!} \right] \\
&\times \left[\sum_{n_4}^{\infty} e^{-i\frac{\gamma(1)}{2} n_4 t} \frac{|\alpha_4|^{2n_4}}{n_4!} \right] \left[\sum_{n_5}^{\infty} e^{-i\frac{\gamma(2)}{2} n_5 t} \frac{|\alpha_5|^{2n_5}}{n_5!} \right] \\
&= \alpha_1 e^{\sum_{j=1}^5 -|\alpha_i|^2} \times e^{|\alpha_1|^2 e^{-i\zeta t}} \times e^{|\alpha_2|^2 e^{-i\frac{\gamma(1)}{2} t}} \times e^{|\alpha_3|^2 e^{-i\frac{\gamma(2)}{2} t}} \times e^{|\alpha_4|^2 e^{-i\frac{\gamma(1)}{2} t}} \times e^{|\alpha_5|^2 e^{-i\frac{\gamma(2)}{2} t}},
\end{aligned}$$

since we have a homogenous system, then we obtain the order parameter in an one-dimensional optical lattice as

$$\phi^{(1)}(t) = \alpha \exp \left[-|\alpha|^2 \left(5 - e^{-i\zeta t} - 2e^{-i\gamma(1)t} - 2e^{-i\gamma(2)t} \right) \right] = \alpha \exp \left[|\alpha|^2 F_1(t) \right].$$

Note $|\phi^{(1)}(t)| = |\alpha|$ at $t = 0$. Our following analysis will focus on the phase factor part $F_1(t)$ which is given by

$$F_1(t) = -[5 - e^{-i\zeta t} - 2e^{-i\gamma(1)t} - 2e^{-i\gamma(2)t}]. \quad (3.12)$$

In general, we expect the two-body interactions to result in a collapse and revival of the superfluid order [107, 114]. The collapse occurs when the many particle state evolves away from a coherent state, then the property of having a macroscopic phase vanishes. The collapse dynamics can be obtained by analyzing the real part of $F_1(t)$

in the vicinity of $t = 0$. therefore, a Taylor expansion up to second order in t yields

$$\text{Re}[F_1(t \rightarrow 0)] \approx -\left[\frac{\zeta^2}{2} + \gamma^2(1) + \gamma^2(2)\right]t^2 = -\frac{1}{2}\left(\frac{t}{\tau_1}\right)^2, \quad (3.13)$$

where τ_1 is the collapse time, given as

$$\tau_1 \approx \frac{1}{\sqrt{\zeta^2 + 2\gamma^2(1) + 2\gamma^2(2)}}. \quad (3.14)$$

This expression clearly indicates that the collapse is faster, the stronger the two-body interaction. The possibility of revivals of the initial state is strongly determined by the long-range part of the interaction. Complete revivals occur when all phase factors appearing in exponential terms of $F_1(t)$ are simultaneously multiples of⁴ 2π , i.e., $\xi = \gamma(1) = \gamma(2) = 2n\pi$, which makes the phase factor equals $F_1(t) = 0$ leading to $\phi^{(1)}(t) = \alpha$. As the ratios between the various possible interaction strengths are in general irrational, complete revivals are unlikely and one can rather expect partial revivals at a finite time.

3.2.2.2. Two-dimensional lattice

In two dimensions the truncation of the interaction to atoms whose indices obey $|j - k| \leq 2$ means that we have to take into account at most next-next-nearest neighbour interactions. This yields

$$F_2(t) = -[13 - e^{-i\zeta t} - 4e^{-i\gamma(1)t} - 4e^{-i\gamma(\sqrt{2})t} - 4e^{-i\gamma(2)t}], \quad (3.15)$$

and a collapse time

$$\tau_2 \approx \frac{1}{\sqrt{\zeta^2 + 4\gamma^2(1) + 4\gamma^2(\sqrt{2}) + 4\gamma^2(2)}}. \quad (3.16)$$

In particular, we intend to study $F_2(t)$ as a function of the ratio between the lattice spacing d and the length scale R_{SC} which demarcates the soft core of the effective interaction potential among Rydberg-dressed atoms. In Fig.(3.5) we present data for $d/R_{\text{SC}} = \{0.7, 1.0, 1.5\}$. The smaller d/R_{SC} the more terms of the long-range tail of the interaction actually contribute to the denominator of τ_2 . This leads to a more

⁴Owing to the fact that $\exp(\pm 2\pi i) = 1$

rapid collapse of the order parameter the smaller d/R_{SC} becomes, which is clearly shown by the data. In fact, all dimensions have in common that for $d/R_{\text{SC}} > 1$, the behaviour of the function $F_D(t)$ is determined mainly by the on-site and nearest-neighbour interaction. Compared to those the other interaction terms are negligible which is owed to the fast drop of the soft-core interaction potential at large inter-site separations. To demonstrate this explicitly, we calculate $F_2(t)$ by neglecting interaction beyond nearest neighbours, i.e., $\gamma(m) = 0$ for $m > 1$. The results and a comparison with the full calculation are shown in Fig.(3.5,b) and Fig.(3.5,c). For $d/R_{\text{SC}} = 0.7$ the two calculations deviate already beyond $\zeta t = 2$. However, for $d/R_{\text{SC}} = 1.5$ agreement for much longer times (here until $\zeta t = 30$) is achieved. Thus, for sufficiently short times the contribution of the long-range interaction terms to the dynamical evolution of $F_2(t)$ is strongly suppressed.

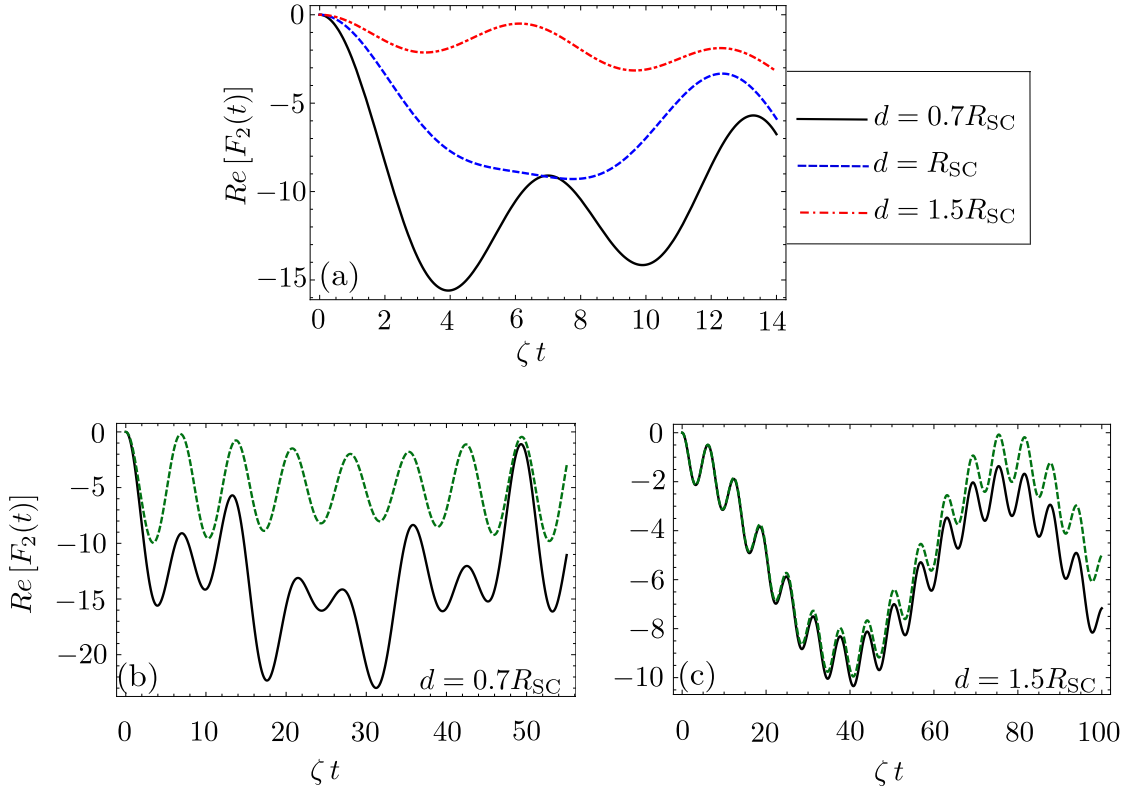


Figure 3.5.: (a) Dynamical evolution of $F_2(t)$ for various values of d/R_c . (b, c) Dotted green curves show calculations merely taking into account the on-site and nearest-neighbour interaction. Solid lines show calculations including all interactions up to next-next-nearest neighbours.

3.2.2.3. Three-dimensional lattice

In this case one obtains

$$F_3(t) = -[33 - e^{-i\zeta t} - 6e^{-i\gamma(1)t} - 12e^{-i\gamma(\sqrt{2})t} - 8e^{-i\gamma(\sqrt{3})t} - 6e^{-i\gamma(2)t}], \quad (3.17)$$

with a corresponding collapse time

$$\tau_3 \approx \frac{1}{\sqrt{\zeta^2 + 6\gamma^2(1) + 12\gamma^2(\sqrt{2}) + 8\gamma^2(\sqrt{3}) + 6\gamma^2(2)}}. \quad (3.18)$$

Generally the collapse time becomes shorter for higher dimensional systems, since the number of contributing interaction terms grows with increasing dimensions (as a consequence of the increasing coordination number).

3.3. Interference pattern

Our aim in this section is to gain information from such a trapped ensemble of atoms via the interference pattern. The method is to simultaneously switch off the optical lattice trapping potential and the Rydberg excitation laser. When one switches off the laser potential traps, the atoms expand ballistically due to the sudden disappearance of the confinement potential. After a time-of-flight period (a few m sec), an interference pattern of the spatial density distribution (see Fig.(3.3,c)) is formed and made visible by taking an absorption image of the atomic cloud. Therefore, the dynamical evolution of the superfluid order can be made visible from an interference experiment as was shown in Ref.[107].

3.3.1. Quasi-momentum distribution

In an interference experiment, we usually measure the expectation value of the spatial density (correlation function), i.e.,

$$\rho(\mathbf{r}, t) = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \rangle, \quad (3.19)$$

where $\hat{\Psi}(\mathbf{r})$ is the bosonic field operator. As we have seen earlier, in the single band approximation the bosonic field operator can be written in terms of the Wannier function expressed in Eq.(3.3). After the expansion (after the time of flight t_{ex}), the Wannier function becomes time-dependent and reads [115]

$$w(\mathbf{r} - \mathbf{r}_j, t) = \frac{1}{\sqrt{\xi}\sqrt{\pi}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_j)^2}{2\xi(t)^2}\right) \exp\left(\frac{i\hbar t_{\text{ex}}}{m\xi^2} \frac{(\mathbf{r} - \mathbf{r}_j)^2}{2\xi(t)^2}\right) e^{-i\theta}, \quad (3.20)$$

where: $\xi(t) = \xi \sqrt{1 + \left(\frac{\hbar t_{\text{ex}}}{m\xi}\right)^2}$ is the time-dependent Wannier function width, and $\theta = \frac{1}{2} \arctan\left(\frac{\hbar t_{\text{ex}}}{m\xi^2}\right)$. Therefore, we can write Eq.(3.19) as

$$\begin{aligned} \rho(\mathbf{r}, t) &= \left\langle \sum_j^L w^*(\mathbf{r} - \mathbf{r}_j, t) \hat{b}_j \sum_k^L w(\mathbf{r} - \mathbf{r}_k, t) \hat{b}_k \right\rangle \\ &= \sum_j^L \sum_k^L \frac{1}{\sqrt{\xi}\sqrt{\pi}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_j)^2}{2\xi(t)^2}\right) \exp\left(-\frac{i\hbar t_{\text{ex}}}{m\xi^2} \frac{(\mathbf{r} - \mathbf{r}_j)^2}{2\xi(t)^2}\right) e^{i\theta} \\ &\quad \frac{1}{\sqrt{\xi}\sqrt{\pi}} \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_k)^2}{2\xi(t)^2}\right) \exp\left(\frac{i\hbar t_{\text{ex}}}{m\xi^2} \frac{(\mathbf{r} - \mathbf{r}_k)^2}{2\xi(t)^2}\right) e^{-i\theta} \langle \hat{b}_j^\dagger \hat{b}_k \rangle. \end{aligned}$$

Assuming that after the expansion we have $\xi(t) \gg \mathbf{r}_j$, then

$$\rho(\mathbf{r}, t) = \frac{1}{\xi(t)\sqrt{\pi}} \sum_{jk}^L \exp\left(-\frac{\mathbf{r}^2}{\xi(t)^2}\right) \exp\left(\frac{i\hbar t_{\text{ex}}}{m\xi^2} \frac{(\mathbf{r}_j - \mathbf{r}_k)^2}{\xi(t)^2}\right) \langle \hat{b}_j^\dagger \hat{b}_k \rangle.$$

For sufficiently long expansion times, the Wannier states will expand to be much larger than the total extent of the sites initially occupied in the optical lattice [115]. We can then, via the *far-field approximation*, write approximately (using the Taylor expansion)

$$\xi(t) \approx \frac{\hbar t_{\text{ex}}}{m\xi}, \quad (3.21)$$

rearranging the spatial distribution we get

$$\rho(\mathbf{r}, t) = \frac{m}{\hbar t_{\text{ex}}} \rho(\mathbf{k}, t),$$

where: $\mathbf{k} = \frac{m\mathbf{r}}{\hbar t_{\text{ex}}}$ is the momentum and,

$$\rho(\mathbf{k}, t) = \frac{\xi}{\sqrt{\pi}} \exp\left(-\frac{\mathbf{k}^2}{1/\xi^2}\right) \sum_{jk}^L e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_k)} \langle \hat{b}_j^\dagger \hat{b}_k \rangle,$$

is the momentum distribution density. If we denote:

$$|\phi(\mathbf{k}, t)|^2 = \frac{\xi}{\sqrt{\pi}} \exp\left(-\frac{\mathbf{k}^2}{1/\xi^2}\right) \quad S(\mathbf{k}) = \sum_{jk}^L e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_k)} \langle \hat{b}_j^\dagger \hat{b}_k \rangle.$$

Then the momentum distribution is obtained as

$$\rho(\mathbf{k}, t) = |\phi(\mathbf{k}, t)|^2 S(\mathbf{k}), \quad (3.22)$$

where:

- $\phi(\mathbf{k}, t)$ is the Fourier transform of the Wannier function. It can be seen that the amplitude of the function decreases with increasing the expansion time, i.e., $\mathbf{k} = \frac{P}{\hbar} = \frac{m\mathbf{v}}{\hbar} = \frac{m\mathbf{r}}{\hbar t_{\text{ex}}} \longrightarrow \mathbf{k} \sim 1/t_{\text{ex}}$. This function has no information of the original Hamiltonian in Eq.(3.5).
- $S(\mathbf{k})$ is the quasi-momentum distribution (which sometimes it is called: visibility). This function depends on the Hamiltonian in Eq.(3.5) which provides useful information about the many-body system and the long-range interaction. Our following study will be centred on the behaviour of this function.

Consequently, the interference pattern is characterised by the quasi-momentum distribution given by [116, 117]

$$S(\mathbf{k}) = \sum_{jk}^L e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_k)} \langle \hat{b}_j^\dagger \hat{b}_k \rangle. \quad (3.23)$$

Let us now study the effect of the Rydberg-dressing on $S(\mathbf{k})$. We will consider here merely on-site and nearest-neighbour interactions of the extended BH model. This approximation is well justified provided that $d/R_c > 1$, as shown previously. We furthermore will only focus on one- and two-dimensional lattices.

In order to calculate $S(\mathbf{k})$, we first evaluate the time-dependent matrix elements of the single-particle density matrix, i.e., $\langle \hat{b}_j^\dagger \hat{b}_k \rangle = \langle \text{SF}(t) | \hat{b}_j^\dagger \hat{b}_k | \text{SF}(t) \rangle$, where we consider that $|\text{SF}(t)\rangle$ is given by Eq.(3.11) with $|\text{SF}(t=0)\rangle$ is expressed in Eq.(3.9). Thus, the matrix elements are calculated as

$$\begin{aligned}
\text{If } j = k & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = |\alpha|^2 = \frac{N}{L} \\
\text{If } |j - k| = 1 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = |\alpha|^2 e^{-2|\alpha|^2 [1 - \cos(\zeta t - \gamma(1)t)]} e^{-2(2D-1)|\alpha|^2 [1 - \cos \gamma(1)t]} \\
\text{If } |j - k| = \sqrt{2} & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = |\alpha|^2 e^{-2|\alpha|^2 [1 - \cos \zeta t] - 4(D-1)|\alpha|^2 [1 - \cos \gamma(1)t]} \quad (3.24) \\
\text{If } |j - k| = 2 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = |\alpha|^2 e^{-2|\alpha|^2 [1 - \cos \zeta t] - 2(2D-1)|\alpha|^2 [1 - \cos \gamma(1)t]} \\
\text{If } |j - k| > 2 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = |\alpha|^2 e^{-2|\alpha|^2 [1 - \cos \zeta t]} e^{-4D|\alpha|^2 [1 - \cos \gamma(1)t]}.
\end{aligned}$$

Using this data we obtain the following results:

3.3.1.1. One-dimensional lattice

In order to be able to distinguish contributions of the on-site and nearest-neighbour interaction, we start with a situation where only the on-site interaction is present. This corresponds to a scenario that was experimentally studied in Ref.[107] and in case of the Rydberg-dressed atoms this is realised when $d/R_{SC} \gg 1$. The quasi-momentum distribution $S(k_x)$ changes as a function of time as shown in Fig.(3.6,a). Two main features can be identified:

- i. First, at $t = 0$, $S(k_x)$ is centred around $k_x = 0$. As the interaction time grows $S(k_x)$ collapses to flat distribution and at an even later time ($\zeta t = 2\pi$) it revives to its original value.
- ii. The second feature is that the periodicity of $S(k_x)$ does not depend on k_x (although the amplitude does). This is a direct consequence of the fact that the correlation function is factorisable, i.e., $\langle \hat{b}_j^\dagger \hat{b}_k \rangle = \langle \hat{b}_j^\dagger \rangle \langle \hat{b}_k \rangle$ for all j and k [118]. The time-dependence thus becomes a global factor of $S(k_x)$.

This changes in the presence of the nearest-neighbour interaction, i.e., $\gamma(1) \neq 0$. Due to a nonzero $\gamma(1)$, $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ is no longer factorizable but depends on the relative distance between respective sites as shown in Eqs.(3.24). This gives rise to strikingly

different features in the quasi-momentum distribution. An example of this is shown in Fig.(3.6,b) for $d/R_c = 1.5$ where $\gamma(1) \approx 0.08\zeta$. The noteworthy feature here is that the time-dependence of $S(k_x)$ depends on the quasi-momentum k_x . For example, at $\zeta t = 2\pi$, we find that $S(k_x)$ revives partially along $k_x = 0$ as in Fig.(3.6,c), while along $k_x = \pi$ it shows a clearly different oscillation pattern as in Fig.(3.6,d).

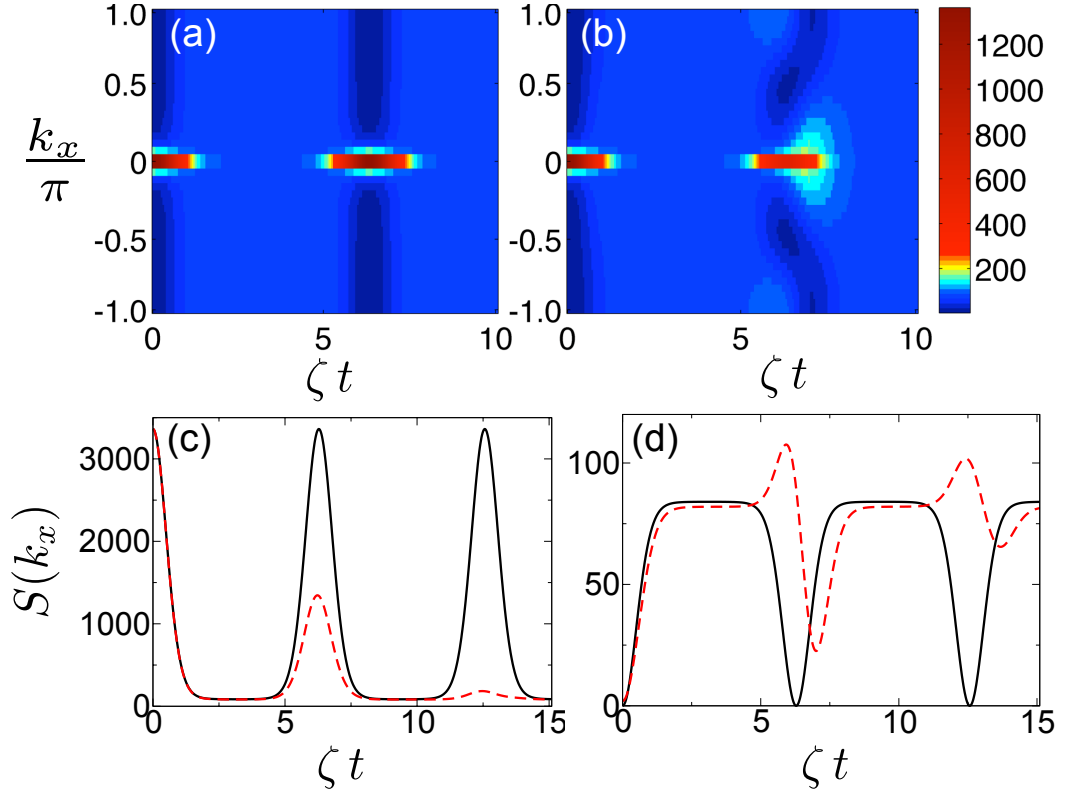


Figure 3.6.: (Color online) Quasi-momentum distribution of $N = 82$ atoms released from a one-dimensional optical lattice with $L = 41$ sites. (a) On-site interaction only, i.e. $\gamma(m) = 0$ (corresponding to $d/R_c \gg 1$), (b) On-site and nearest-neighbour interaction for $d/R_c = 1.5$ ($\gamma(1) \approx 0.08\zeta$). (c,d) Cuts through $S(k_x)$ at different values of the quasi-momentum. The panels show cuts along $k_x = 0$ (c) and $k_x = \pi$ (d). The solid/dashed curves correspond to the parameters of panel (a)/(b).

An additional calculation for the matrix elements $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ is carried out using the many-body state expressed in Eq.(3.6) instead of the coherent state in Eq.(3.9) where we have obtained⁵

⁵Full derivation can be found in the Appendix G

$$\begin{aligned}
\text{If } j = k & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = \frac{N}{L} \\
\text{If } |j - k| = 1 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = \frac{N}{L} \left[1 - \frac{4}{L} + \frac{2}{L} \cos(a - ab) + \frac{2}{L} \cos ab \right]^{N-1} \\
\text{If } |j - k| = 2 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = \frac{N}{L} \left[1 - \frac{4}{L} + \frac{2}{L} \cos(a) + \frac{2}{L} \cos ab \right]^{N-1} \\
\text{If } |j - k| = 3 & \quad \langle \hat{b}_j^\dagger \hat{b}_k \rangle = \frac{N}{L} \left[1 - \frac{6}{L} + \frac{2}{L} \cos(\alpha) + \frac{4}{L} \cos ab \right]^{N-1},
\end{aligned} \tag{3.25}$$

with $a = \zeta t$ and $b = \gamma(1)/\zeta$. It can be obviously noticed from the comparison between both methods visualized in Fig.(3.7) that both of them are quite identical. Therefore, whether the interference visibility is calculated via Eq.(3.6) or Eq.(3.9) the results are exactly alike.

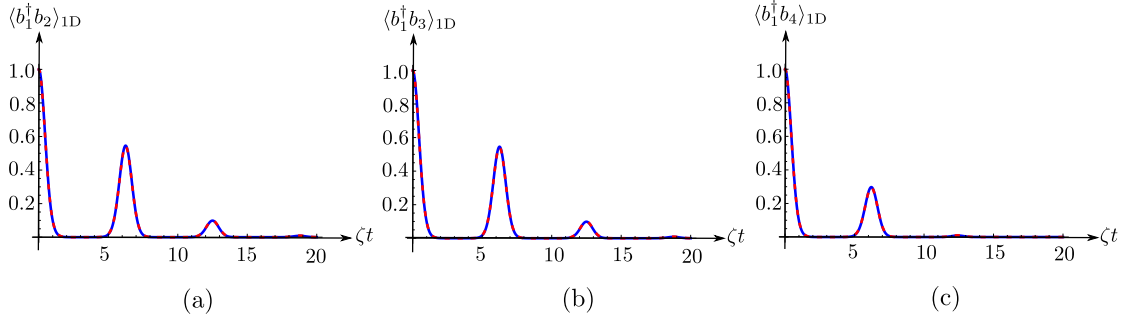


Figure 3.7.: The matrix elements of the single-particle density matrix, $\langle b_j^\dagger b_k \rangle$ when $|j - k| = 1, 2, 3$ in (a), (b), (c), respectively, plotted using the initial superfluid state as a many-body state expressed in Eq.(3.6) as in the blue solid line, and using the coherent state in Eq.(3.9) as the dashed red line shows in one dimensional optical lattice. With $\gamma(1) = 0.08\zeta$.

3.3.1.2. Two-dimensional lattice

Let us now turn to the discussion of the interference pattern that emerges in the case in which the atoms are released from a two-dimensional optical lattice. In order to have a reference we again calculate at first the interference patterns for vanishing nearest-neighbour interaction. The main features in the interference pattern can be captured by analysing time slices taken at $\zeta t = 0, \pi/2$ and 2π . This data is shown in Fig.(3.8,a-c). Like in the one-dimensional case the time-evolution is periodic showing a first revival at $\zeta t = 2\pi$ and the expected periodicity [107]. In Fig.(3.8,d-f), we

present the interference pattern that is obtained in case of a finite nearest-neighbour interaction ($d/R_c = 1.45$ and $\gamma(1) \approx 0.1g$) using the same time slices. We find that the height of the peaks of $S(\mathbf{k})$ in Fig.(3.8,f) is lowered compared to Fig.(3.8,c). The most striking feature is, however, the appearance of additional interference maxima in between the ones that occurred previously in the case of pure on-site interactions. These peaks occur because the nearest-neighbour interaction $\gamma(1)$ actually affects (indirectly) the phase relation between atoms that are separated by a distance $\sqrt{2}d$ (next-nearest neighbours $\gamma(\sqrt{2})$) as shown in Eqs.(3.24).

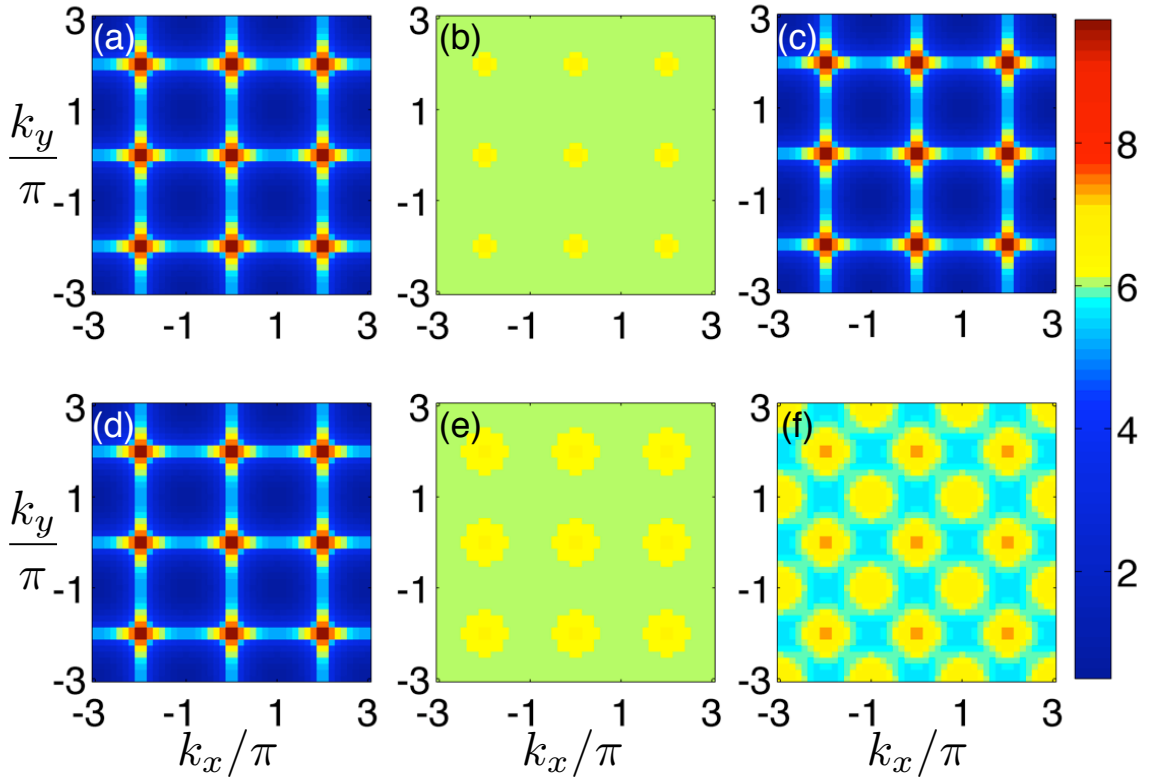


Figure 3.8.: (Color online) Natural logarithm of the quasi-momentum distribution $S(\mathbf{k})$ of atoms released from a two-dimensional 15×15 -lattice and an average particle number in each sites of $|\alpha|^2 = 2$. The figures show snapshots taken different times: $\zeta t = 0$ [(a) and (d)], $\zeta t = \pi/2$ [(b) and (e)] and $\zeta t = 2\pi$ [(c) and (f)]. Panels (a)-(c) show data that has been obtained by taking only on-site interactions into account. The data shown in panels (d)-(f) includes also nearest-neighbour interactions.

3.4. Conclusion

In conclusion, we have shown that Rydberg-dressed atoms in an optical lattice give rise to an extended BH model. In particular, we have studied the dynamical evolution of an atomic superfluid under the influence of Rydberg dressing. The emerging long-range interactions result in a rapid collapse of the superfluid order parameter and in general allow only for partial revivals. Moreover, we have demonstrated that interference experiments can directly reveal the interaction between Rydberg-dressed atoms. The hallmark here is the emergence of additional interference maxima. In addition, the time-dependence of the quasi-momentum distribution is no longer a global factor. This leads to a time-dependence which strongly depends on value of the quasi-momentum.

We expect that our predictions can be probed in current experiments using Rydberg atoms in lattices, e.g. the one presented in Ref.[119] by Viteau *et al.* In this particular experiment Rydberg D-states of rubidium-87 with principal quantum numbers in the range $n = 55 - 80$ are excited and the lattice spacing can be tuned within $0.42 \mu\text{m} < d < 13 \mu\text{m}$. If one instead excites a Rydberg S-state with $n = 60$ and uses a laser with the parameters $\Delta = 2\pi \times 15 \text{ MHz}$ and $\Omega = 2\pi \times 0.5 \text{ MHz}$ one obtains $R_c \approx 4 \mu\text{m}$ as the characteristic length scale of the soft-core potential. This leaves sufficient freedom for tuning the ratio d/R_c . The typical revival time of the interference signal evaluates to $t_0 \approx 27 \text{ ms}$. This has to be compared with the effective lifetime of dressed ground state atoms, $\tau_{\text{eff}} = |\Delta/\Omega|^2 \times \tau_{\text{Ryd}}$ where τ_{Ryd} is the bare lifetime of the Rydberg state since we need to have a long lifetime for the Rydberg atom in order to be able to observe the revival dynamics. Using the above parameters, we obtain $\tau_{\text{eff}} = 225 \text{ ms}$, which leads to a coherence time that in principle should permit the observation of the predicted dynamics.

CHAPTER 4

Dynamic splitting of a BEC with long-range interactions

Up to this chapter, our focus has been on the study of dynamics of Bose-Einstein condensate (BEC) in time-independent potential traps. In the current chapter, it is with a great interest to take it further and investigate these dynamics in a time-dependent adiabatic potential trap.

The evolution of a system under a slowly varying Hamiltonian, the so called *adiabatic evolution*, has been a well-studied problem in both classical and quantum mechanics [120] and an important method of preparation and control of quantum states. This theorem indicates that an initial non-degenerate eigenstate remains to be an instantaneous eigenstate when the Hamiltonian changes slowly in time comparing to the level spacing [121].

In this chapter we study N repulsively contact-interacting bosonic atoms of zero temperature forming a Bose-Einstein condensate. This ensemble is studied using the non-linear time-dependent Schrödinger equation or the so-called Gross-Pitaevskii equation.

The structure of this chapter is organised as follows. Firstly, we introduce in section (4.1) the adiabatic transformation method where we present the dynamical variable of the process, the so-called “the adiabatic switching function” in subsection (4.1.1). The behaviour of the ground state of an N -atom ensemble as a response to the adiabatic potential change and the strength of the contact-interaction is presented in section (4.2) where a numerical method known as “imaginary time propagation method (ITPM)” is studied in subsection (4.2.1) in order to get the initial state of the numerical calculation. Eventually, this chapter ends with a conclusion in section (4.3) that summarizes the results being presented.

4.1. Adiabatic transformation of the harmonic oscillator potential

Initially, we consider in our system N non-interacting bosonic atoms trapped in a harmonic oscillator potential $V_{\text{ho}}(x)$ at $t = 0$, and these atoms reside in their ground state $\psi_{\text{ho}}^{(0)}(x, t = 0)$. Now, we are going to slowly (adiabatically) change the potential from a harmonic oscillator potential $V_{\text{ho}}(x) = \frac{1}{2}m\omega^2x^2$ from an initial time $t = 0$ into a double-well potential $V_{\text{dw}}(x) = \gamma x^4 - \beta x^2$ at a final time $t = t_{\text{max}}$ as it schematically depicted in Fig(4.1). This transformation is very interesting because of the dramatic change in the structure of the wave functions from the beginning till the end [122].

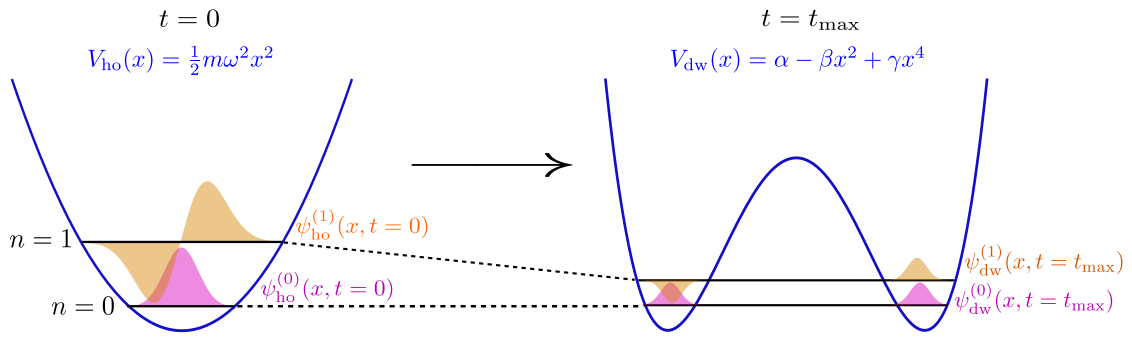


Figure 4.1.: Schematic illustration of the adiabatic transformation of the harmonic oscillator potential from $t = 0$ to a double-well potential at $t = t_{\text{max}}$ where $\psi_{\text{ho}}^{(0,1)}(x, t = 0)$ and $\psi_{\text{dw}}^{(0,1)}(x, t = t_{\text{max}})$ are the ground and the first excited states for the harmonic and the double-well potentials, respectively.

In a problem where the Hamiltonian $\hat{H}(t)$ changes in a continuous way from an initial time $t = 0$ to a final time $t = t_{\text{max}}$, the quantum¹ adiabatic theorem states that, if the system initially begins in a non-degenerate eigenstate of a simple Hamiltonian $\hat{H}(t = 0)$ for which the solution is analytically known², then the wave function is propagated using a time-varying Hamiltonian from $t = 0$ to $t = t_{\text{max}}$ with a certain propagation time. The wave function and its energy at the final time will be the corresponding eigenvalue and eigenfunction of the new Hamiltonian $\hat{H}(t = t_{\text{max}})$ [122]. Therefore, if the initial state of our system was the ground state of the harmonic oscillator potential, i.e., $\psi_{\text{ho}}^{(0)}(x, t = 0)$, then after a certain adiabatic time

¹We will not discuss the classical adiabatic switching method in our system since it fails completely in describing the change in the wave functions [122].

²It is due to simplicity to choose an analytically known solution for the initial state of the adiabatically evolving system.

$t \gg 0$, the system would reach the ground state of the double-well potential, i.e., $\psi_{\text{dw}}^{(0)}(x, t = t_{\text{max}})$, at $t = t_{\text{max}}$.

In order for the quantum adiabatic switching to be numerically efficient, i.e., ultimately converges to the ground state of the double-well potential at $t = t_{\text{max}}$, it is necessary to find a propagation method which takes maximum advantage of the fact that the time-dependent wave function $\psi(x, t)$ is almost an eigenstate at all times [122]. Therefore, to demonstrate this transformation, the time-dependent potential is chosen to be given by:

$$\mathcal{V}_{\text{td}}(x, t) = V_{\text{ho}}(x) + \lambda(t) [V_{\text{dw}}(x) - V_{\text{ho}}(x)], \quad (4.1)$$

where $\lambda(t)$ is an adiabatic switching function which will be thoroughly discussed in the next subsection. This expression shows that the process of turning off the harmonic oscillator potential and switching on the double-well potential depends mainly on the nature and the structure of the adiabatic switching function.

4.1.1. Adiabatic switching function

As we have seen in Eq.(4.1), $\lambda(t)$ is a time-dependent adiabatic switching function. This function changes, over the time interval $0 \leq t \leq t_{\text{max}}$, from $\lambda(t = 0) = 0$ to $\lambda(t = t_{\text{max}}) = 1$. To have the maximum convergence to the adiabatic limit, this function must satisfy the following properties:

1. Ideally, the switching function should be smooth, i.e., be continuous with a continuous first derivative.
2. It has a zero first derivative at both the start and end of the switching, i.e., at $t = 0$ and $t = t_{\text{max}}$,

$$\left. \frac{d\lambda(t)}{dt} \right|_{t=0} = \left. \frac{d\lambda(t)}{dt} \right|_{t=t_{\text{max}}} = 0.$$

The reason for this condition is explained as follows. In the adiabatic switching one starts with a system at a certain state (the ground state in our case), but the system then starts to lag behind the Hamiltonian as the switching takes place. By using a switching function whose derivative is initially zero, the

system will not go far from its initial ground state so abruptly. Similarly, by finishing with zero derivative, the system is given a chance to catch up with the final form of the Hamiltonian.

3. In order to make the energy states of the time-dependent potential realise the potential's change, the maximum rate of change of $\lambda(t)$ with respect to t should be as small as possible in the adiabatic region [123] comparing to the frequency Ω between the time-dependent ground $E_0(t)$ and first excited $E_1(t)$ states

$$\frac{d\lambda(t)}{dt} \ll \Omega \sim \frac{\Delta E(t)}{\hbar}.$$

For that matter, we introduce the following adiabatic function, illustrated in Fig(4.2).

$$\lambda(t) = \sin^2\left(\frac{\pi t}{2t_{\max}}\right). \quad (4.2)$$

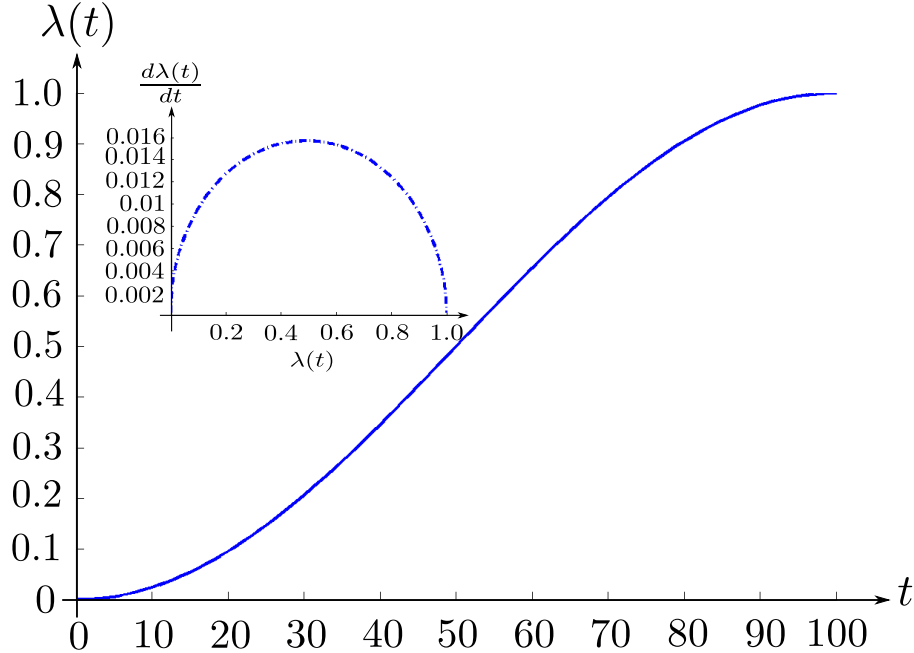


Figure 4.2.: (a) The adiabatic switching functions $\lambda(t)$ as a function of time. (b) The first derivative of the adiabatic functions $d\lambda(t)/dt$.

It is obvious that $\lambda(t)$ satisfies the first two adiabatic conditions. Regarding the third condition, since initially at $t = 0$, the system is assumed to be in a non-degenerate eigenstate of $\hat{H}(x, t = 0)$ specified by a quantum number $n = 0$, i.e., $\psi_{\text{ho}}^{(0)}(x, t = 0)$,

then, in the adiabatic limit, and assuming no degeneracies occur, the wave function will change with time such that it remains the instantaneous eigenfunction of the Hamiltonian $\hat{H}(x, t)$ with the same quantum number [123] until the end of the adiabatic process at $t = t_{\max}$ where the wave function represents the ground state of the double-well potential, i.e., $\psi_{\text{dw}}^{(0)}(x, t = t_{\max})$. Hence, if the adiabatic process is carried out on a time-scale which is much longer than the relaxation time of the system³, then in practice, this process is described by an infinite number of quasi-static Schrödinger equations (at each time step t) which can be written as

$$\begin{aligned} \hat{H}(x, t)\psi(x, t) &= E(t)\psi(x, t) \\ \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \mathcal{V}_{\text{td}}(x, t) \right] \psi(x, t) &= E(t)\psi(x, t), \end{aligned} \quad (4.3)$$

where: $\psi(x, t)$, $E(t)$ are the quasi-static eigenstates and eigenenergies, respectively. To numerically diagonalise the Hamiltonian $\hat{H}(x, t)$ we need to scale this equation to natural units where we obtain

$$\left[-\frac{d^2}{dq^2} + \tilde{\mathcal{V}}_{\text{td}}(q, \tau) \right] \tilde{\psi}(q, \tau) = \epsilon(\tau) \tilde{\psi}(q, \tau). \quad (4.4)$$

Here $q = \frac{x}{\xi}$ and $\tau = t\omega$ are the dimensionless spatial and time variables, $\epsilon(\tau) = \frac{2m\xi^2}{\hbar^2} E(t)$ is the time-dependent eigenenergies. The time-dependent potential is $\tilde{\mathcal{V}}_{\text{td}}(q, \tau) = \tilde{V}_{\text{ho}}(q) + \lambda_i(\tau) [\tilde{V}_{\text{dw}}(q) - \tilde{V}_{\text{ho}}(q)]$ where $\tilde{V}_{\text{ho}}(q) = l'q^2$ is the harmonic oscillator potential with $l' = \frac{m^2\omega^2\xi^4}{\hbar^2}$, and $\tilde{V}_{\text{dw}} = -\tilde{\beta}'q^2 + \tilde{\gamma}'q^4$ is the double-well potential with $\tilde{\beta}' = \frac{2\beta\xi^4m}{\hbar^2}$ and $\tilde{\gamma}' = \frac{2\gamma\xi^6m}{\hbar^2}$. As shown in Fig.(4.3, a), the energy difference $\Delta\epsilon(\tau) = \epsilon_1(\tau) - \epsilon_0(\tau)$ is plotted as a function of the adiabatic switching function $\lambda(\tau)$. At $t = 0$, the energy difference is equal to $\Delta\epsilon(\tau = 0) = 1$ which corresponds to the energy difference between any two eigenstates of the harmonic oscillator potential. However, $\Delta\epsilon(\tau = \tau_{\max}) \sim 10^{-11}$ which corresponds to the energy difference between the first two eigenstates of the double-well potential that usually represents the numerical tunnelling rate between both wells as was discussed in the subsubsection (2.1.4.1). Moreover, in Fig.(4.3, b) the energy difference $\Delta\epsilon'(\tau) = \epsilon_2(\tau) - \epsilon_1(\tau)$

³The relaxation time is the typical time-scale for the system to return to equilibrium after being suddenly disturbed.

increases from $\Delta\epsilon'(\tau = 0) = 1$ to $\Delta\epsilon'(\tau = \tau_{\max}) \sim 1.5$. This can be understood from the double-well energy states structure as was shown in Fig.(2.5) where we have seen that ϵ_1 is far from ϵ_2 but close to ϵ_0 . The spectrum of the first four eigenenergies as a function of $\lambda(\tau)$ is illustrated in Fig.(4.4).

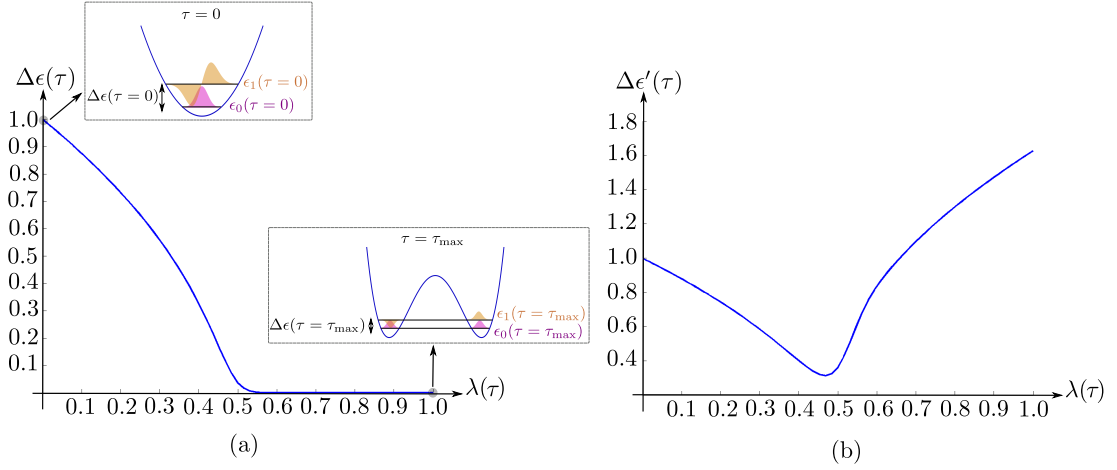


Figure 4.3.: (a): the energy difference $\Delta\epsilon(\tau)$ between the ground state $\epsilon_0(\tau)$ and the first excited state $\epsilon_1(\tau)$ of the time-dependent potential as a function of the adiabatic switching functions $\lambda(\tau)$. (b): the energy difference $\Delta\epsilon'(\tau)$ between the second $\epsilon_2(\tau)$ and the first excited states $\epsilon_1(\tau)$.

To ensure that the third adiabatic condition is entirely fulfilled, we first obtain the quasi-static ground state of the double-well potential, i.e., $\tilde{\psi}_{\text{dw}}^{(0)}(q, \tau = \tau_{\max})$, which is the solution of Eq.(4.4) at $\tau = \tau_{\max}$, and then, after choosing the initial state to be the ground state of the harmonic oscillator potential, i.e., $\tilde{\Psi}(q, \tau = 0) = \tilde{\psi}_{\text{ho}}^{(0)}(q, \tau = 0)$ we integrate the dimensionless version of the time-dependent Schrödinger equation that is given by

$$i \frac{\partial \tilde{\Psi}(q, \tau)}{\partial \tau} = \hat{\mathcal{H}}(q, \tau) \tilde{\Psi}(q, \tau) = \left(-l \frac{d^2}{dq^2} + \tilde{\mathcal{V}}_{\text{td}}(q, \tau) \right) \tilde{\Psi}(q, \tau), \quad (4.5)$$

where $\tilde{\mathcal{V}}_{\text{td}}(q, \tau) = \tilde{V}_{\text{ho}}(q) + \lambda_i(\tau) (\tilde{V}_{\text{dw}}(q) - \tilde{V}_{\text{ho}})$ is the dimensionless time-dependent potential where the harmonic potential is $\tilde{V}_{\text{ho}}(q) = \frac{1}{4l} q^2$ with $l = \frac{\hbar}{2m\xi^2\omega}$, and $\tilde{V}_{\text{dw}}(q) = \tilde{\gamma} q^4 - \tilde{\beta} q^2 - \frac{1}{4l} q^2$ is the double-well potential with $\tilde{\gamma} = \frac{\beta \xi^4}{\hbar \omega}$ and $\tilde{\beta} = \frac{\alpha \xi^2}{\hbar \omega}$. Therefore, if the following quantity is fulfilled

$$I = |\langle \tilde{\Psi}(q, \tau_{\max}) | \tilde{\psi}_{\text{dw}}^{(0)}(q, \tau = \tau_{\max}) \rangle|^2 = 1, \quad (4.6)$$

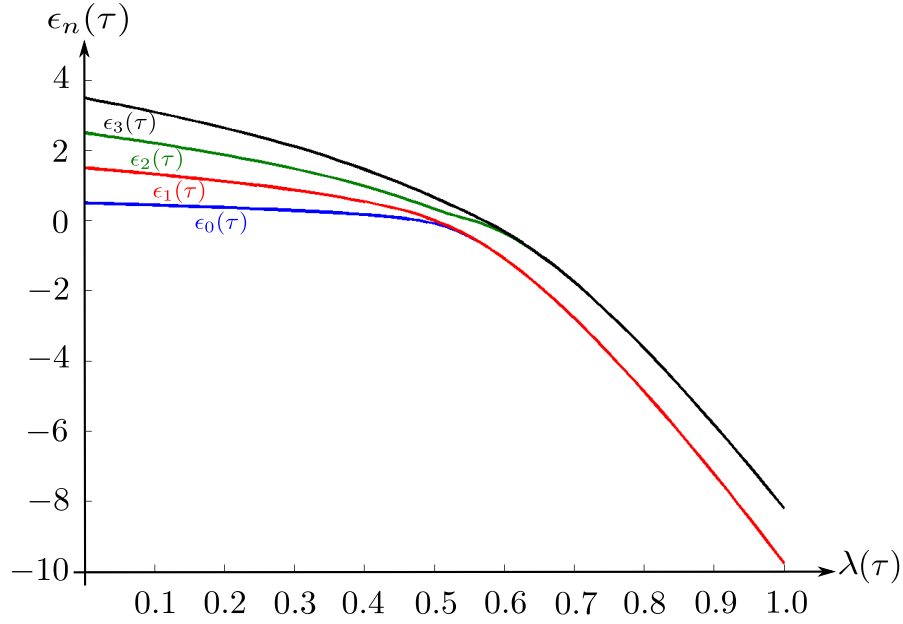


Figure 4.4.: The first four eigenenergies spectrum $\epsilon_n(\tau)$ with $n = 0, 1, 2, 3$ as a function of the adiabatic switching function $\lambda(\tau)$.

then it means that as the system begins from the ground state of the harmonic oscillator potential at $\tau = 0$, it will reach the adiabatically connected ground state of the double-well potential at $\tau = \tau_{\max}$ after a certain adiabatic propagation time $\tau_{\max}$. Fig(4.5) shows that for an adiabatic process lifetime $\tau_{\max} = 10^3$, the quantity in Eq.(4.6) equals zero at $\tau = 0$, and as time passes by, the value increases until the end of the adiabatic passage at $\tau = \tau_{\max}$ where it equals to an exact unity, i.e., $|\langle \tilde{\Psi}(q, \tau_{\max}) | \tilde{\psi}_{\text{dw}}^{(0)}(q, \tau = \tau_{\max}) \rangle|^2 = 1$.

As a result, since our adiabatic switching function $\lambda(t)$, expressed in Eq.(4.2), satisfies all the three adiabatic conditions, then by using this adiabatic function, and solving the time-dependent Schrödinger equation in Eq.(4.5), we can see how the probability density changes over time as shown in Fig.(4.6). At the beginning of the adiabatic process at $\tau = 0$ the probability density represents the ground state of the harmonic oscillator. As time passes by $\tau > 0$, the particle will adiabatically follow the same state that, as a result of the potential change, deforms and inclines to be composed of two peaks until the end of the switching time at $\tau = \tau_{\max}$ where it shows the probability density of the ground state of the double-well potential. Moreover, we have seen that in the limit of non-interacting regime, we use the time-dependent

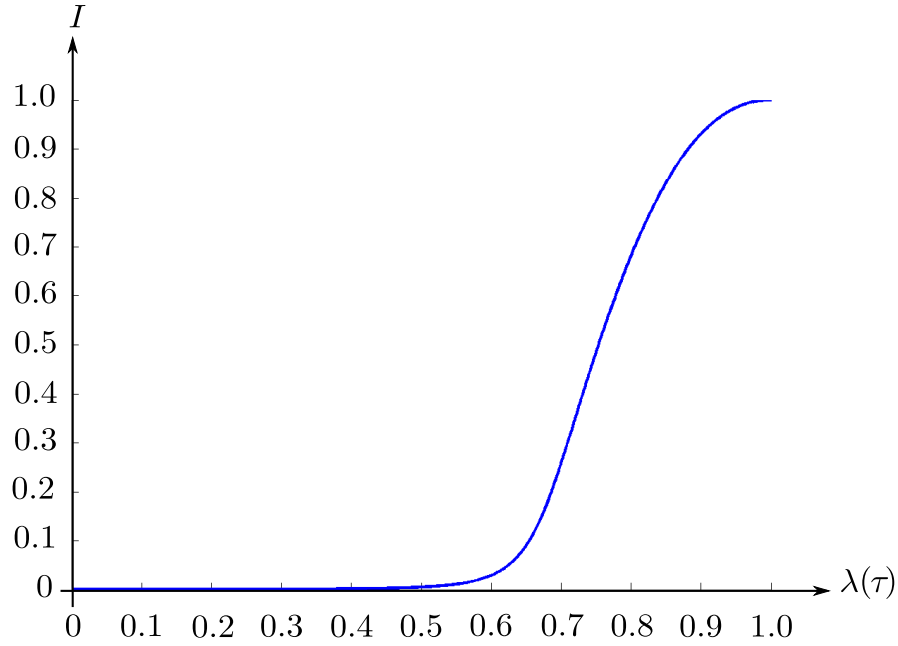


Figure 4.5.: The closeness $I = |\langle \tilde{\Psi}(q, \tau_{\max}) | \tilde{\psi}_{\text{dw}}^{(0)}(q, \tau = \tau_{\max}) \rangle|^2$, with $\tau_{\max} = 10^3$, $l = 0.5$, $\tilde{\beta} = 0.40$ and $\tilde{\gamma} = 0.01$.

(and quasi-static) Schrödinger equation in Eq.(4.4) to express the adiabatic process which is described by a time-dependent potential $\mathcal{V}_{\text{td}}(x, t)$ that depends mainly on the structure of the adiabatic switching function $\lambda(t)$.

4.2. Splitting of an interacting BEC

Initially, we consider N bosonic atoms trapped in a harmonic oscillator potential and these atoms interact via repulsive contact-interaction $a > 0$ with a is the s-wave scattering length. From the theoretical point of view, and similarly to what we have seen earlier, the properties and the dynamics of this condensate are usually described by the mean-field equation for the condensate wave function, i.e., the time-dependent non-linear Gross-Pitaevskii equation (GPE), which is given by:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega x^2 + g_{1D} |\Psi(x, t)|^2 \right) \Psi(x, t), \quad (4.7)$$

where: $g_{1D} \sim a$ is the one-dimensional coupling constant which determines the strength of the interatomic interaction and proportional to the s-wave scattering length. The dimensionless version of this equation is expressed as

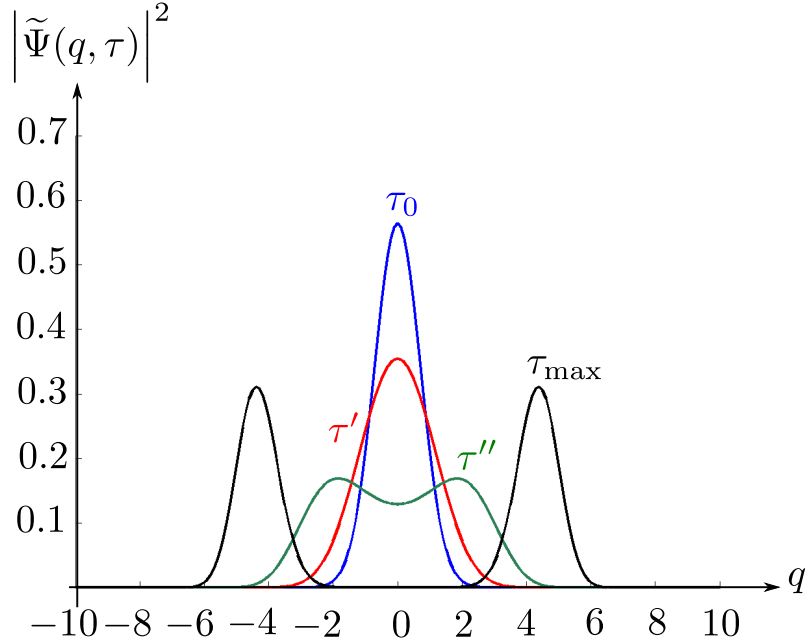


Figure 4.6.: The probability density of the ground state wave function of N non-interacting atoms trapped in a time-dependent Hamiltonian from $\tau_0 = 0$ until $\tau = \tau_{\max}$ with $\tau_0 = 0 < \tau' = 500 < \tau'' = 600 < \tau_{\max} = 10^3$, $l = 0.5$, $\tilde{\beta} = 0.40$ and $\tilde{\gamma} = 0.01$.

$$\begin{aligned}
 i \frac{\partial \tilde{\Psi}(q, \tau)}{\partial \tau} &= \hat{\mathcal{N}}(\tilde{\Psi}) \tilde{\Psi}(q, \tau) \\
 &= \left(-l \frac{\partial^2}{\partial q^2} + \frac{1}{4l} q^4 + \tilde{g}_{1D} |\tilde{\Psi}(q, \tau)|^2 \right) \tilde{\Psi}(q, \tau),
 \end{aligned} \tag{4.8}$$

where: $\hat{\mathcal{N}}(\tilde{\Psi})$ is the non-linear Hamiltonian, $l = \frac{\hbar}{2m\xi^2\omega}$ and $\tilde{g}_{1D} = \frac{g_{1D}}{\hbar\omega}$. Our purpose now is to solve the GPE and get its ground state. In general, finding an analytical solution for it is quite difficult. However, it is possible to get the ground state to a good accuracy using a mathematical trick known as *imaginary time propagation method* (ITPM).

4.2.1. Imaginary time propagation method (ITPM)

Imaginary time propagation method is a reliable and easily-implemented method of obtaining the ground state of the system by propagation in imaginary time [30]. In general, finding the ground state wave function directly from the Hamiltonian

for a quantum system is difficult, with only a few known exactly solvable systems. However, this mathematical trick makes it possible to approximate a ground state wave function to a good accuracy. The convergence can, however, be accelerated in practice by choosing $\tilde{\Psi}(q, \tau = 0)$ appropriately [124].

The algorithm for this method can be put in order as following:

- i. **Substitute** the imaginary time $i\tau = \nu$ instead of the real time τ in the GPE in Eq.(4.8) via the so-called, Wick rotation, i.e., $\tau \longrightarrow i\tau = \nu$. Then we write :

$$i \frac{\partial \tilde{\Psi}}{\partial \tau} = \hat{\mathcal{N}}(\tilde{\Psi}) \tilde{\Psi} \quad \longrightarrow \quad \frac{\partial \tilde{\Psi}}{\partial (i\tau)} = \frac{\partial \tilde{\Psi}}{\partial \nu} = -\hat{\mathcal{N}}(\tilde{\Psi}) \tilde{\Psi}.$$

Since the formal solution for Eq.(4.8) is given by:

$$\tilde{\Psi}(q, \tau) = \exp(-i\hat{\mathcal{N}}\tau) \tilde{\Psi}(q, \tau = 0), \quad (4.9)$$

then after propagating GPE in imaginary time, this solution changes to

$$\tilde{\Psi}(q, \nu) = \exp(-\hat{\mathcal{N}}\nu) \tilde{\Psi}(q, \nu = 0). \quad (4.10)$$

Expanding the initial state $\tilde{\Psi}(q, \nu = 0)$ in the basis of eigenfunctions φ_n ,

$$\tilde{\Psi}(q, \nu = 0) = \sum_n c_n \varphi_n(q) \quad \text{where: } c_n = \langle \varphi_n(q) | \tilde{\Psi}(q, \nu = 0) \rangle,$$

allows us to write the time-evolution in Eq.(4.10) as

$$\tilde{\Psi}(q, \nu) = \sum_n \exp(-\epsilon_n \nu) c_n \varphi_n(q). \quad (4.11)$$

It can be seen from Eq.(4.10) and Eq.(4.11) that the unitary time-evolution has turned into an exponential decay. Crucially, the eigenenergy governs the decay rate, and so the eigenstate with the lowest energy, i.e. the ground state of the system, decays slowest [30]. In this way, in general, for a sufficiently long time integration $\nu \rightarrow \infty$ and under the action of $\exp(-\epsilon_n \nu)$, the initial state converges asymptotically to the ground state, i.e., $\tilde{\Psi}(q, \nu) \rightarrow e^{-\epsilon_0 \nu} c_0 \varphi_0$, since the other exponentials decay more rapidly. [125].

- ii. **Split** equally the imaginary time interval into N_ν imaginary time steps with an equal distance between each step equal to $d\nu$.
- iii. **Solve** the equation $\frac{\partial \tilde{\Psi}}{\partial \nu} = -\hat{\mathcal{N}}(\tilde{\Psi})\tilde{\Psi}$ at each imaginary time step.
- iv. **Renormalise** the resulting state after each imaginary time step. The reason behind the renormalisation is because the Gross-Pitaevskii equation does not conserve the norm, i.e., the inner product of two states changes with time⁴.

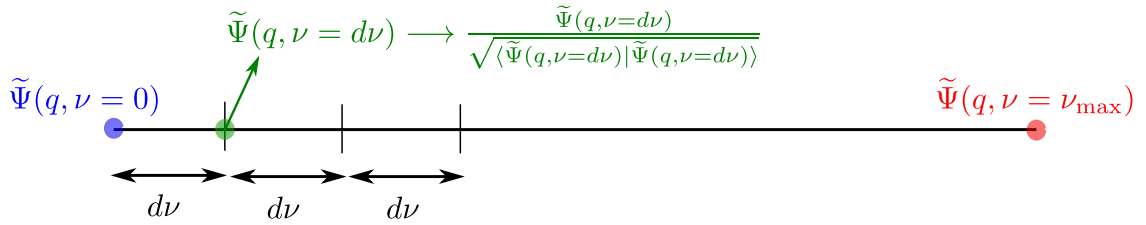


Figure 4.7.: Imaginary time propagation method (ITPM).

Fig.(4.8, a) shows the ground state probability density for the dimensionless GPE propagating in imaginary time for different strengths of the contact-interaction $\tilde{g}_{1D}$. it can be seen that the probability density in the non-interacting limit $\tilde{g}_{1D} = 0$ represents the ground state of the harmonic oscillator potential. As the contact-interaction increases, the probability density takes the shape of an inverted parabola.

After we have obtained the ground state of N contact-interacting atoms trapped in a harmonic oscillator potential using ITPM, we now, consider this state as an initial state for the same N atoms but this time they are trapped in a time-dependent potential $\tilde{\mathcal{V}}_{td}(q, \tau)$. Then, solving the time-dependant and dimensionless GPE in real time illustrates the change of the corresponding adiabatic probability density for a certain contact-interaction strength,

⁴The unitary time-evolution equation is given by: $\tilde{\Psi}(\tau) = e^{-i\hat{\mathcal{N}}\tau}\tilde{\Psi}(\tau = 0)$. The inner product of the state $\tilde{\Psi}(\tau)$ is calculated as (bearing in mind that $\hat{\mathcal{N}}$ is a hermitian operator):

$$\langle \tilde{\Psi}(\tau) | \tilde{\Psi}(\tau) \rangle = \langle e^{i\hat{\mathcal{N}}\tau} \tilde{\Psi}(\tau = 0) | e^{-i\hat{\mathcal{N}}\tau} \tilde{\Psi}(\tau = 0) \rangle = e^{i\hat{\mathcal{N}}\tau} e^{-i\hat{\mathcal{N}}\tau} \langle \tilde{\Psi}(\tau = 0) | \tilde{\Psi}(\tau = 0) \rangle = 1.$$

But in case of GPE in imaginary time propagation, the inner product changes with time, i.e.,

$$\langle \tilde{\Psi}(\nu) | \tilde{\Psi}(\nu) \rangle = \langle e^{-\hat{\mathcal{N}}\nu} \tilde{\Psi}(\nu = 0) | e^{-\hat{\mathcal{N}}\nu} \tilde{\Psi}(\nu = 0) \rangle = e^{-\hat{\mathcal{N}}\nu} e^{-\hat{\mathcal{N}}\nu} \langle \tilde{\Psi}(\nu = 0) | \tilde{\Psi}(\nu = 0) \rangle = e^{-2\hat{\mathcal{N}}\nu}.$$

$$i \frac{\partial \tilde{\Psi}(q, \tau)}{\partial \tau} = \left(-l \frac{d^2}{dq^2} + \tilde{\mathcal{V}}_{\text{td}}(q, \tau) + \tilde{g}_{1\text{D}} |\tilde{\Psi}(q, \tau)|^2 \right). \quad (4.12)$$

Fig(4.8, b) shows how the adiabatic ground state density of the GPE changes over time and for different contact-interaction values. It can be seen that the ground state density of the double-well potential gets broader and more parabolic by increasing the strength of the interaction .

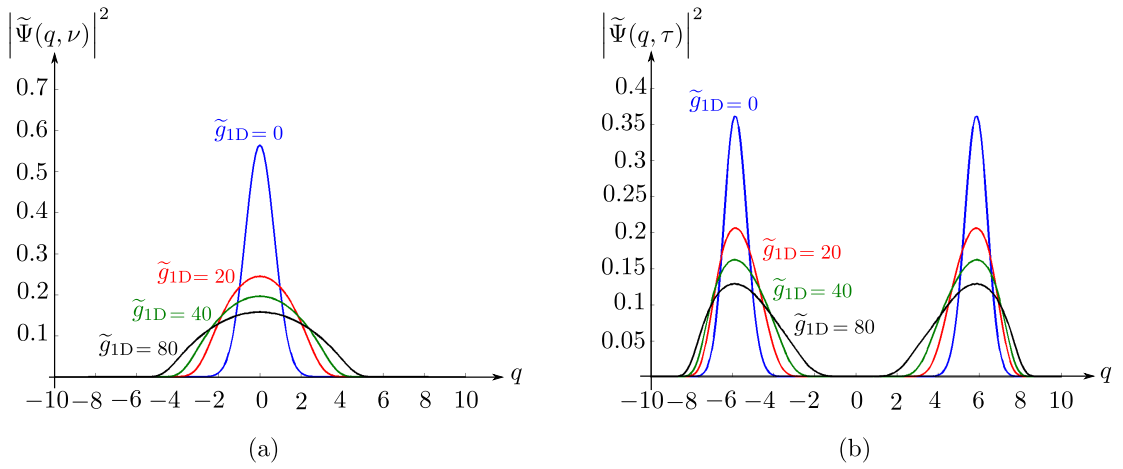


Figure 4.8.: (a) The probability density of the ground state wave function for N contact-interacting atoms trapped in a harmonic oscillator potential for different interaction values $\tilde{g}_{1\text{D}}$ and calculated using the imaginary time propagation method (ITPM) where ν is the imaginary time and $l = 0.5$. (b) The probability density of the ground state wave function of N contact-interacting atoms at the end of the adiabatic process, i.e., $t = t_{\text{max}}$, for different interaction values d and calculated using the real time propagation τ , where $\tau_{\text{max}} = 10^3$, $l = 0.5$, $\tilde{\beta} = 0.70$ and $\tilde{\gamma} = 0.01$.

4.3. Conclusion

To sum up, we have analysed a system of N contact-interacting bosons that undergo an adiabatic evolution transformation of the external potential trap. The adiabatic process depends mainly on the dynamical variable, the so-called adiabatic switching function $\lambda(t)$ that have to satisfy certain conditions to maximise the rate of convergence of the energy to its adiabatic limit.

For N contact-interacting bosonic atoms, the dynamics were governed by the time-dependent non-linear Gross-Pitaevskii equation where we have investigated

the time-evolution of the ground-state probability density and the spectrum of the eigenenergies. To numerically solve such a system, a mathematical trick, known as imaginary time propagation method, was required to get the system's initial state. Therefore, and depending on the resulting initial state, we managed via solving the time-dependent Schrödinger equation in real time to notice the change of the probability density at the end of the adiabatic process for different contact-interaction strengths.

CHAPTER 5

Summary and outlook

To conclude this thesis, we would like to make a brief summary of its content. Also, we mention possible directions of future work.

In chapter 1, three theoretical background topics have been presented. We have started with investigating the basic concepts of Bose-Einstein condensate (BEC). Since the dynamics of a dilute and interacting gas is governed by Gross-Pitaevskii equation (GPE), we have studied its analytical derivation along with its validity conditions. The fundamentals of the interaction between a two-level atom and an semiclassical electromagnetic field has been investigated leading to introduce the concept of a periodic optical trapping potential. The final topic has covered the characteristics and features of Rydberg atoms. Rydberg-dressing has been analysed where we have analytically derived the soft-core dressing interaction.

In chapter 2, different shapes and dimensions of static multi-well potential traps have been selected: one-dimensional double- and triple-well potentials and a two-dimensional quadruple-well potential. In this chapter we studied an ensemble of Rydberg-dressed atoms trapped in multi-well potentials within the mean-field theory using GPE. It has been shown that atoms share a common Rabi-oscillatory feature in the non-interacting limit (Rabi regime) regardless of the shape of the confinement. In the linear-limit (Josephson regime) double- and quadruple-well potentials exhibit similar dynamics. However, in the non-linear interacting limit (Fock regime) an interesting phenomenon has appeared, the so-called macroscopic quantum self-trapping (MQST), where the atoms at a critical interaction strength prefer to locate in a certain well. In the double-well potential the tunnelling has been completely suppressed, while in the triple- and quadruple-potentials the MQST has been non-pure where part of the atoms tend to leave their initial wells to generate a form of tunnelling whereas the rest of the atoms stays trapped. Interestingly, when the initial conditions of the atom-number for four condensates in the quadruple-well potential trap are completely different, a nearly pure MQST is observed which is pretty much similar to the double-well potential case.

We have expanded our investigation in Chapter 3 to study an ensemble of Rydberg-dressed atoms loaded into an optical lattice forming a superfluid state. The extended Bose-Hubbard model (EBH) has been used to describe both, the time-evolution of the order parameter and interference pattern of the atoms in different optical lattice

dimensions. We have shown that, due to the long-range interaction terms, only partial revivals can be expected when studying the time-evolution of the superfluid order parameter. In addition, the long-range interaction effects can also be revealed when investigating the interference pattern based on the quasi-momentum distribution function.

Lastly, in Chapter 4, a dynamical potential trap has been adopted in a way that it begins as a harmonic oscillator and ends as a double-well potential. An ensemble of contact-interacting bosonic atoms loaded in a time-dependent potential has been described through the mean-field approach using GPE.

Finally, among the most interesting candidates for further investigations is including the tunnelling term in the extended Bose-Hubbard Hamiltonian, which has been neglected in Chapter 3, in order to notice its effect on both the time-evolution of the superfluid order parameter along with the interference pattern. Additionally, we might investigate the dynamics of an ensemble of long-ranged interacting Rydberg-dressed atoms trapped in a dynamical potential trap.

APPENDICES

APPENDIX A

Gross-Pitaevskii equation derivation.

The Gross-Pitaevskii equation (GPE) describes a zero temperature and an interacting Bose-Einstein condensate (BEC) for which the scattering length between atoms a is smaller than the spacing between atoms. To derive the GP equation, we start from the many-body Hamiltonian describing N interacting atoms via atom-atom interaction $V_{\text{int}}(r, r')$ and trapped in an external potential $V_{\text{ext}}(r)$, i.e.,

$$\hat{H} = \int dr \hat{\Psi}^\dagger(r) \hat{H}_0 \hat{\Psi}(r) + \frac{1}{2} \int dr dr' \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r') \hat{\Psi}(r), \quad (\text{A.1})$$

where $\hat{H}_0 = -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r)$ is the single-atom Hamiltonian, and $\hat{\Psi}(r)$, $\hat{\Psi}^\dagger(r)$ are the annihilation and creation bosonic field operators, respectively. Since the field operator is indeed an operator, its time evolution is given by Heisenberg equation,

$$i\hbar \frac{\partial \hat{\Psi}(r)}{\partial t} = [\hat{\Psi}(r), \hat{H}] = [\hat{\Psi}(r), \hat{H}_1] + [\hat{\Psi}(r), \hat{H}_2], \quad (\text{A.2})$$

where $\hat{H}_1 = \int dr \hat{\Psi}^\dagger(r) \hat{H}_0 \hat{\Psi}(r)$ and $\hat{H}_2 = \frac{1}{2} \int dr dr' \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r') \hat{\Psi}(r)$. Our purpose now is to calculate both commutators. Starting with the first one we find, after changing the variable in $\hat{H}_1$ from r to r' ,

$$\begin{aligned}
[\hat{\Psi}(r), \hat{H}_1] &= \hat{\Psi}(r) \hat{H}_1 - \hat{H}_1 \hat{\Psi}(r) \\
&= \int dr' \hat{\Psi}(r) \hat{\Psi}^\dagger(r') \hat{H}_0 \hat{\Psi}(r') - \int dr' \hat{\Psi}^\dagger(r') \hat{H}_0 \hat{\Psi}(r') \hat{\Psi}(r) \\
&= \int dr' (\hat{\Psi}^\dagger(r') \hat{\Psi}(r) + \delta(r - r')) \hat{H}_0 \hat{\Psi}(r') - \int dr' \hat{\Psi}^\dagger(r') \hat{H}_0 \hat{\Psi}(r) \hat{\Psi}(r') \\
&= \int dr' \hat{\Psi}^\dagger(r') \hat{\Psi}(r) \hat{H}_0 \hat{\Psi}(r') + \int dr' \delta(r - r') \hat{H}_0 \hat{\Psi}(r') \\
&\quad - \int dr' \hat{\Psi}^\dagger(r') \hat{\Psi}(r) \hat{H}_0 \hat{\Psi}(r') \\
&= \int dr' \delta(r - r') \hat{H}_0 \hat{\Psi}(r') \\
&= \hat{H}_0 \hat{\Psi}(r).
\end{aligned} \tag{A.3}$$

Now, we calculate the second commutator, after changing the variable in $\hat{H}_2$, similarly to what has been done previously, where $r \rightarrow r'$ and $r' \rightarrow r''$, then one obtains,

$$\begin{aligned}
[\hat{\Psi}(r), \hat{H}_2] &= \left[\hat{\Psi}(r), \frac{1}{2} \int d' dr'' V_{\text{int}}(r', r'') \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \hat{\Psi}(r') \right] \\
&= \frac{1}{2} \int d' dr'' V_{\text{int}}(r', r'') \underbrace{[\hat{\Psi}(r), \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \hat{\Psi}(r')]}_I.
\end{aligned} \tag{A.4}$$

It can be seen that as the particle interaction operator depends only on the relative distance between both atoms, then it can be put outside the commutator of the field operators. In order to evaluate this commutator, we need to calculate I . To simplify this quantity, the following identity is used,

$$[A, BC] = B[A, C] + [A, B]C,$$

so if $A = \hat{\Psi}(r)$, $B = \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'')$ and $C = \hat{\Psi}(r'') \hat{\Psi}(r')$, then we write,

$$\begin{aligned}
I &= \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'') [\hat{\Psi}(r), \hat{\Psi}(r'') \hat{\Psi}(r')] + [\hat{\Psi}(r), \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'')] \hat{\Psi}(r'') \hat{\Psi}(r') \\
&= \hat{\Psi}^\dagger(r') \hat{\Psi}^\dagger(r'') \{ \hat{\Psi}(r'') [\hat{\Psi}(r), \hat{\Psi}(r')] + [\hat{\Psi}(r), \hat{\Psi}(r'')] \hat{\Psi}(r') \} + \\
&\quad \{ \hat{\Psi}^\dagger(r') [\hat{\Psi}(r), \hat{\Psi}^\dagger(r'')] + [\hat{\Psi}(r), \hat{\Psi}^\dagger(r')] \hat{\Psi}^\dagger(r'') \} \hat{\Psi}(r'') \hat{\Psi}(r').
\end{aligned} \tag{A.5}$$

As the field operators satisfy the commutation relations, i.e., $[\hat{\Psi}(r), \hat{\Psi}^\dagger(r')] = \delta(r - r')$, $[\hat{\Psi}(r), \hat{\Psi}(r')] = [\hat{\Psi}^\dagger(r), \hat{\Psi}^\dagger(r')] = 0$, therefore, Eq.(A.5) becomes,

$$I = \hat{\Psi}^\dagger(r')\hat{\Psi}(r'')\hat{\Psi}(r')\delta(r - r'') + \delta(r - r')\hat{\Psi}^\dagger(r'')\hat{\Psi}(r'')\hat{\Psi}(r').$$

Inserting into Eq.(A.4) we have,

$$\begin{aligned} [\hat{\Psi}(r), \hat{H}_2] &= \frac{1}{2} \int d' dr'' V_{\text{int}}(r', r'') \hat{\Psi}^\dagger(r') \hat{\Psi}(r'') \hat{\Psi}(r') \delta(r - r'') \\ &\quad + \frac{1}{2} \int d' dr'' V_{\text{int}}(r', r'') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \hat{\Psi}(r') \delta(r - r') \\ &= \frac{1}{2} \int dr' V_{\text{int}}(r', r) \hat{\Psi}^\dagger(r') \hat{\Psi}(r) \hat{\Psi}(r') + \frac{1}{2} \int dr'' V_{\text{int}}(r, r'') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \hat{\Psi}(r) \\ &= \frac{1}{2} \int dr' V_{\text{int}}(r', r) \hat{\Psi}^\dagger(r') \hat{\Psi}(r') \hat{\Psi}(r) + \frac{1}{2} \int dr'' V_{\text{int}}(r, r'') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \hat{\Psi}(r) \\ &= \frac{1}{2} \left[\int dr' V_{\text{int}}(r', r) \hat{\Psi}^\dagger(r') \hat{\Psi}(r') + \int dr'' V_{\text{int}}(r, r'') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \right] \hat{\Psi}(r) \\ &= \frac{1}{2} \left[\int dr' V_{\text{int}}(r, r') \hat{\Psi}^\dagger(r') \hat{\Psi}(r') + \int dr'' V_{\text{int}}(r, r'') \hat{\Psi}^\dagger(r'') \hat{\Psi}(r'') \right] \hat{\Psi}(r), \end{aligned}$$

where the last step is done based on the fact that the atom-atom interaction depends only on the absolute value of the relative distance between both atoms, i.e., $V_{\text{int}}|r', r| = V_{\text{int}}|r, r'|$. It can be easily noticed that both integrals inside the squared brackets in the last expression are exactly the same with different labels. Therefore, mathematically speaking, these integrals are identical. Thus, the second commutator reads as

$$[\hat{\Psi}(r), \hat{H}_2] = \int dr' \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r') \hat{\Psi}(r). \quad (\text{A.6})$$

Substituting Eq.(A.3) and Eq.(A.6) in Heisenberg equation in Eq.(A.2) we get,

$$\begin{aligned} i\hbar \frac{\partial \Psi(r)}{\partial t} &= \hat{H}_0 \hat{\Psi}(r) + \int dr' \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r') \hat{\Psi}(r) \\ &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + \int dr' \hat{\Psi}^\dagger(r') V_{\text{int}}(r, r') \hat{\Psi}(r') \right] \hat{\Psi}(r), \end{aligned}$$

which is the time-dependent non-linear Gross-Pitaevskii equation.

APPENDIX B

The effective Hamiltonian of a system of two Rydberg-dressed atoms.

The effective Hamiltonian for a system that is composed of two Rydberg-dressed atoms, where a far off-resonant laser dressing the electronic ground state $|g\rangle$ with a Rydberg $|r\rangle$ state, is obtained by applying the perturbation theory to the fourth order, i.e.,

$$\hat{H}_{\text{eff}} = \hat{H}_{\text{n}}^{(0)} + \hat{H}_{\text{n}}^{(1)} + \hat{H}_{\text{n}}^{(2)} + \hat{H}_{\text{n}}^{(3)} + \hat{H}_{\text{n}}^{(4)}. \quad (\text{B.1})$$

For simplicity, we will denote the basis $\{|g_1g_2\rangle, |g_1r_2\rangle, |r_1g_2\rangle, |r_1r_2\rangle\}$ as $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$, respectively, as Fig(B.1) shows. The energy of the state $|0\rangle$ where both atoms are in their ground states is assumed to be $E_0 = 0$, and the states $|1\rangle, |2\rangle$ have energies equal to $E_1 = E_2 = \hbar\Delta$, however the state $|3\rangle$ has the energy of $E_3 = 2\hbar\Delta + V_{12}$ with V_{12} is the van der Waals interaction. The coupling strength between $|0\rangle$ and $|1\rangle, |2\rangle$ equals to $U_{01} = U_{02} = \hbar\Omega/2$ which is the same as the coupling strength between $|1\rangle, |2\rangle$ and $|3\rangle$ where $U_{13} = U_{23} = \hbar\Omega/2$, bearing in mind that the couplings

$$U_{00} = U_{11} = U_{22} = U_{33} = U_{03} = U_{30} = 0,$$

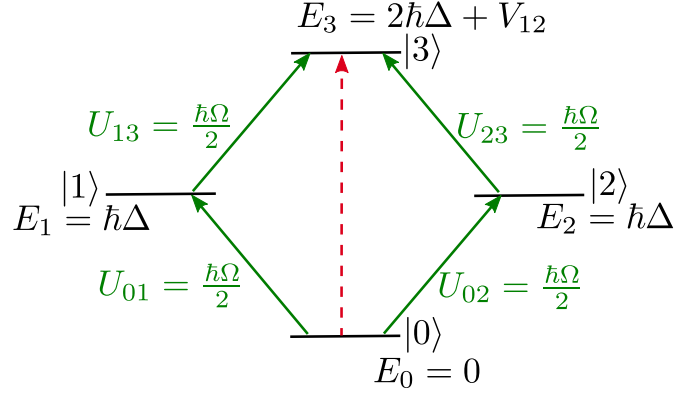


Figure B.1.: Energy level scheme which consists of the basis $\{|g_1g_2\rangle, |g_1r_2\rangle, |r_1g_2\rangle, |r_1r_2\rangle\} = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ respectively. The energy for both atoms when they are in their ground state is assumed to be equal to zero $E_0 = 0$, where the states $|1\rangle, |2\rangle$ have the energy of $E_0 = E = 1 = \hbar\Delta$. When both atoms are in their Rydberg state $|3\rangle$, their energy is the sum of $E_3 = \hbar\Delta + V_{12}$. The coupling is allowed between states $|0\rangle \leftrightarrow |1\rangle, |0\rangle \leftrightarrow |2\rangle$ and $|1\rangle \leftrightarrow |3\rangle, |2\rangle \leftrightarrow |3\rangle$ (solid green line), but is forbidden in the case of $|0\rangle \leftrightarrow |3\rangle$ (dotted red line), and the coupling energies are equal to $\hbar\Omega/2$.

are forbidden due to the selection rules. Let us start by computing the values of the first fifth orders of the perturbation theory. The zeroth order perturbation term is given by

$$\hat{H}_n^{(0)} = E_n = E_0 = 0, \quad (\text{B.2})$$

where n denotes the ground state. The first order perturbation term,

$$\hat{H}_n^{(1)} = U_{nn} = U_{00} = 0, \quad (\text{B.3})$$

and that is because there is no coupling between both ground states as it violates the selection rules. The second order perturbation term,

$$\hat{H}_n^{(2)} = \sum_{j \neq n} \frac{|U_{nj}|^2}{(E_n - E_j)} = \frac{|U_{01}|^2}{E_0 - E_1} + \frac{|U_{02}|^2}{E_0 - E_2} = \frac{\left(\frac{\hbar\Omega}{2}\right)^2}{-\hbar\Delta} + \frac{\left(\frac{\hbar\Omega}{2}\right)^2}{-\hbar\Delta} = -2 \frac{\left(\frac{\hbar\Omega}{2}\right)^2}{\hbar\Delta}, \quad (\text{B.4})$$

where $j = 1, 2$ which represents all the possible states that couple with the state $|0\rangle$. The third order perturbation term,

$$\begin{aligned}
\hat{H}_n^{(3)} &= \sum_{j \neq n} \sum_{\alpha \neq n} \frac{U_{nj} U_{j\alpha} U_{\alpha n}}{(E_n - E_j)(E_n - E_\alpha)} - U_{nn} \sum_{j \neq n} \frac{|U_{nj}|^2}{(E_n - E_j)^2} \\
&= \frac{U_{01} U_{13} U_{30}}{(E_0 - E_1)(E_0 - E_3)} + \frac{U_{02} U_{23} U_{30}}{(E_0 - E_2)(E_0 - E_3)} - U_{00} \frac{|U_{01}|^2}{(E_0 - E_1)^2} - U_{00} \frac{|U_{02}|^2}{(E_0 - E_2)^2} \\
&= 0,
\end{aligned} \tag{B.5}$$

where $U_{30} = U_{03} = U_{00} = 0$ with $\alpha = 1, 2, 3$ represents the states that couples $|0\rangle$ with $|1\rangle, |2\rangle$, and $|1\rangle, |2\rangle$ with $|3\rangle$. The fourth order perturbation term,

$$\begin{aligned}
\hat{H}_n^{(4)} &= \sum_{j \neq n} \sum_{\alpha \neq n} \sum_{\beta \neq n} \frac{U_{nj} U_{j\alpha} U_{\alpha\beta} U_{\beta n}}{(E_n - E_j)(E_n - E_\alpha)(E_n - E_\beta)} - \sum_{j \neq n} \sum_{\alpha \neq n} \frac{U_{nj} U_{n\alpha} U_{nn} U_{\alpha n}}{(E_n - E_j)(E_n - E_\alpha)^2} \\
&\quad - \sum_{j \neq n} \sum_{\alpha \neq n} \frac{U_{nj} U_{n\alpha} U_{nn} U_{\alpha n}}{(E_n - E_j)^2 (E_n - E_\alpha)} + \sum_{j \neq n} \frac{|U_{nj}|^2 |U_{nn}|^2}{(E_n - E_j)^3} - \hat{H}_{nn}^2 \sum_{j \neq n} \frac{|U_{nj}|^2}{(E_n - E_j)^2} \\
&= \sum_{j \neq n} \sum_{\alpha \neq n} \sum_{\beta \neq n} \frac{U_{nj} U_{j\alpha} U_{\alpha\beta} U_{\beta n}}{(E_n - E_j)(E_n - E_\alpha)(E_n - E_\beta)} - \sum_{j \neq n} \frac{|U_{nj}|^2}{(E_n - E_j)} \sum_{j \neq n} \frac{|U_{nj}|^2}{(E_n - E_j)^2} \\
&= \frac{U_{01} U_{13} U_{32} U_{20}}{(E_0 - E_1)(E_0 - E_3)(E_0 - E_1)} + \frac{U_{02} U_{23} U_{31} U_{10}}{(E_0 - E_2)(E_0 - E_3)(E_0 - E_1)} \\
&\quad + \frac{U_{01} U_{13} U_{32} U_{20}}{(E_0 - E_1)(E_0 - E_3)(E_0 - E_2)} + \frac{U_{02} U_{23} U_{32} U_{20}}{(E_0 - E_2)(E_0 - E_3)(E_0 - E_2)} \\
&\quad - \frac{|U_{01}|^2 |U_{01}|^2}{(E_0 - E_1)(E_0 - E_1)^2} - \frac{|U_{02}|^2 |U_{02}|^2}{(E_0 - E_2)(E_0 - E_2)^2} - \frac{|U_{01}|^2 |U_{02}|^2}{(E_0 - E_1)(E_0 - E_2)^2} \\
&\quad - \frac{|U_{02}|^2 |U_{01}|^2}{(E_0 - E_2)(E_0 - E_1)^2} \\
&= -\frac{4\left(\frac{\hbar\Omega}{2}\right)^4}{\hbar^2 \Delta^2 (2\hbar\Delta + V_{12})} + \frac{4\left(\frac{\hbar\Omega}{2}\right)^4}{\hbar^3 \Delta^3}.
\end{aligned} \tag{B.6}$$

Summing the results of Eqs.(B.2, B.3, B.4, B.5, B.6), as in Eq(B.1), yields,

$$\begin{aligned}
\hat{H}_{\text{eff}} &= \hat{H}_n^{(0)} + \hat{H}_n^{(1)} + \hat{H}_n^{(2)} + \hat{H}_n^{(3)} + \hat{H}_n^{(4)} \\
&= 0 + 0 - 2 \frac{\left(\frac{\hbar\Omega}{2}\right)^2}{\hbar\Delta} + 0 - \frac{4\left(\frac{\hbar\Omega}{2}\right)^4}{\hbar^2 \Delta^2 (2\hbar\Delta + V_{12})} + \frac{4\left(\frac{\hbar\Omega}{2}\right)^4}{\hbar^3 \Delta^3} \\
&= 2\hbar \left(\frac{\left(\frac{\Omega}{2}\right)^4}{\Delta^3} - \frac{\left(\frac{\Omega}{2}\right)^2}{\Delta} \right) + \frac{2\hbar \left(\frac{\Omega}{2}\right)^4}{\Delta^3} \left(\frac{V_{12}}{2\hbar\Delta + V_{12}} \right).
\end{aligned}$$

APPENDIX C

An optical setup to create a double-well potential.

The aim in this appendix is to present an optical setup to produce a double-well potential for one three-level V -type rubidium atom ^{87}Rb using two crossed, focused and far-off-resonant lasers. Our scheme focuses on rubidium's D_2 transition, as illustrated in Fig(C.1), since it is of much more relevance to current quantum and atom optics experiments, because it has a cycling transition that is used for cooling and trapping ^{87}Rb which is between the state $5^2\text{S}_{\frac{1}{2}}(F=2)$ and $5^2\text{P}_{\frac{3}{2}}(F=3)$.

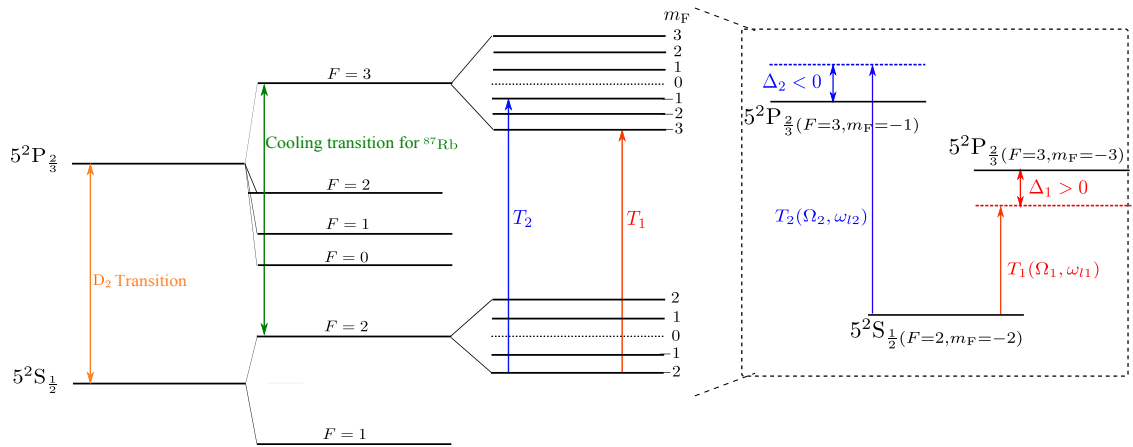


Figure C.1.: Hyperfine energy level diagram for the D_2 line for ^{87}Rb . the cycling cooling transition is shown in green. The two lasers producing the double-well potential are shown as two transitions; red T_1 and blue T_2 .

The configuration we use is based on three hyperfine states; the ground state $5^2S_{\frac{1}{2}}(F=2, m_F=-2)$ which is coupled with $5^2P_{\frac{3}{2}}(F=3, m_F=-3)$ by a red-detuned laser, i.e., $\Delta_1 > 0$, and with $5^2P_{\frac{3}{2}}(F=3, m_F=-1)$ by a blue-detuned one, i.e., $\Delta_2 < 0$. Each of the coupling laser fields are assumed to have a three-dimensional Gaussian profile that can be expressed as

$$\vec{E}_i(x, y, z) = E_{0i} \hat{e}_i \frac{w_i}{w_i(x)} \exp(ik_i x) \exp\left(-\frac{y^2 + z^2}{w_i(x)^2}\right),$$

where, $E_{0i}, w_i, k_i, \hat{e}_i$ are the amplitudes, waists, wave vectors and the unit polarisations, respectively. $w_i(x)$ is the beam width which is given by $w_i(x) = w_i \sqrt{1 + (x/x_{ri})^2}$ where x_{ri} is Rayleigh length, with $i = 1, 2$. Inserting the Rayleigh length formula into the previous equations gives

$$\vec{E}_i(x, y, z) = \frac{E_{0i} \hat{e}_i}{\sqrt{1 + \left(\frac{x}{x_{ri}}\right)^2}} \exp(ik_i x) \exp\left\{-\frac{y^2 + z^2}{w_i^2 \left[1 + \left(\frac{x}{x_{ri}}\right)^2\right]}\right\}.$$

In order to make these two beams interfere and produce a trapping potential, they must be linearly rotated around a specific axis, (z), for example, with a certain angle (θ). In order to get the new coordinates for the electric field $\vec{E}(x', y', z')$, the rotation matrix $R_{\theta, z}$ must be applied on the old ones $\vec{E}(x, y, z)$, i.e., $\vec{E}(x', y', z') = R_{\theta, z} \vec{E}(x, y, z)$. Therefore, one writes,

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{cases} x' = y \sin \theta + x \cos \theta \\ y' = y \cos \theta - x \sin \theta \\ z' = z \end{cases}.$$

Thus, the expressions of both laser beams lead to

$$\vec{E}_i(x, y, z) = \frac{E_{0i} \hat{e}_i}{\sqrt{1 + \left(\frac{x \cos \theta - y \sin \theta}{x_{ri}}\right)^2}} \exp[ik_i(x \cos \theta - y \sin \theta)] \exp\left\{-\frac{(y \cos \theta + x \sin \theta)^2 + z^2}{w_i^2 \left[1 + \left(\frac{x \cos \theta - y \sin \theta}{x_{ri}}\right)^2\right]}\right\}. \quad (C.1)$$

We have seen in subsection (2.1.1) that the ground state energy shift resulting from the interaction between both Gaussian laser beams and the three-level atom which also represents the double-well potential trap is calculated via applying the second order perturbation theory on the system Hamiltonian expressed in Eq.(2.2) which results,

$$V_{\text{dw}}(x, y, z) \approx A_1 |\vec{E}_1(x, y, z)|^2 + A_2 |\vec{E}_2(x, y, z)|^2. \quad (\text{C.2})$$

where: $A_i = \frac{|d_i|^2}{4\hbar\Delta_i}$ with $i = 1, 2$. Therefore, to get a more applicable double-well trap potential expression, Taylor expansion in higher dimensions is applied on Eq.(C.1) at the centre of both Gaussian beams, i.e., $x_0 = y_0 = z_0 = 0$. Taylor expansion in three dimensions is given by (where the second order expansion is applied on y, z axes and the fourth order on x axis),

$$\begin{aligned} |E(x, y, z)|^2 \simeq & |E(x_0, y_0, z_0)|^2 + \frac{\partial |E(x_0, y_0, z_0)|^2}{\partial x} (x - x_0) + \frac{\partial |E(x_0, y_0, z_0)|^2}{\partial y} (y - y_0) \\ & + \frac{\partial |E(x_0, y_0, z_0)|^2}{\partial z} (z - z_0) + \frac{1}{2!} \left[\frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial x^2} (x - x_0)^2 \right. \\ & + \frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial y^2} (y - y_0)^2 + \frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial z^2} (z - z_0)^2 \Big] \\ & + \frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial x \partial y} (x - x_0)(y - y_0) + \frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial y \partial z} (y - y_0)(z - z_0) \\ & + \frac{\partial^2 |E(x_0, y_0, z_0)|^2}{\partial x \partial z} (x - x_0)(z - z_0) + \frac{1}{3!} \frac{\partial^3 |E(x_0, y_0, z_0)|^2}{\partial x^3} (x - x_0)^3 \\ & + \frac{1}{4!} \frac{\partial^4 |E(x_0, y_0, z_0)|^2}{\partial x^4} (x - x_0)^4. \end{aligned}$$

This gives after evaluating the derivatives of $E(x, y, z)$, and substituting them in Eq.(C.2),

$$V_{\text{dw}}(x, y, z) = \alpha - \beta x^2 + \gamma x^4 - \delta y^2 - \sigma z^2 + \eta xy,$$

where:

$$\alpha = A_1 E_{01}^2 + A_2 E_{02}^2$$

$$\begin{aligned}
\beta &= \frac{A_1 E_{01}^2 \cos^2 \theta}{x_{r1}^2} + \frac{2A_1 E_{01}^2 \sin^2 \theta}{w_1^2} + \frac{A_2 E_{02}^2 \cos^2 \theta}{x_{r2}^2} + \frac{2A_2 E_{02}^2 \sin^2 \theta}{w_2^2} \\
\gamma &= \frac{A_1 E_{01}^2 \cos^4 \theta}{x_{r1}^4} + \frac{2A_1 E_{01}^2 \sin^4 \theta}{w_1^4} + \frac{4A_1 E_{01}^2 \cos^2 \theta \sin^2 \theta}{x_{r1}^2 w_1^2} \\
&\quad + \frac{A_2 E_{02}^2 \cos^4 \theta}{x_{r2}^4} + \frac{2A_2 E_{02}^2 \sin^4 \theta}{w_2^4} + \frac{4A_2 E_{02}^2 \cos^2 \theta \sin^2 \theta}{x_{r2}^2 w_2^2} \\
\delta &= \frac{A_1 E_{01}^2 \sin^2 \theta}{x_{r1}^2} + \frac{2A_1 E_{01}^2 \cos^2 \theta}{w_1^2} + \frac{A_2 E_{02}^2 \sin^2 \theta}{x_{r2}^2} + \frac{2A_2 E_{02}^2 \cos^2 \theta}{w_2^2} \\
\sigma &= \frac{2A_1 E_{01}^2}{w_1^2} + \frac{2A_2 E_{02}^2}{w_2^2} \\
\eta &= \frac{2A_1 E_{01}^2 \sin \theta \cos \theta}{x_{r1}^2} - \frac{4A_1 E_{01}^2 \sin \theta \cos \theta}{w_1^2} + \frac{2A_2 E_{02}^2 \sin \theta \cos \theta}{x_{r2}^2} - \frac{4A_2 E_{02}^2 \sin \theta \cos \theta}{w_2^2}.
\end{aligned}$$

For a very small θ , the previous pre-factors can be reduced considering that $\cos \theta \approx 1$ and $\sin \theta \approx 0$ where we find

$$\begin{aligned}
\alpha &= A_1 E_{01}^2 + A_2 E_{02}^2 & \beta &= \frac{A_1 E_{01}^2}{x_{r1}^2} + \frac{A_2 E_{02}^2}{x_{r2}^2} & \gamma &= \frac{A_1 E_{01}^2}{x_{r1}^4} + \frac{A_2 E_{02}^2}{x_{r2}^4} \\
\delta &= \frac{2A_1 E_{01}^2}{w_1^2} + \frac{2A_2 E_{02}^2}{w_2^2} & \sigma &= \frac{2A_1 E_{01}^2}{w_1^2} + \frac{2A_2 E_{02}^2}{w_2^2} & \eta &= 0.
\end{aligned}$$

Consequently, the three-dimensional double-well potential is formulated as

$$V_{\text{dw}}(x, y, z) = \alpha - \beta x^2 + \gamma x^4 - \delta(y^2 + z^2),$$

assuming that $\delta = \sigma$. It is worth mentioning that the rotation angle, θ , has a very important role in shaping the double-well potential especially when it comes to the height of the potential barrier where it becomes higher when θ gets smaller.

Laser quantity	T ₁	T ₂
Laser frequency ω_l (Hz)	$2\pi \times 384.158 \times 10^{12}$	$2\pi \times 384.298 \times 10^{12}$
Wave vector k (c m ⁻¹)	12814.147	12818.816
Dipole transition d (C m)	2.534×10^{-29}	0.6543×10^{-29}
Detuning Δ (Hz)	4.398×10^{11}	-4.398×10^{11}
Laser waist w_0 (m)	5×10^{-6}	10×10^{-6}
Laser power P (Watt)	0.003	3.199
Electric field amplitude $E_0(\text{V m}^{-1}) = \sqrt{\frac{2P}{\pi w_0^2}}$	9434.9	142730
Rabi frequency $\Omega(\text{Hz}) = \frac{E_0 d}{\hbar}$	3.608×10^8	1.409×10^9
Rayleigh length $x_r(\text{m}) = \frac{w_0^2 k}{2}$	0.000016	0.000064
Effective spontaneous emission rate $\Gamma_{\text{eff}} = \Gamma_e \frac{\Omega^2}{\Delta^2}$	25.651	26.086

Table C.1.: Lasers parameters.

Double-well quantity	Strength
$\alpha(\hbar\text{Hz})$	-4.3×10^{-27}
$\beta(\hbar\text{Hz m}^{-2})$	5.6×10^{-20}
$\gamma(\hbar\text{Hz m}^{-4})$	4×10^{-9}
$\delta(\hbar\text{Hz m}^{-2})$	3.4×10^{-17}
Potential minimum on x axis $x_{\min}(\text{m}) = \sqrt{\frac{\beta}{2\gamma}}$	2.6×10^{-6}
Well separation $d(\text{m}) = 2 x_{\min} $	5.3×10^{-6}
Trapping frequency on x axis $\omega_x(\text{Hz}) = \sqrt{\frac{4\beta}{m}}$	$2\pi \times 199.882$
Trapping frequencies on y, z axes $\omega_{y,z}(\text{Hz}) = \sqrt{\frac{2\delta}{2m}}$	$2\pi \times 3485.3$
Length scale on x axis $\xi_x(\text{m}) = \sqrt{\frac{\hbar}{\sqrt{4\beta m}}}$	7.62831×10^{-7}
Length scales on y, z axes $\xi_{y,z}(\text{m}) = \sqrt{\frac{\hbar}{\sqrt{2\delta m}}}$	1.82682×10^{-7}
Potential barrier $\Delta V(\text{Hz}) = \frac{\beta^2}{4\gamma}$	$2\pi \times 305.541$

Table C.2.: Double-well potential parameters.

APPENDIX D

The analytical derivation of the tunnelling rate in a symmetric double-well potential trap.

The analytical expression of the tunnelling rate in a symmetric double-well potential shown in Eq.(2.18) is derived as follows. We start by writing the tunnelling rate as:

$$J = -\langle \phi_L(x) | \hat{H}(x) | \phi_R(x) \rangle,$$

where $\hat{H}(x)$ and $\phi_{L,R}(x)$ are the time-independent one-dimensional Hamiltonian of one atom trapped in a double-well potential and the localised Gaussian wave functions for the left and right wells, respectively. Therefore, we write,

$$J = -\left\langle \left(\frac{1}{\xi_L^2 \pi} \right)^{\frac{1}{4}} \exp \left[-\frac{(x + x_{\min})^2}{2\xi_L^2} \right] \left| \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} - \beta x^2 \right| \left(\frac{1}{\xi_R^2 \pi} \right)^{\frac{1}{4}} \exp \left[-\frac{(x - x_{\min})^2}{2\xi_R^2} \right] \right\rangle.$$

Since the double-well potential is symmetric, then both Gaussian widths are equal, i.e., $\xi_L = \xi_R = \sqrt{\frac{\hbar}{m\omega_x}} = \xi$, with $\omega_x = \sqrt{\frac{4\beta}{m}}$ being the double-well trapping frequency.

To simplify the problem, the tunnelling rate is formulated as

$$J = -\left(\frac{1}{\xi^2\pi}\right)^{\frac{1}{2}}\left[\frac{-\hbar^2}{2m}A - \beta B\right] \quad (\text{D.1})$$

where we have denoted:

$$\begin{aligned} A &= \left\langle \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] \left| \frac{d^2}{dx^2} \right| \exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] \right\rangle \\ &= \int_{-\infty}^{+\infty} \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] \frac{d^2}{dx^2} \left(\exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] \right) dx, \end{aligned}$$

and,

$$\begin{aligned} B &= \left\langle \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] \left| x^2 \right| \exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] \right\rangle \\ &= \int_{-\infty}^{+\infty} \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] x^2 \exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] dx. \end{aligned}$$

Let us study each bracket analytically. Starting with the **the first bracket** A we find,

$$\begin{aligned} A &= \int_{-\infty}^{+\infty} \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] \frac{d^2}{dx^2} \left(\exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] \right) dx \\ &= \int_{-\infty}^{+\infty} \exp\left[-\frac{(x+x_{\min})^2}{2\xi^2}\right] \exp\left[-\frac{(x-x_{\min})^2}{2\xi^2}\right] \left[\frac{(x-x_{\min})^2 - \xi^2}{\xi^4} \right] dx \\ &= \int_{-\infty}^{+\infty} \exp\left[-\frac{(x+x_{\min})^2 + (x-x_{\min})^2}{2\xi^2}\right] \left[\frac{(x-x_{\min})^2 - \xi^2}{\xi^4} \right] dx \\ &= \int_{-\infty}^{+\infty} \exp\left[-\frac{x^2 + x_{\min}^2}{\xi^2}\right] \left[\frac{(x-x_{\min})^2 - \xi^2}{\xi^4} \right] dx \\ &= \exp\left[-\frac{x_{\min}^2}{\xi^2}\right] \frac{1}{\xi^2} \int_{-\infty}^{+\infty} \exp\left[-\frac{x^2}{\xi^2}\right] \left[\frac{(x-x_{\min})^2}{\xi^2} - 1 \right] dx \end{aligned}$$

Assuming that:

$$y = \frac{x}{\xi} \implies x = y\xi \implies dx = \xi dy$$

then we can write:

$$\begin{aligned}
A &= \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \frac{1}{\xi} \int_{-\infty}^{+\infty} e^{-y^2} \left[\frac{(y\xi - x_{\min})^2}{\xi^2} - 1 \right] dy \\
&= \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \frac{1}{\xi} \left\{ \int_{-\infty}^{+\infty} e^{-y^2} \left[y^2 + \frac{x_{\min}^2}{\xi^2} - 2\frac{x_{\min}}{\xi}y - 1 \right] dy \right\} \\
&= \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \frac{1}{\xi} \left\{ \int_{-\infty}^{+\infty} e^{-y^2} y^2 dy + \frac{x_{\min}^2}{\xi^2} \int_{-\infty}^{+\infty} e^{-y^2} dy - 2\frac{x_{\min}}{\xi} \int_{-\infty}^{+\infty} e^{-y^2} y dy - \int_{-\infty}^{+\infty} e^{-y^2} dy \right\} \\
&= \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \frac{1}{\xi} \left\{ \underbrace{\int_{-\infty}^{+\infty} e^{-y^2} y^2 dy}_{I_1} + \left[\frac{x_{\min}^2}{\xi^2} - 1 \right] \underbrace{\int_{-\infty}^{+\infty} e^{-y^2} dy}_{I_2} - 2\frac{x_{\min}}{\xi} \underbrace{\int_{-\infty}^{+\infty} e^{-y^2} y dy}_{I_3} \right\}.
\end{aligned} \tag{D.2}$$

We need to calculate I_1 , I_2 , and I_3 . To do that, we begin with I_1 :

$$I_1 = \int_{-\infty}^{+\infty} e^{-y^2} y^2 dy = 2 \int_0^{+\infty} e^{-y^2} y^2 dy = \int_0^{+\infty} e^{-t} t^{\frac{3}{2}-1} dt = \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{2}, \tag{D.3}$$

with Γ being the Gamma special function, and we have changed the variable such that:

$$y^2 = t \implies 2y dy = dt \implies dy = \frac{dt}{2y} \implies dy = \frac{1}{2} t^{-\frac{1}{2}} dt.$$

For I_2 we obtain,

$$I_2 = \int_{-\infty}^{+\infty} e^{-y^2} dy = 2 \int_0^{+\infty} e^{-y^2} dy = \int_0^{+\infty} e^{-t} t^{\frac{1}{2}-1} dt = \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \tag{D.4}$$

after assuming that:

$$y = \sqrt{t} \implies dy = \frac{1}{2\sqrt{t}} dt.$$

Similarly for I_3 we get,

$$I_3 = \int_{-\infty}^{+\infty} e^{-y^2} y dy = 2 \int_0^{+\infty} e^{-y^2} y dy = \int_0^{+\infty} e^{-t} dt = \Gamma(1) = 1, \tag{D.5}$$

with the assumption of:

$$y^2 = t \implies 2ydy = dt \implies dy = \frac{dt}{2y} \implies dy = \frac{1}{2}t^{-\frac{1}{2}}dt.$$

Substituting Eqs.(D.3,D.4,D.5) in Eq.(D.2), one can write:

$$A = \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \frac{1}{\xi} \left\{ \left(\frac{\sqrt{\pi}}{2} \right) + \left[\frac{x_{\min}^2}{\xi^2} - 1 \right] (\sqrt{\pi}) - 2 \frac{x_{\min}}{\xi} (1) \right\}. \quad (D.6)$$

Analogously for **the second bracket** B , we write,

$$\begin{aligned} B &= \int_{-\infty}^{+\infty} \exp \left[-\frac{(x+x_{\min})^2}{2\xi^2} \right] x^2 \exp \left[-\frac{(x-x_{\min})^2}{2\xi^2} \right] dx \\ &= \int_{-\infty}^{+\infty} \exp \left[-\frac{(x+x_{\min})^2 + (x-x_{\min})^2}{2\xi^2} \right] x^2 dx \\ &= \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \int_{-\infty}^{+\infty} \exp \left[-\frac{x^2}{\xi^2} \right] x^2 dx. \end{aligned}$$

Changing the variable yields to:

$$y = \frac{x}{\xi} \implies x = y\xi \implies dx = \xi dy,$$

therefore, one obtains,

$$B = \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \xi^3 \int_{-\infty}^{+\infty} e^{-y^2} y^2 dy = \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \xi^3 \left(\frac{\sqrt{\pi}}{2} \right) \quad (D.7)$$

after we once again change the variable according to:

$$y^2 = t \implies 2ydy = dt \implies dy = \frac{dt}{2y} \implies dy = \frac{1}{2}t^{-\frac{1}{2}}dt.$$

Consequently, we insert both Eq.(D.6) and Eq.(D.7) in Eq.(D.1), we obtain:

$$J = -\frac{\xi^2}{\sqrt{\pi}} \exp \left[-\frac{x_{\min}^2}{\xi^2} \right] \left\{ \frac{-\hbar^2}{2m} \frac{1}{\xi^4} N1 - \beta N2 \right\},$$

where:

$$N1 = \left(\frac{\sqrt{\pi}}{2} \right) + \left[\frac{x_{\min}^2}{\xi^2} - 1 \right] (\sqrt{\pi}) - 2 \frac{x_{\min}}{\xi} (1), \quad N2 = \frac{\sqrt{\pi}}{2} \quad \text{dimensionless numbers.}$$

APPENDIX E

The matrix elements η for the triple- and quadruple-well potentials .

In this appendix we list the entire matrix elements of an one-dimensional triple- and two-dimensional quadruple-well potentials. starting with **an one-dimensional triple-well potential**, we find for the left, right and middle wells, respectively, the following:

$$\begin{aligned}\eta_{L1,R1,M1} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R,M}(x')|^2 |\phi_{L,R,M}(x)|^2 \\ \eta_{L2,R2,M2} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,M}(x') \phi_{L,R,L}(x') \phi_{M,M,M}(x) \phi_{L,R,M}(x) \\ \eta_{L3,R3,M3} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R,M}(x')|^2 \phi_{R,L,R}(x) \phi_{L,R,M}(x) \\ \eta_{L4,R4,M4} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{M,M,L}(x')|^2 |\phi_{L,R,M}(x)|^2 \\ \eta_{L5,R5,M5} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{M,M,L}(x')|^2 \phi_{M,M,L}(x) \phi_{L,R,M}(x) \\ \eta_{L6,R6,M6} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,L}(x') \phi_{M,M,L}(x') \phi_{R,L,R}(x) \phi_{L,R,M}(x) \\ \eta_{L7,R7,M7} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{R,L,R}(x')|^2 |\phi_{L,R,M}(x)|^2 \\ \eta_{L8,R8,M8} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,R}(x') \phi_{R,L,L}(x') \phi_{M,M,R}(x) \phi_{L,R,M}(x) \\ \eta_{L9,R9,M9} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{R,L,R}(x')|^2 \phi_{R,L,R}(x) \phi_{L,R,M}(x)\end{aligned}$$

$$\begin{aligned}
\eta_{L10,R10,M10} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,L}(x) \phi_{L,R,M}(x) \phi_{L,R,M}(x') \phi_{M,M,M}(x') \\
\eta_{L11,R11,M11} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,M}(x') \phi_{M,M,L}(x') \phi_{M,M,L}(x) \phi_{L,R,M}(x) \\
\eta_{L12,R12,M12} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,M}(x') \phi_{M,M,L}(x') \phi_{R,L,R}(x) \phi_{L,R,M}(x) \\
\eta_{L13,R13,M13} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') |\phi_{L,R,M}(x)|^2 \phi_{L,R,M}(x') \phi_{R,L,R}(x') \\
\eta_{L14,R14,M14} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,L}(x') \phi_{R,L,R}(x') \phi_{M,M,M}(x) \phi_{L,R,M}(x) \\
\eta_{L15,R15,M15} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{L,R,M}(x') \phi_{R,L,R}(x') \phi_{R,L,R}(x) \phi_{L,R,M}(x) \\
\eta_{L16,R16,M16} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{M,M,M}(x') \phi_{R,L,R}(x') \phi_{L,R,L}(x) \phi_{L,R,M}(x) \\
\eta_{L17,R17,M17} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{M,M,L}(x') \phi_{R,L,R}(x') \phi_{M,M,L}(x) \phi_{L,R,M}(x) \\
\eta_{L18,R18,M18} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dx V_{\text{SC}}(x, x') \phi_{M,M,R}(x') \phi_{R,L,R}(x') \phi_{R,L,L}(x) \phi_{L,R,M}(x).
\end{aligned}$$

However, for a **two-dimensional quadruple-well potential** we have:

$$\begin{aligned}
\eta_{i1} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_3(x', y')|^2 \phi_3(x, y) \\
\eta_{i2} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_3(x', y')|^2 \phi_2(x, y) \\
\eta_{i3} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_3(x', y')|^2 \phi_0(x, y) \\
\eta_{i4} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_3(x', y')|^2 \phi_1(x, y) \\
\eta_{i5} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_2(x', y')|^2 \phi_3(x, y) \\
\eta_{i6} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_2(x', y')|^2 \phi_2(x, y) \\
\eta_{i7} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_2(x', y')|^2 \phi_0(x, y) \\
\eta_{i8} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_2(x', y')|^2 \phi_1(x, y) \\
\eta_{i9} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_0(x', y')|^2 \phi_3(x, y) \\
\eta_{i10} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_0(x', y')|^2 \phi_2(x, y) \\
\eta_{i11} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_0(x', y')|^2 \phi_0(x, y) \\
\eta_{i12} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_0(x', y')|^2 \phi_1(x, y) \\
\eta_{i13} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) |\phi_0(x', y')|^2 \phi_3(x, y)
\end{aligned}$$

$$\begin{aligned}\eta_{i39} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) \phi_0(x, y) \phi_0(x', y') \phi_1(x', y') \\ \eta_{i40} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy dx' dy' V_{\text{SC}}(x, y, x', y') \phi_i(x, y) \phi_1(x, y) \phi_0(x', y') \phi_1(x', y').\end{aligned}$$

With $i = 0, 1, 2, 3$ represent the four wells.

APPENDIX F

Poisson distribution of non-interacting atoms in a superfluid state.

To prove that N non-interacting atoms in a superfluid state have a poissonian distribution, we need to evaluate the expectation value of $\langle \hat{b}_i^\dagger \hat{b}_i \rangle$. Therefore, we start by writing the many-body Fock state for these atoms where,

$$\begin{aligned} |\text{SF}\rangle &= \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{L}} \sum_{j=1}^L b_j^\dagger \right]^N |0\rangle \\ &= \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N \left(\sum_{j=1}^L b_j^\dagger \right)^N |0\rangle \\ &= \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N \left(\hat{b}_i^\dagger + \sqrt{L-1} \hat{B}^\dagger \right)^N |0\rangle, \end{aligned}$$

where: $\hat{B}^\dagger = \frac{1}{\sqrt{L-1}} \sum_{i \neq j=1}^{L-1} \hat{b}_j^\dagger$. Thus, the expectation value of the atom number $\hat{b}_i^\dagger \hat{b}_i$ can be written as

$$\langle \hat{b}_i^\dagger \hat{b}_i \rangle = \langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle = \left\langle \langle 0 | \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N (\hat{b}_i + \sqrt{L-1} \hat{B})^N | \hat{b}_i^\dagger \hat{b}_i | \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N (\hat{b}_i^\dagger + \sqrt{L-1} \hat{B}^\dagger)^N | 0 \rangle \right\rangle.$$

Let us begin by evaluating this bracket from the right, where we write,

$$\begin{aligned} \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle &= \hat{b}_i^\dagger \hat{b}_i \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N (\hat{b}_i^\dagger + \sqrt{L-1} \hat{B}^\dagger)^N | 0 \rangle \\ &= \frac{1}{\sqrt{N!}} \hat{b}_i^\dagger \hat{b}_i \left(\frac{1}{\sqrt{L}} \hat{b}_i^\dagger + \sqrt{\frac{L-1}{L}} \hat{B}^\dagger \right)^N | 0 \rangle. \end{aligned}$$

Since the binomial coefficients theorem is given by $(x+y)^r = \sum_k \binom{r}{k} x^k y^{r-k}$, then we write,

$$\begin{aligned} \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle &= \frac{1}{\sqrt{N!}} \hat{b}_i^\dagger \hat{b}_i \sum_k \binom{N}{k} \left(\frac{1}{\sqrt{L}} \right)^k (\hat{b}_i^\dagger)^k \left(\sqrt{\frac{L-1}{L}} \right)^{N-k} (\hat{B}^\dagger)^{N-k} | 0 \rangle \\ &= \frac{1}{\sqrt{N!}} \left(\frac{L-1}{L} \right)^N \sum_k \binom{N}{k} \left(\sqrt{\frac{1}{L-1}} \right)^k \hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger)^k (\hat{B}^\dagger)^{N-k} | 0 \rangle. \end{aligned}$$

Therefore, the expectation value expression becomes,

$$\begin{aligned} \langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle &= \left\langle \langle 0 | \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{L}} \right)^N (\hat{b}_i + \sqrt{L-1} \hat{B})^N | \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-1}{L}} \right)^N \sum_k \binom{N}{k} \left(\sqrt{\frac{1}{L-1}} \right)^k \hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger)^k (\hat{B}^\dagger)^{N-k} | 0 \rangle \right\rangle \\ &= \left\langle \langle 0 | \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-1}{L}} \right)^N \sum_m \binom{N}{m} \left(\sqrt{\frac{1}{L-1}} \right)^m (\hat{b}_i)^m (\hat{B})^{N-m} | \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-1}{L}} \right)^N \sum_k \binom{N}{k} \left(\sqrt{\frac{1}{L-1}} \right)^k \hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger)^k (\hat{B}^\dagger)^{N-k} | 0 \rangle \right\rangle, \end{aligned}$$

where after simplification we have

$$\begin{aligned} \langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle &= \frac{1}{N!} \left(\frac{L-1}{L} \right)^N \sum_{k,m}^N \binom{N}{k} \binom{N}{m} \left(\frac{1}{L-1} \right)^{\frac{k+m}{2}} \\ &\quad \langle 0_b | (\hat{b}_i)^m \hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger)^k | 0_b \rangle \langle 0_B | (\hat{B})^{N-m} (\hat{B}^\dagger)^{N-k} | 0_B \rangle. \end{aligned} \quad (\text{F.1})$$

Based on the following relations

$$|r\rangle = \frac{(\hat{S}_x^\dagger)^r}{\sqrt{r!}} |0_S\rangle \quad \langle r| = \langle 0_S| \frac{(\hat{S}_x)^r}{\sqrt{r!}},$$

both brackets can be easily evaluated where we get

$$\begin{aligned} \langle 0_b | (\hat{b}_i)^m \hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger)^k | 0_b \rangle &= \sqrt{k!m!} \langle m | \hat{b}_i^\dagger \hat{b}_i | k \rangle \\ \langle 0_B | (\hat{B})^{N-m} (\hat{B}^\dagger)^{N-k} | 0_B \rangle &= (N-m)! \delta_{k,m} \quad \text{when } k = m. \end{aligned}$$

Inserting in Eq.(F.1) we obtain,

$$\langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle = \frac{1}{N!} \left(\frac{L-1}{L} \right)^N \sum_{k,m}^N \binom{N}{k} \binom{N}{m} \left(\frac{1}{L-1} \right)^{\frac{k+m}{2}} \sqrt{k!m!} \langle m | \hat{b}_i^\dagger \hat{b}_i | k \rangle (N-m)! \delta_{k,m}.$$

Assuming that $k = m$ which leads to $\delta_{k,m} = 1$, and bearing in mind that the binomial defines as $\binom{N}{k} = \frac{N!}{k!(N-k)!}$, then we have

$$\begin{aligned} \langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle &= \frac{1}{N!} \left(\frac{L-1}{L} \right)^N \sum_k^N \binom{N}{k} \frac{N!}{k!(N-k)!} \left(\frac{1}{L-1} \right)^k \langle k | \hat{b}_i^\dagger \hat{b}_i | k \rangle (N-k)! \\ &= \left(\frac{L-1}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{1}{L-1} \right)^k \langle k | \hat{b}_i^\dagger \hat{b}_i | k \rangle \\ &= \left(\frac{L-1}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{1}{L-1} \right)^k \sqrt{k} \langle k | \hat{b}_i^\dagger | k-1 \rangle \\ &= \left(\frac{L-1}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{1}{L-1} \right)^k \sqrt{k} \sqrt{k} \langle k | k \rangle \\ &= \sum_k^N \binom{N}{k} \left(1 - \frac{1}{L} \right)^{N-k} \left(\frac{1}{L} \right)^k k, \end{aligned}$$

and the term $\binom{N}{k} \left(1 - \frac{1}{L}\right)^{N-k} \left(\frac{1}{L}\right)^k$ is nothing but the Poissonian distribution.

In the thermodynamic limit where $N \rightarrow \infty$ we find

$$\begin{aligned} \lim_{N \rightarrow \infty} \left[\binom{N}{k} \left(1 - \frac{1}{L}\right)^{N-k} \left(\frac{1}{L}\right)^k \right] &= \lim_{N \rightarrow \infty} \left[\binom{N}{k} \left(1 - \frac{1}{L}\right)^N \left(1 - \frac{1}{L}\right)^{-k} \left(\frac{1}{L}\right)^k \right] \\ &= \lim_{N \rightarrow \infty} \left[\frac{N!}{k!(N-k)!} \left(1 - \frac{1}{L}\right)^N \left(1 - \frac{1}{L}\right)^{-k} \left(\frac{1}{L}\right)^k \right]. \end{aligned}$$

Supposing that $\lambda = \frac{N}{L}$, then we have

$$\lim_{N \rightarrow \infty} \left[\frac{N!}{k!(N-k)!} \left(1 - \frac{\lambda}{N}\right)^N \left(1 - \frac{\lambda}{N}\right)^{-k} \left(\frac{\lambda}{N}\right)^k \right],$$

but as $\lim_{N \rightarrow \infty} \left[\left(1 - \frac{\lambda}{N}\right)^N \right] = e^{-\lambda}$ and $\lim_{N \rightarrow \infty} \left[\left(1 - \frac{\lambda}{N}\right)^{-k} \right] = 1$, then we write the limitation as,

$$\lim_{N \rightarrow \infty} \left[\frac{N!}{k!(N-k)!} \left(\frac{\lambda}{N}\right)^k \right] = \lim_{N \rightarrow \infty} \left[\frac{N!}{N^k(N-k)!} \right] e^{-\lambda} \left(\frac{\lambda^k}{k!}\right),$$

and as, $\lim_{N \rightarrow \infty} \left[\frac{N!}{N^k(N-k)!} \right] = 1$, thus the expectation value of the atom number takes the form of

$$\langle \hat{b}_i^\dagger \hat{b}_i \rangle = \langle \text{SF} | \hat{b}_i^\dagger \hat{b}_i | \text{SF} \rangle = \sum_k \underbrace{e^{-\lambda} \left(\frac{\lambda^k}{k!}\right)}_{f_{\text{Poisson}}} k = \sum_k f_{\text{Poisson}}(k) k.$$

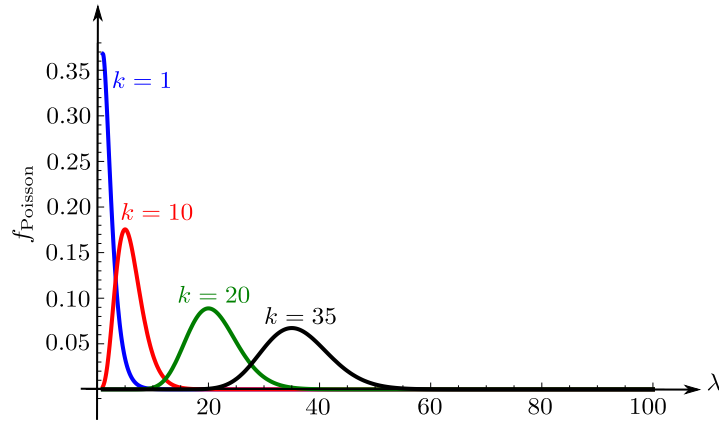


Figure F.1.: Poisson distribution.

APPENDIX G

Matrix elements $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ of the quasi-momentum distribution $S(\mathbf{k})$ for one-dimensional optical lattice using a many-body Fock state.

For an one-dimensional optical lattice, we derive in this appendix the formula of the matrix elements $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ which considered the most significant part of the quasi-momentum distribution expressed in Eq.(3.23). For this reason, when $j = k$, we begin by witting the initial many-body Fock state, which is a perfect superfluid state, as

$$|\text{SF}(t=0)\rangle = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{L}} \sum_{j=1}^L b_j^\dagger \right]^N |0\rangle.$$

We can write this state as:

$$|\text{SF}(t=0)\rangle = \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{3}{L}} \right)^N \left(A^\dagger + \sqrt{\frac{L-3}{3}} B^\dagger \right)^N |0\rangle, \quad (\text{G.1})$$

where:

$$\hat{A}^\dagger = \frac{1}{\sqrt{3}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger) \quad \hat{B}^\dagger = \frac{1}{\sqrt{L-3}} \sum_{j=4}^L \hat{b}_j^\dagger.$$

Since there are two nearest neighbors for site k , then, there are three sites involving in the calculation, i.e., k , $k+1$ and $k-1$. We can write the extended Bose-Hubbard Hamiltonian $\hat{\mathcal{H}}_{\text{EBH}}$ (after neglecting the tunnelling) as:

$$\hat{\mathcal{H}}_{\text{EBH}} = \frac{\zeta}{2} \sum_j^L n_j(n_j - 1) + \frac{1}{2} \sum_{jk} V_{\text{SC}}^{jk}(r_j - r_k) n_j n_k \quad (\text{G.2})$$

where:

$$\zeta = \frac{2\Omega^4}{\Delta^3} \quad V_{\text{SC}}^{jk}(r_j - r_k) = \frac{\zeta R_{\text{SC}}^6}{d^6 + R_{\text{SC}}} = \zeta\gamma,$$

with d , Δ , Ω and R_{SC} are the lattice spacing, detuning, Rabi frequency and soft-core potential radius, respectively. The unitary operator of the system can be written as:

$$\begin{aligned} \hat{U} &= \prod_j^L \hat{U}_j = \hat{U}_1 \hat{U}_2 \hat{U}_3 \prod_{j=4}^L \hat{U}_j = \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{U}_4 \dots \hat{U}_L) \\ \hat{U}^\dagger &= \prod_j^L \hat{U}_j^\dagger = \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \prod_{j=4}^L \hat{U}_j^\dagger = \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger). \end{aligned} \quad (\text{G.3})$$

Using equations (G.1) and (G.3), we write the correlation function expression as:

$$\langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle = \langle \text{SF}(t=0) | \hat{U}^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} | \text{SF}(t=0) \rangle,$$

thus,

$$= \left\langle \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{3}{L}} \right)^N \langle 0 | \left(\hat{A} + \sqrt{\frac{L-3}{3}} \hat{B} \right)^N \left| U^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} \right| \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{3}{L}} \right)^N \left(\hat{A}^\dagger + \sqrt{\frac{L-3}{3}} \hat{B}^\dagger \right)^N | 0 \rangle \right\rangle.$$

Let us calculate this bracket from the right:

$$\hat{U}^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} | \text{SF}(t=0) \rangle = \hat{U}^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{3}{L}} \right)^N \left(\hat{A}^\dagger + \sqrt{\frac{L-3}{3}} \hat{B}^\dagger \right)^N | 0 \rangle.$$

Using Eq.(G.3) we write:

$$\begin{aligned} \hat{U}^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} |\text{SF}(t=0)\rangle &= \frac{1}{\sqrt{N!}} \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{U}_4 \dots \hat{U}_L) \\ &\quad \left(\sqrt{\frac{3}{L}} \hat{A}^\dagger + \sqrt{\frac{L-3}{L}} \hat{B}^\dagger \right)^N |0\rangle. \end{aligned}$$

Applying the binomial theorem, i.e., $(x+y)^r = \sum_k^r \binom{r}{k} y^k x^{r-k}$, we write the righthand side of the bracket as

$$\begin{aligned} \hat{U}^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U} |\text{SF}(t=0)\rangle &= \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-3}{L}} \right)^N \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{U}_4 \dots \hat{U}_L) \sum_k^N \binom{N}{k} \\ &\quad \left(\sqrt{\frac{3}{L-3}} \right)^k (\hat{A}^\dagger)^k (\hat{B}^\dagger)^{N-k} |0\rangle. \end{aligned}$$

Now we can estimate the entire bracket:

$$\begin{aligned} \langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle &= \left\langle \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{3}{L}} \right)^N \langle 0 | \left(\hat{A} + \sqrt{\frac{L-3}{3}} \hat{B} \right)^N \left| \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-3}{L}} \right)^N \right. \right. \\ &\quad \left. \left. \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{U}_4 \dots \hat{U}_L) \sum_k^N \binom{N}{k} \left(\sqrt{\frac{3}{L-3}} \right)^k \right. \right. \\ &\quad \left. \left. (\hat{A}^\dagger)^k (\hat{B}^\dagger)^{N-k} |0\rangle \right\rangle \right. \\ &= \left\langle \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-3}{L}} \right)^N \sum_m^N \binom{N}{m} \left(\sqrt{\frac{3}{L-3}} \right)^m \langle 0 | (A)^m (B)^{N-m} \right. \\ &\quad \left. \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{L-3}{L}} \right)^N \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{U}_4 \dots \hat{U}_L) \sum_k^N \binom{N}{k} \right. \\ &\quad \left. \left(\sqrt{\frac{3}{L-3}} \right)^k (A^\dagger)^k (B^\dagger)^{N-k} |0\rangle \right\rangle, \end{aligned}$$

therefore,

$$\begin{aligned}
\langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle &= \frac{1}{N!} \left(\frac{L-3}{L} \right)^N \sum_k^N \sum_m^N \binom{N}{k} \binom{N}{m} \left(\frac{3}{L-3} \right)^{\frac{k+m}{2}} \\
&\quad \langle 0_A | (\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{A}^\dagger)^k | 0_A \rangle \\
&\quad \langle 0_B | (\hat{B})^{N-m} (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) (\hat{U}_4 \dots \hat{U}_L) (\hat{B}^\dagger)^{N-k} | 0_B \rangle
\end{aligned} \tag{G.4}$$

We see that there are two brackets that have to be calculated:

$$\langle 0_A | (\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{A}^\dagger)^k | 0_A \rangle,$$

and

$$\langle 0_B | (\hat{B})^{N-m} (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) (\hat{U}_4 \dots \hat{U}_L) (\hat{B}^\dagger)^{N-k} | 0_B \rangle.$$

Calculating the first bracket, $\langle 0_A | (\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{A}^\dagger)^k | 0_A \rangle$, from the right gives,

$$(\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{A}^\dagger)^k | 0_A \rangle = (\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \sqrt{k!} | k \rangle.$$

Therefore, we write,

$$\begin{aligned}
\langle 0_A | (\hat{A})^m \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 (\hat{A}^\dagger)^k | 0_A \rangle &= \langle \sqrt{m!} \langle m | | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \sqrt{k!} | k \rangle \rangle \\
&= \sqrt{k! m!} \langle m | | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle.
\end{aligned}$$

where:

$$|k\rangle = \frac{(\hat{A}^\dagger)^k}{\sqrt{k!}} | 0_A \rangle = \frac{1}{\sqrt{k!}} \left[\frac{1}{\sqrt{3}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger) \right]^k | 0_A \rangle$$

$$\langle m | = \langle 0_A | \frac{(\hat{A})^m}{\sqrt{m!}} = \langle 0_A | \frac{1}{\sqrt{m!}} \left[\frac{1}{\sqrt{3}} (\hat{b}_1 + \hat{b}_2 + \hat{b}_3) \right]^m.$$

Likewise for the second bracket, $\langle 0_B | (\hat{B})^{N-m} (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger) (\hat{U}_4 \dots \hat{U}_L) (\hat{B}^\dagger)^{N-k} | 0_B \rangle$, where calculating from the right leads to,

$$(\hat{B})^{N-m}(\hat{U}_4^\dagger \dots \hat{U}_L^\dagger)(\hat{U}_4 \dots \hat{U}_L)(\hat{U}^\dagger)^{N-k}|0_B\rangle = (\hat{U})^{N-m}(\hat{U}_4^\dagger \dots \hat{U}_L^\dagger)(\hat{U}_4 \dots \hat{U}_L)\sqrt{(N-k)!|N-k\rangle},$$

thus, the whole second bracket is obtained as,

$$\begin{aligned} \langle 0_B | (\hat{B})^{N-m}(\hat{U}_4^\dagger \dots \hat{U}_L^\dagger)(\hat{U}_4 \dots \hat{U}_L)(\hat{B}^\dagger)^{N-k} | 0_B \rangle &= \\ \left\langle \sqrt{(N-m)!|N-m\rangle} \left| (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger)(\hat{U}_4 \dots \hat{U}_L) \sqrt{(N-k)!|N-k\rangle} \right\rangle &= \\ = \sqrt{(N-k)!(N-m)!} \underbrace{\langle N-m | (\hat{U}_4^\dagger \dots \hat{U}_L^\dagger)(\hat{U}_4 \dots \hat{U}_L) | N-k \rangle}_{=1} &= \\ = \sqrt{(N-k)!(N-m)!} \langle N-m | N-k \rangle &= \\ = \sqrt{(N-k)!(N-m)!} \delta_{km}. \end{aligned}$$

After we have got the formulae of both brackets, we substitute them in Eq.(G.4) to derive the general expression for the correlation function, then we find:

$$\begin{aligned} \langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle &= \frac{1}{N!} \left(\frac{L-3}{L} \right)^N \sum_k^N \sum_m^N \binom{N}{k} \binom{N}{m} \left(\frac{3}{L-3} \right)^{\frac{k+m}{2}} \\ &\quad \sqrt{m!k!} \langle m | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle \sqrt{(N-k)!(N-m)!} \delta_{km}. \end{aligned}$$

The delta function is equal to $\delta_{km} = 1$ if and only if $k = m$, then we write the previous expression as:

$$\begin{aligned} \langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle &= \frac{1}{N!} \left(\frac{L-3}{L} \right)^N \sum_k^N \binom{N}{k} \binom{N}{k} \left(\frac{3}{L-3} \right)^k \\ &\quad k! \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle (N-k)! \\ &= \frac{1}{N!} \left(\frac{L-3}{L} \right)^N \sum_k^N \binom{N}{k} \frac{N!}{k!(N-k)!} \left(\frac{3}{L-3} \right)^k \\ &\quad k! \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle (N-k)!, \end{aligned}$$

hence,

$$\langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle = \left(\frac{L-3}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{3}{L-3} \right)^k \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle. \quad (\text{G.5})$$

In order to solve this function, it is obvious that $\langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle$ has to be calculated. To do that, it has been mentioned earlier that:

$$|k\rangle = \frac{1}{\sqrt{k!}} \left[\frac{1}{\sqrt{3}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger) \right]^k |0\rangle \quad \langle k| = \frac{1}{\sqrt{k!}} \langle 0| \left[\frac{1}{\sqrt{3}} (\hat{b}_1 + \hat{b}_2 + \hat{b}_3) \right]^k,$$

where: k is the number of particles in the three lattice sites. Evaluating from the right leads to:

$$\begin{aligned} \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 |k\rangle &= \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left[\frac{1}{\sqrt{3}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger) \right]^k |0\rangle \\ &= \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger)^k |0\rangle \\ &= \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \sum_n^k \binom{k}{n} (\hat{b}_1^\dagger + \hat{b}_2^\dagger)^n (\hat{b}_3^\dagger)^{k-n} |0\rangle \\ &= \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \sum_n^k \sum_p^n \binom{k}{n} \binom{n}{p} \\ &\quad (\hat{b}_1^\dagger)^p (\hat{b}_2^\dagger)^{n-p} (\hat{b}_3^\dagger)^{k-n} |0\rangle \\ &= \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \sum_n^k \sum_p^n \binom{k}{n} \binom{n}{p} \\ &\quad \sqrt{p!(n-p)!(k-n)!} |p, n-p, k-n\rangle. \end{aligned}$$

Therefore, the bracket is obtained as:

$$\begin{aligned} \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \left\langle \frac{1}{\sqrt{k!}} \langle 0| \left[\frac{1}{\sqrt{3}} (\hat{b}_1 + \hat{b}_2 + \hat{b}_3) \right]^k \right| \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \\ &\quad \sum_n^k \sum_p^n \binom{k}{n} \binom{n}{p} \sqrt{p!(n-p)!(k-n)!} |p, n-p, k-n\rangle \Bigg\rangle, \end{aligned}$$

hence,

$$\begin{aligned} \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \left\langle \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \sum_r \sum_y \binom{k}{r} \binom{r}{y} \sqrt{y!(r-y)!(k-r)!} \langle y, r-y, k-r | \right. \\ &\quad \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 \frac{1}{\sqrt{k!}} \left(\frac{1}{\sqrt{3}} \right)^k \sum_n \sum_p \binom{k}{n} \binom{n}{p} \\ &\quad \left. \sqrt{p!(n-p)!(k-n)!} | p, n-p, k-n \rangle \right\rangle, \end{aligned}$$

then we can write:

$$\begin{aligned} \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \frac{1}{k!} \left(\frac{1}{3} \right)^k \sum_n \sum_p \sum_r \sum_y \binom{k}{n} \binom{n}{p} \binom{k}{r} \binom{r}{y} \\ &\quad \sqrt{p!(n-p)!(k-n)!} \sqrt{y!(r-y)!(k-r)!} \\ &\quad \langle y, r-y, k-r | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | p, n-p, k-n \rangle. \end{aligned} \quad (\text{G.6})$$

In order to get the value of the bracket $\langle y, r-y, k-r | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | p, n-p, k-n \rangle$, we have to get the unitary operator expression for the interacting lattice sites. As the system is governed by the Hamiltonian given by Eq.(G.2), and as we are studying the expectation value of $\langle \hat{b}_1^\dagger \hat{b}_1 \rangle$, then we need to take into account the interaction between atoms in lattice site (1) and the nearest neighbour lattice sites which are (2) and (L). Therefore, we write the expression of the Hamiltonian as:

$$\hat{\mathcal{H}}_{\text{EBH}} = \frac{\zeta}{2} [n_1(n_1 - 1)] + \frac{1}{2} V_{\text{SC}}^{12} n_1 n_2 + \frac{1}{2} V_{\text{SC}}^{1L} n_1 n_L,$$

or:

$$\hat{\mathcal{H}}_{\text{EBH}} = \frac{\zeta}{2} [n_1(n_1 - 1)] + \frac{\Omega^4}{\Delta^3} \beta_{12} n_1 n_2 + \frac{\Omega^4}{\Delta^3} \beta_{1L} n_1 n_L,$$

where:

$\beta_{12} = \beta_{1L} = \beta = \frac{R_{\text{SC}}^6}{d^6 + R_{\text{SC}}^6}$, n_1, n_2, n_L : is the number of particles in the lattice site (1), (2) and (L), respectively. Substituting the indices of each lattice site yields:

$$\hat{\mathcal{H}}_{\text{EBH}} = \frac{\zeta}{2} [p(p - 1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n - p) + p(k - n)].$$

After getting the expression of the Hamiltonian for the interacting sites, the unitary operator expression can be obtained directly:

$$\hat{U} = e^{-i\hat{\mathcal{H}}_{\text{EBH}}t} = \exp \left\{ -i \left[\frac{\zeta}{2} [p(p-1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n-p) + p(k-n)] \right] t \right\}.$$

calculating the bracket from the right gives:

$$\begin{aligned} \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 |p, n-p, k-n\rangle &= \\ \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \exp \left\{ -i \left[\frac{\zeta}{2} [p(p-1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n-p) + p(k-n)] \right] t \right\} & \\ |p, n-p, k-n\rangle & \\ = \exp \left\{ -i \left[\frac{g}{2} [p(p-1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n-p) + p(k-n)] \right] t \right\} U_1^\dagger U_2^\dagger U_3^\dagger \hat{b}_1^\dagger \hat{b}_1 & \\ |p, n-p, k-n\rangle & \\ = \exp \left\{ -i \left[\frac{g}{2} [p(p-1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n-p) + p(k-n)] \right] t \right\} U_1^\dagger U_2^\dagger U_3^\dagger p & \\ |p, n-p, k-n\rangle. & \end{aligned}$$

As the conjugate of the unitary operator $\hat{U}$ is given by

$$\hat{U}^\dagger = e^{i\hat{\mathcal{H}}_{\text{EBH}}t} = \exp \left\{ i \left[\frac{\zeta}{2} [y(y-1)] + \frac{\Omega^4}{\Delta^3} \beta [y(r-y) + y(k-r)] \right] t \right\},$$

then, we write:

$$\begin{aligned} \langle y, r-y, k-r | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 |p, n-p, k-n\rangle & \\ = \exp \left\{ -i \left[\frac{\zeta}{2} [p(p-1)] + \frac{\Omega^4}{\Delta^3} \beta [p(n-p) + p(k-n)] \right] t \right\} & \\ \exp \left\{ i \left[\frac{\zeta}{2} [y(y-1)] + \frac{\Omega^4}{\Delta^3} \beta [y(r-y) + y(k-r)] \right] t \right\} & \\ p \langle y, r-y, k-r | p, n-p, k-n\rangle, & \end{aligned}$$

so,

$$\begin{aligned}
& \langle y, r-y, k-r | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | p, n-p, k-n \rangle = \\
& \exp \left\{ -i \left[\frac{\zeta}{2} \left[p(p-1) - y(y-1) \right] + \frac{\Omega^4}{\Delta^3} \beta \left[p(n-p) - y(r-y) + p(k-n) - y(k-r) \right] t \right\} \\
& p \delta_{y,p} \delta_{r-y, n-p} \delta_{k-r, k-n}.
\end{aligned}$$

Let us put the previous bracket in equation (G.6):

$$\begin{aligned}
\langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \frac{1}{k!} \left(\frac{1}{3} \right)^k \sum_n^k \sum_p^n \sum_r^k \sum_y^r \binom{k}{n} \binom{n}{p} \binom{k}{r} \binom{r}{y} \sqrt{p!(n-p)!(k-n)!} \\
& \sqrt{y!(r-y)!(k-r)!} \\
& \langle y, r-y, k-r | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | p, n-p, k-n \rangle.
\end{aligned}$$

Inserting the value of the last bracket gives

$$\begin{aligned}
\langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \frac{1}{k!} \left(\frac{1}{3} \right)^k \sum_n^k \sum_p^n \sum_r^k \sum_y^r \binom{k}{n} \binom{n}{p} \binom{k}{r} \binom{r}{y} \\
& \exp \left\{ -i \left[\frac{\zeta}{2} \left[p(p-1) - y(y-1) \right] + \frac{\Omega^4}{\Delta^3} \beta \left[p(n-p) - y(r-y) + p(k-n) - y(k-r) \right] t \right\} \\
& p \delta_{y,p} \delta_{r-y, n-p} \delta_{k-r, k-n} \sqrt{p!(n-p)!(k-n)!} \sqrt{y!(r-y)!(k-r)!}.
\end{aligned}$$

In order to get: $\delta_{y,p} = \delta_{r-y, n-p} = \delta_{k-r, k-n} = 1$, the following equalities must be achieved

$$y = p \quad r - y = n - p \quad k - r = k - n,$$

then the expression of the bracket yields:

$$\begin{aligned}
\langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \frac{1}{k!} \left(\frac{1}{3} \right)^k \sum_n^k \sum_p^n \binom{k}{n} \binom{n}{p} \binom{k}{n} \binom{n}{p} \\
& \exp \left\{ -i \left[\frac{\zeta}{2} \left[p(p-1) - (p)(p-1) \right] + \frac{\Omega^4}{\Delta^3} \beta \left[p(n-p) - (p)(n-p) + (p)(k-n) - (p)(k-n) \right] t \right\} \\
& \sqrt{p!(n-p)!(k-n)!(p)!(n-p)!(k-n)!(p)}.
\end{aligned}$$

Since the binomial coefficients are given by the formula

$$\binom{k}{n} = \frac{k!}{n!(k-n)!},$$

then, we write,

$$\begin{aligned} \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle &= \left(\frac{1}{3} \right)^k \sum_n^k \sum_p^n \binom{k}{n} \frac{n! k! n! \sqrt{p!(n-p)!(k-n)!(p)!(n-p)!(k-n)!(p)}}{p!(n-p)! n!(k-n)! p!(n-p)! k!} \\ &= \left(\frac{1}{3} \right)^k \sum_n^k \sum_p^n \binom{k}{n} \frac{n!}{(p-1)!(n-p)!}. \end{aligned}$$

Mathematica can be used to simplify this expression, and get the following:

$$\text{Simplify} \left[\frac{1}{3^k} \text{Sum} \left[\text{Binomial}[\mathbf{k}, \mathbf{n}] \frac{\mathbf{n}!}{(\mathbf{p}-1)! (\mathbf{n}-\mathbf{p})!}, \{\mathbf{n}, 0, \mathbf{k}\}, \{\mathbf{p}, 0, \mathbf{n}\} \right] \right]$$

$\frac{k}{3}$

which gives,

$$\langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle = \frac{k}{3}.$$

Now, We put this value in Eq.(G) where we find:

$$\begin{aligned} \langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle &= \left(\frac{L-3}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{3}{L-3} \right)^k \langle k | \hat{U}_1^\dagger \hat{U}_2^\dagger \hat{U}_3^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{U}_1 \hat{U}_2 \hat{U}_3 | k \rangle \\ &= \left(\frac{L-3}{L} \right)^N \sum_k^N \binom{N}{k} \left(\frac{3}{L-3} \right)^k \frac{k}{3} \end{aligned}$$

Again, we can use Mathematica to simplify this expression even more:

$$\text{Simplify} \left[\left(\frac{\mathbf{L}-3}{\mathbf{L}} \right)^{\mathbf{N}} \text{Sum} \left[\text{Binomial} [\mathbf{N}, \mathbf{k}] \left(\frac{3}{\mathbf{L}-3} \right)^{\mathbf{k}} \frac{\mathbf{k}}{3}, \{\mathbf{k}, 0, \mathbf{N}\} \right] \right]$$

$$\frac{\left(\frac{-3+\mathbf{L}}{\mathbf{L}} \right)^{\mathbf{N}} \left(\frac{\mathbf{L}}{-3+\mathbf{L}} \right)^{\mathbf{N}}}{\mathbf{L}}$$

Resultantly, it can be readily concluded that the correlation function for a single lattice site for interacting atoms via long-range interactions with its nearest neighboring sites is written as:

$$\langle \text{SF}(t) | \hat{b}_1^\dagger \hat{b}_1 | \text{SF}(t) \rangle = \frac{N}{L}. \quad (\text{G.7})$$

Pursuing the same previous analytical steps, we can obtain the formulae of the matrix elements $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ in case of $j \neq k$. For instance, when $|j - k| = 1$, Eq.(G.1) becomes

$$|\text{SF}(t=0)\rangle = \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{4}{L}} \right)^N \left(A^\dagger + \sqrt{\frac{L-4}{4}} B^\dagger \right)^N |0\rangle,$$

where, $\hat{A}^\dagger = \frac{1}{\sqrt{4}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger + \hat{b}_4^\dagger)$ and $\hat{B}^\dagger = \frac{1}{\sqrt{L-4}} \sum_{j=5}^L \hat{b}_j^\dagger$, since there are four contributing lattice sites to the study. Similarly, when $|j - k| = 2$, we obtain,

$$|\text{SF}(t=0)\rangle = \frac{1}{\sqrt{N!}} \left(\sqrt{\frac{5}{L}} \right)^N \left(A^\dagger + \sqrt{\frac{L-5}{5}} B^\dagger \right)^N |0\rangle,$$

where, $\hat{A}^\dagger = \frac{1}{\sqrt{5}} (\hat{b}_1^\dagger + \hat{b}_2^\dagger + \hat{b}_3^\dagger + \hat{b}_4^\dagger + \hat{b}_5^\dagger)$ and $\hat{B}^\dagger = \frac{1}{\sqrt{L-5}} \sum_{j=6}^L \hat{b}_j^\dagger$, and so on so forth for higher lattice sites number.

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