Ultracold Atoms in Optical Cavities

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*Als meus pares*

*Reality is merely an illusion albeit a very persistent one.*

Albert Einstein
Abstract

This thesis summarizes the research work we did in the past years, which focuses on the theoretical study of quantum effects of ordered atomic structures interacting with the quantum electric field of an optical resonator. Within this work we investigated the quantum properties of the light at the cavity output, emitted by this kind of system, and the quantum state of the atoms confined by the light fields of the cavity mode. Following one possible partition, we have organized the thesis in two parts.

The first part of the thesis is devoted to the quantum properties of the light at the output of optical cavities, in which atoms are confined. After a brief introduction on the basics of atom-photon interactions, we show theoretically, that two atomic dipoles in a resonator can behave as a quantum non-linear medium, whose response can be controlled through the interatomic distance inside the resonator. We identify the parameter regime, for which the system operates as a parametric amplifier, based on the atoms' collective dipole cascade emission. Moreover we also determine the corresponding squeezing spectrum of the field at the cavity output. Within this model we assume that the atoms are strongly confined by an external potential. Nevertheless, this configuration could result from atom trapping by the mechanical forces of the cavity field.

The second part of the thesis studies the quantum ground state of an ultracold atomic gas trapped inside an optical resonator by the mechanical effects of atom-photon interactions. Due to the strong coupling regime, the ultracold atomic gas feels a quantum potential, where the fluctuations at the single photon level may be relevant in determining the trapping conditions. This potential depends on the atomic distribution, which at the same time determines the intracavity-field amplitude. Here, after a brief introduction on ultracold atoms in optical lattices, we study the low temperature
physics of an ultracold atomic gas in the quantum potential formed inside a pumped cavity, by mapping the dynamics to an effective Bose-Hubbard model. We predict the existence of non-compressible states of the atomic gas, and determine a phase diagram as a function of the cavity parameters. Novel effects are encountered, such as the existence of overlapping stability regions corresponding to competing insulator-like states when the laser pumps the cavity, to provide one example out of many.

At the end of the thesis a concluding chapter presents some general outlooks to this thesis work.
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PART I

Quantum non-linear optics with ultracold atoms
Quantum light sources are an essential tool for implementing quantum computation and information protocols. In particular, squeezed light sources are a basic element of quantum information with continuous variables [1, 2, 3, 4, 5, 6, 7, 8, 9]. Several experiments have demonstrated the possibility of implementing a controlled generation of quantum light [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21].

A well known system, already used since the late eighties, for generating quantum light is the optical parametric oscillator (OPO) [22, 23]. The OPO was previously studied in the framework of non-linear optics [24, 25]. The OPO is usually accomplished with a non-linear crystal placed in a resonator. In these crystals, the macroscopical polarization responds non-linearly to the applied electric field. The crystal symmetries enhance some non-linear response over others, and as a result, the nature of the interaction produces photons in pairs at the resonator output [23, 26] exhibiting non-classical correlations. In the optical parametric oscillator, the atoms composing the crystal are only virtually excited and it is the geometry of the crystal what determines its response.

On the microscopic side, recent studies have revealed that a single atom can constitute a non-linear optical medium operating in the quantum regime [27, 28, 29, 30]. Here, the important ingredient is the control of the microscopic interaction between photons and the atomic degrees of freedom.

In the first part of this thesis we show that two atoms confined inside an optical resonator can act as a peculiar nonlinear medium for light. Here, the nonlinear response is the result of two dipoles confined in a standing wave cavity and driven by a laser, as sketched in Fig.1. Accordingly, here the microscopic details determine the effective dynamics. Such microscopic dynamics allow us to identify parameters which permit us to coherently
control the system response.

In particular we show how the interatomic distances, inside the resonator, control the linear-nonlinear response of the medium. Moreover, we will show how the system response can be switched from a parametric amplifier to a Kerr medium, just by varying the intensity of the driving laser.

The system presented in this part of the thesis has some theoretical idealizations. Nevertheless, we have taken care being as close as possible to experimental realizations. Some of those include experiments where confinement of a single or few atoms has been achieved inside optical cavities with nanometric precision [31, 12, 11, 10, 32, 33, 13]. These experiments, among others, aim at the controlled generation of quantum light, and eventually to the realization of atomic interfaces for quantum networks [11, 10, 1, 34, 21, 2]. It is in this context that the work presented in this thesis can find applications. Further outlooks of this work are discussed in the conclusions.

Figure 1: Two atoms are confined inside a high-finesse optical resonator, their dipoles are driven by a laser and coupled to a cavity mode. The quantum state of the field at the cavity output can be controlled by the interatomic distance inside the resonator, and the laser intensity and detuning. A detecting apparatus measures the field at the cavity output.

The first part of this thesis is organized as follows. In chapter 1 we present an overview on atom-photon interactions. In chapter 2, we introduce the system and its theoretical description, and highlight how the dependence of the interatomic distances determines the non-linear response of the system. Moreover we derive the effective Hamiltonian that describes different nonlinear dynamics. In the third chapter we characterize the statistical properties of the light at the cavity output when the system operates
as an optical parametric oscillator [22, 23, 26]. This analysis is both analytical and numerical. In this last chapter we also study the effect of atomic motion on the emitted light, by using a semiclassical model for the atomic motion. Finally, in the conclusions we provide some outlook of the work presented in the first part of the thesis.
In this chapter we review some concepts and basic theoretical tools which will be used in this thesis. First, we introduce the basic Hamiltonian describing the interaction of an atom with the quantum electromagnetic field. Then the effects of spontaneous emission and cavity decay on the coupled dynamics of dipole and cavity field are introduced with the formalism of the master equation.

1.1 Two-level atom

In this thesis, we consider the interaction of atoms with the quantized electromagnetic field, whereby the atom electronic states which are relevantly involved in the dynamics are an electronic ground state and an electronic excited state, constituting a dipole transition. In this regime the atom is well approximated by a two-level quantum system, and we can restrict the atomic Hilbert space to two states, the ground and the excited states of the dipolar transition which we denote by \( |g\rangle \) and \( |e\rangle \), respectively. This two-level approximation refers to single atoms, and it is valid for sufficiently weak electromagnetic fields when multiphoton processes can be neglected\(^1\). We denote by \( \hat{H}_{\text{at}} \) the corresponding Hamiltonian which reads

\[
\hat{H}_{\text{at}} = \hbar \omega_0 |e\rangle \langle e| \tag{1.1}
\]

\(^1\)In an atomic vapor the approximation breaks down at high densities, when the single atom picture is not valid anymore \[35\].
being $\omega_0$ the dipole transition frequency, and where we have set the energy of the ground state to zero. Hence, a generic state of the two level transition is given by $|\varphi\rangle = \alpha |e\rangle + \beta |g\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$. In this reduced Hilbert space, we define the non hermitian spin-flip operators $\hat{\sigma} = |g\rangle \langle e|$ and $\hat{\sigma}^\dagger$ its adjoint. They fulfill the commutation relations $[\hat{\sigma}^\dagger, \hat{\sigma}] = \hat{\sigma}_z$, $[\hat{\sigma}_z, \hat{\sigma}^\dagger] = 2\hat{\sigma}^\dagger$, $[\hat{\sigma}_z, \hat{\sigma}] = -2\hat{\sigma}$ with $\hat{\sigma}_z = |e\rangle \langle e| - |g\rangle \langle g|$.

The atomic dipole operator $\hat{\vec{d}} = e\hat{\vec{r}}_e$, where $\hat{\vec{r}}_e$ is the position operator of the valence electron with respect to the center of mass of the atom, is defined on the reduced Hilbert space as

$$\hat{\vec{d}} = \vec{d}\left(\hat{\sigma}^\dagger + \hat{\sigma}\right), \quad (1.2)$$

where $\vec{d} = \langle e| \hat{\vec{d}}|g\rangle$ is the dipole matrix element of the atomic transition which we assumed to be real. We have also used $\langle e| \hat{\vec{d}}|e\rangle = 0 = \langle g| \hat{\vec{d}}|g\rangle$ because of parity selection rules.

### 1.2 Atom-Photon interactions

We now consider the interaction of the atomic dipole with the quantum electromagnetic field. Let us denote by $\hat{H}$ the Hamiltonian describing the coupled dynamics of atom and electromagnetic field. We decompose it into the sum of the terms

$$\hat{H} = \hat{H}_{at} + \hat{H}_f + \hat{H}_{int} \quad (1.3)$$

where $\hat{H}_{at}$ is given by Eq.(1.1), and $\hat{H}_f$ is the Hamiltonian for the electromagnetic field given by

$$\hat{H}_f = \hbar \sum_j \omega_j \hat{b}^\dagger_j \hat{b}_j \quad (1.4)$$

The operators $\hat{b}_j$ and $\hat{b}^\dagger_j$ are the creation and annihilation operators for a photon in the mode $j$ at frequency $\omega_j$ and obey the commutation relations

$$[\hat{b}_j, \hat{b}^\dagger_{j'}] = \delta_{jj'} \quad (1.5a)$$

$$[\hat{b}_j, \hat{b}_{j'}] = [\hat{b}^\dagger_j, \hat{b}^\dagger_{j'}] = 0. \quad (1.5b)$$
The term $\hat{H}_{int}$ describes the atom-field interaction. In the electric dipole approximation\(^2\) it takes the form

$$\hat{H}_{int} = -\hat{\vec{d}} \cdot \hat{\vec{E}}_{j,\varepsilon}(\vec{r})$$  \hspace{1cm} (1.6)$$

where $\hat{\vec{d}}$ is the atomic dipole operator defined in Eq.

$$\hat{\vec{E}}_{j,\varepsilon}(\vec{r}) = \sum_{j,\vec{\varepsilon}} \sqrt{\frac{\hbar \omega_j}{2\epsilon_0 V}} \vec{e} f_j(\vec{r}) \hat{b}_j + H.c.$$  \hspace{1cm} (1.7)$$

Here, $\epsilon_0$ is the vacuum permittivity, $V$ is the quantization volume and $\vec{e}$ the polarization vector. The functions $f_j(\vec{r})$ are the orthonormal mode functions giving the spatial dependence of the field. These mode functions fulfill $\int_V d\vec{r} |f_j|^2 = 1$.

By inserting Eq.

$$\hat{H}_{int} = \hbar \sum_{j,\vec{\varepsilon}} g_{j,\varepsilon}(\vec{r}) \left( \hat{\sigma}^\dagger + \hat{\sigma} \right) \left( \hat{b}_j + \hat{b}_j^\dagger \right)$$  \hspace{1cm} (1.8)$$

where $g_{j,\varepsilon}(\vec{r})$ is the atom-field coupling strength, which is defined as

$$g_{j,\varepsilon}(\vec{r}) = -\sqrt{\frac{\hbar \omega_j}{2\epsilon_0 V}} \vec{d} \cdot \vec{e} f_j(\vec{r}) / \hbar.$$  \hspace{1cm} (1.9)$$

When expanding the product $(\hat{\sigma}^\dagger + \hat{\sigma}) \left( \hat{b}_j + \hat{b}_j^\dagger \right)$ in Eq.

2 This approximation is based on the assumption that the typical wavelength of the field is much larger than the atomic size, which is of the order of the Bohr radius ($a_B = 0.58\AA$). In general, this is a good approximation for optical transitions, where the optical wavelengths are several thousands of $\AA$.\footnote{This approximation is based on the assumption that the typical wavelength of the field is much larger than the atomic size, which is of the order of the Bohr radius ($a_B = 0.58\AA$). In general, this is a good approximation for optical transitions, where the optical wavelengths are several thousands of $\AA$.}
1. Atom-Photon Interactions: Basics

strengths, $|g_{je}(\vec{r})| \ll \omega_0, \omega_j$. Under these conditions the processes which do not conserve the energy of the unperturbed system (i.e., $\hat{b}_j^{\dagger}\hat{\sigma}^{\dagger}$ and $\hat{b}_j\hat{\sigma}$) are very unlikely to occur and so they can be safely neglected. This approximation is called the Rotating Wave Approximation (RWA).

After performing the RWA, the interaction Hamiltonian reads

$$\hat{H}_{\text{int}} = \hbar \sum_{j,e} g_{je} \langle \vec{r} \rangle \left( \hat{b}_j^{\dagger}\hat{\sigma}^{\dagger} + \hat{\sigma}^{\dagger}\hat{b}_j \right)$$  \hspace{1cm} (1.10)

The quantum description of the interaction between matter and radiation introduces an intrinsic radiative instability of the atomic excited state. In fact, let us consider that the system is initially prepared in the state $|\phi_i\rangle = |e,0\rangle$, where $|e,0\rangle = |e\rangle \otimes |0\rangle$, corresponding to the atom in the internal excited state and the field in the vacuum state. State $|\phi_i\rangle$ is coupled quasi-resonantly by Eq.(1.10) to a manifold of states $|\phi_f\rangle = |g,1_j\rangle$ by processes where the atom is deexcited emitting a photon into the mode $j$. In first order perturbation theory the transition rate from $|\phi_i\rangle$ to $|\phi_f\rangle$ is given by [36]

$$\Gamma_{i\rightarrow f} = \frac{2\pi}{\hbar} \left| \langle \phi_f | \hat{H}_{\text{int}} | \phi_i \rangle \right|^2 \delta (E_i - E_f)$$  \hspace{1cm} (1.11)

In free space, when the volume $V \rightarrow \infty$, the states $|g,1_j\rangle$ form a continuum. In this limit we can replace the sum in Eq.(1.10) by an integral

$$\sum_j \rightarrow \int d\vec{k} \sum_{\epsilon_j, \vec{k}} \rho_{at}(\vec{k}, \epsilon)$$  \hspace{1cm} (1.12)

where $\rho_{at}(\vec{k}, \epsilon)$ is the density of states of the electromagnetic field at a fixed polarization $\epsilon$ and wavevector $\vec{k}$. The one-to-many transition probability per unit of time from the state $|\phi_i\rangle$ to a set of final states $|\phi_f\rangle$ is given by [36]

$$\gamma = \frac{2\pi}{\hbar} \left| \langle \phi_f | \hat{H}_{\text{int}} | \phi_i \rangle \right|^2 \rho_{at}(\omega = \omega_0)$$  \hspace{1cm} (1.13)

By substituting Eq.(1.10), and considering Eq.(1.12), into Eq.(1.13) we obtain the rate of the spontaneous emission of the atomic excited states due to its coupling with the vacuum state of the quantum electromagnetic field [37]

$$\gamma = \frac{d^2\omega_0^3}{3\hbar \pi \epsilon_0 c^3}$$  \hspace{1cm} (1.14)
1.3 Atomic dipole coupled to a single mode resonator

In this section we consider the electromagnetic field to be confined in one dimension by two reflecting mirrors forming a cavity. Due to the boundary conditions imposed by the mirrors of the resonator, the field in the cavity exhibits a discrete spectrum of modes, corresponding to the wavelengths supported by the length of the cavity $L$. We will consider that one of the cavity modes interacts resonantly with the dipole of the atom trapped inside the resonator, while the other modes of the field are far-off resonance of the atomic transition. Thus, we can focus on the dynamics of the interaction of a dipole with a single mode of the electromagnetic field. The electric field operator for the cavity mode is defined as

$$\hat{\mathcal{E}}(\vec{r}) = \sqrt{\frac{\hbar \omega_c}{2\epsilon_0 \epsilon_f}} \hat{a} + \hat{a}^\dagger$$

where now, $V_c$ is the cavity mode volume and $f(\vec{r})$ is a dimensionless mode profile that fulfills the boundary conditions. The boundary conditions impose that the field vanishes at the cavity mirror. The operators $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators of a cavity mode photon at frequency $\omega_c$. As plotted in Fig.(1.1), we assume that the cavity axis corresponds to the $\hat{x}$-axis. By $\vec{k}$ and $\omega_c$, we denote the wave vector and frequency of the cavity mode, such that $\omega_c = c|\vec{k}|$ and $\vec{k} = \pi/L(m_x,0,0)$ where $m_x$ is a positive integer. Here, we consider a sinusoidal mode profile along the $x$-axis such that $f(\vec{r}) = \sin(kx)$ and the electric field along the cavity axis takes the form

$$\hat{E}(x) = \sqrt{\frac{\hbar \omega_c}{2\epsilon_0 V_c}} (\hat{a} + \hat{a}^\dagger) \sin(kx)$$

where we have assumed that the electromagnetic field is polarized in the $z$ direction.

We denote by $\hat{H}_{\text{cav}}$ the Hamiltonian for the cavity mode, with

$$\hat{H}_{\text{cav}} = \hbar \omega_c \hat{a}^\dagger \hat{a} = \hbar \omega_c \hat{N}$$

where $\hat{N} \equiv \hat{a}^\dagger \hat{a}$ is the hermitian number operator, that indicates the cavity
mode number of photons. By \( \{|n\}\rangle \), we denote the eigenstates of \( \hat{H}_{\text{cav}} \), Eq.(1.17), which are the photon number states also known as Fock states [36], forming a complete and orthonormal basis set. Their energy eigenvalues are \( E_n = \hbar \omega_c n \) with \( n = 0, 1, 2 \ldots \)

![Figure 1.1: Schematic representation of the cavity on the x direction formed by two mirrors. A single mode of the electric field is represented. The darker areas indicates the maxima of the field intensities.](image)

### 1.3.1 The Jaynes-Cummings model

We now study the dynamics of an atomic dipole coupled to the optical mode of a resonator. The interaction of a single mode of the quantized electromagnetic field with the dipole transition of an atom, is found from Eq.(1.6) in the electric dipole approximation and in the RWA. The electric field, reduced now to the single mode of a resonator, is given by Eq. (1.16). The total Hamiltonian is then given by

\[
\hat{H} = \hat{H}_{\text{at}} + \hat{H}_{\text{cav}} + \hat{H}_{\text{cav-at}}
\]

where \( \hat{H}_{\text{cav}} \) and \( \hat{H}_{\text{at}} \) are given by Eq. (1.17) and Eq. (1.1), respectively, while the term that describes the interaction between the single mode and the atomic dipole reads

\[
\hat{H}_{\text{cav-at}} = \hbar g(x) \left( \hat{a}^\dagger \hat{\sigma} + \hat{\sigma}^\dagger \hat{a} \right).
\]

Here, we introduce the atom-field coupling strength

\[
g(x) = -\sqrt{\frac{\hbar \omega_c}{2 \kappa_0 V_c}} d \sin (kx) / \hbar
\]

Hamiltonian (1.18) is called the Jaynes-Cummings Hamiltonian [38]. We
now summarize some basic properties of the dynamics, assuming the atom to be fixed at position \( x \), and set \( g(x) = g \).

In order to solve the Schrödinger equation governed by Eq. (1.18), we introduce a basis that consists of the product of the atomic and cavity mode states sketched in Fig. (1.2)a, i.e. \( |g,n\rangle = |g\rangle \otimes |n\rangle \) and \( |e,n\rangle = |e\rangle \otimes |n\rangle \). These states are eigenstates of \( \hat{H}_{\text{at}} + \hat{H}_{\text{cav}} \) with eigenvalues
\[
\left( \hat{H}_{\text{at}} + \hat{H}_{\text{cav}} \right) |g,n\rangle = \hbar \omega_c n |g,n\rangle , \quad (1.21)
\]
\[
\left( \hat{H}_{\text{at}} + \hat{H}_{\text{cav}} \right) |e,n\rangle = \hbar (\omega_0 + \omega_c n) |e,n\rangle . \quad (1.22)
\]

In particular the states \( |g,n+1\rangle \) and \( |e,n\rangle \) are degenerate when \( \omega_0 = \omega_c \).

As we can see in Fig (1.2)b, close to resonance \( (\omega_c \approx \omega_0) \) they form a series of doublets. The distance between states in the doublets is \( \hbar \Delta_c \), where \( \Delta_c = \omega_c - \omega_0 \).

![Figure 1.2: a) Two level atoms interacting with a quantized field. On the left side we show the energy levels corresponding to the ground state \( |g\rangle \) and the excited state \( |e\rangle \) of the atom with a dipole transition at frequency \( \omega_0 \). On the right side, the energy levels of the cavity mode corresponding to the photon number state are represented. b) Energy levels for the atom + field in absence of interaction. The energy difference between two levels in a manifold is \( \hbar \Delta_c \). The detuning is considered to be positive. Note that when \( \Delta_c = \omega_c - \omega_0 = 0 \) states \( |e,n\rangle \) and \( |g,n+1\rangle \) are degenerate.](image)

The interaction \( \hat{H}_{\text{cav-at}} \) couples the states \( |e,n\rangle \) and \( |g,n+1\rangle \) according to the relations
\[
\hat{H}_{\text{cav-at}} |g,n+1\rangle = \hbar g \sqrt{n+1} |e,n\rangle \\
\hat{H}_{\text{cav-at}} |e,n\rangle = \hbar g \sqrt{n} |g,n+1\rangle \quad (1.23)
\]
while
\[ \hat{H}_{\text{cav-at}} |g, 0\rangle = 0 \quad (1.24) \]

Hence, the state $|g, 0\rangle$ is the only product state that is eigenstate of the total Hamiltonian at eigenvalue $E_0 = 0$. Using this basis, the total Hamiltonian can thus be written as

\[ \hat{H} = \bigoplus_n \tilde{\hat{H}}_n \quad (1.25) \]

The Hamiltonian $\hat{H}$ has a block-diagonal structure as displayed in Fig.(1.3), with block-matrices $\tilde{\hat{H}}_n$ of size 2x2, coupling the pairs of states $\{|g, n+1\rangle, |e, n\rangle \}$, which can be written as

\[ \tilde{\hat{H}}_n = \hbar \omega_0 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \hbar \omega_c \begin{pmatrix} n & 0 \\ 0 & n+1 \end{pmatrix} + \hbar g \begin{pmatrix} 0 & \sqrt{n+1} \\ \sqrt{n+1} & 0 \end{pmatrix} \quad (1.26) \]

\[ \hat{H} = \begin{pmatrix} \ddots & \ddots & \ddots \\ \tilde{\hat{H}}_n & \tilde{\hat{H}}_{n+1} & \ddots \\ \ddots & \ddots & \ddots \end{pmatrix} \]

Figure 1.3: Block diagonal structure of the Jaynes-Cummings Hamiltonian

The structure of Eq.(1.25) allows us to diagonalize $\hat{H}$ by diagonalizing each block $\tilde{\hat{H}}_n$ separately. Using Eq.(1.26), the eigenvalues take the form

\[ E_{\pm,n} = \hbar \left[ \frac{\omega_0}{2} + \omega_c \left( n + \frac{1}{2} \right) \right] \pm \hbar \frac{\Omega_n}{2} \quad (1.27) \]

Here, $\Omega_n$ is the so-called Rabi frequency

\[ \Omega_n = \sqrt{4g^2(n+1) + \Delta_c^2} \quad (1.28) \]

that depends on the number of photons and on the atom-cavity detuning.
The eigenstates of the energy read

\[
\begin{align*}
|+, n\rangle &= \sin \theta_n |g, n+1\rangle + \cos \theta_n |e, n\rangle \\
|-, n\rangle &= \cos \theta_n |g, n+1\rangle - \sin \theta_n |e, n\rangle
\end{align*}
\] (1.29a)

where \( \theta_n \) fulfills the relation

\[
\tan \theta_n = \frac{2g\sqrt{n+1}}{\Omega_n - \Delta_c} \tag{1.30}
\]

The states given in Eqs.(1.29) are a superposition of dipole and field states and are called “dressed states”.

At resonance \( \Delta_c = 0 \), Eq.(1.29a) and Eq.(1.29b) read

\[
\begin{align*}
|+, n\rangle &= \frac{1}{\sqrt{2}} (|e, n\rangle + |g, n+1\rangle) \\
|-, n\rangle &= \frac{1}{\sqrt{2}} (-|e, n\rangle + |g, n+1\rangle)
\end{align*}
\] (1.31a)

and in this limit

\[
\Omega_n (\omega_0 = \omega_c) = 2g\sqrt{n+1}
\]

(1.32)

The Rabi frequency \( \Omega_n \) depends on the number of photons, and scales as the square root of the number of photons of the electromagnetic field.

Let us now study the time evolution governed by the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} |\Psi (t)\rangle = \hat{H} |\Psi (t)\rangle
\]

(1.33)

We assume that the atom is initially prepared in the excited state, and it is resonantly coupled to the cavity mode \( \Delta_c = 0 \), while the cavity mode state is \( |n\rangle \). We expand the initial state in the eigenstates of the Hamiltonian described in Eq.(1.25)

\[
|\Psi (0)\rangle = |e, n\rangle = \frac{1}{\sqrt{2}} (|+, n\rangle - |-, n\rangle)
\]

(1.34)

From Eq. (1.33), at a certain time \( t > 0 \), the state of the system is given by

\[
|\Psi (t)\rangle = \left( e^{-iE_+s t/\hbar} \cos \theta_n |+, n\rangle - e^{-iE_-s t/\hbar} \sin \theta_n |-, n\rangle \right).
\]

(1.35)

Going back to the product basis \( |e, n\rangle, |g, n\rangle \), and by using Eq.(1.27) we
obtain
\[ |\Psi(t)\rangle = e^{-i\omega_0(n+1)t} [-i \sin (\Omega_n t/2) |g,n+1\rangle + \cos (\Omega_n t/2) |e,n\rangle] \]
(1.36)

The probability to find the atom in the excited state is a periodic function that oscillates as a function of time at frequency $\Omega_n/2$, and reads as
\[ p_e(t) = |\langle e,n | \Psi(t) \rangle|^2 = \cos^2 (g\sqrt{n+1}t) . \]
(1.37)

where the relation (1.32) has been used. This behavior is even encountered when the cavity field is initially prepared in the vacuum: in this case, one photon is periodically emitted and reabsorbed by the atom at the frequency $\Omega_0$, which is denoted by the vacuum Rabi frequency.

Let us now consider the situation when the field is initially in a coherent state $|\alpha\rangle$, eigenstate of the annihilation operator $a |\alpha\rangle = \alpha |\alpha\rangle$, with $\alpha$ complex scalar. In the basis of number states it takes the form [22]
\[ |\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle , \]
(1.38)

and it is hence a coherent superposition of number states. Correspondingly, the probability occupation of the photon number state $|n\rangle$ follows the Poisson distribution
\[ P(n) = |\langle n | \alpha \rangle|^2 = e^{-|\alpha|^2} \sum_n \frac{|\alpha|^{2n}}{n!} . \]
(1.39)

with mean photon number $\langle n \rangle = |\alpha|^2$. Evaluating the evolution for the initial state $|e,\alpha\rangle$, one finds that the probability to find the atom in the excited state at time $t$ is given by
\[ p_e(t) = e^{-|\alpha|^2} \sum_n \frac{|\alpha|^{2n}}{n!} \cos^2 (g\sqrt{n+1}t) \]
(1.40)

which is the sum of periodic functions with incommensurate frequencies. As a consequence, the behavior as a function of time is an oscillatory behavior which is damped (collapse), and may reappear when some rephasing among the different oscillatory components takes place (revival) [39]. This is
lustrated in Fig. (1.4) for an initial coherent state of radiation with \( \langle n \rangle = 7 \). Collapse and revivals are a manifestation of the “granular nature” of the electromagnetic field. They have been observed for the first time in microwave cavity quantum electrodynamics experiments, where the coherent dynamics of a microwave single mode field coupled with individual atomic dipoles was realized \([40, 41]\).

![Figure 1.4: Probability \( p_e \) to find the atom in the excited state of a two level atom as a function of the time. The dipole interacts with a coherent state of the field with a mean number of photons \( \langle n \rangle = 7 \).](image)

“Collapse and revivals” are a quantum property of the electromagnetic field, which is lost in the classical limit, when the mean number of photons \( \langle n \rangle \gg 1 \). In this case, for times \( t \ll |\alpha|/g \), we can approximate Eq. (1.40) by the expression

\[
p_e(t) \approx \frac{1}{2} + \frac{1}{2} \cos(|\alpha|gt) e^{-g^2t^2}
\]

showing that now the atomic excitation probability oscillates at period \( |\alpha|/g \), and decays as a Gaussian with width \( 1/g \). The time of the collapse hence gets very large in respect to the oscillation period. The latter is now determined by the mean photon number, and we recover the Rabi oscillations of a dipole in a classical oscillating field \([36]\).

1.4 Master Equation

So far, we have considered the dynamics of quantum systems where the total energy is conserved and the dynamics is Hamiltonian. However, experimental systems are essentially “open”, namely, energy is exchanged and
correlations are established with external environments. As a result, measurements of observables defined on the system, exhibit damping and loss of quantum coherence in the system itself. The theoretical description of these effective dynamics must be necessarily based on a statistical approach. In this section, we consider systems composed by an atom and a cavity mode, which exchange photons with the modes of the external electromagnetic field. We then sketch the basic steps, which lead us to a closed equation for the density matrix of the atom-cavity system, the Born-Markov master equation, where the external electromagnetic field enters into the dynamics through its average correlation functions [42].

Let us generically consider a system $S$ and a reservoir $R$, whose respective Hilbert spaces are denoted by $\mathcal{H}_S$ and $\mathcal{H}_R$. In absence of mutual interactions, the Hamiltonian of the system (reservoir) $S$ ($R$) defined on the Hilbert space $\mathcal{H}_S$ ($\mathcal{H}_R$) is $H_S$ ($H_R$)$^3$. Their total Hilbert space is $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$, and the Hamiltonian describing the dynamics for the coupled system and reservoir degrees of freedom is

$$H = H_S \otimes 1_R + 1_S \otimes H_R + H_{SR}$$

(1.42)

where $1_j$ is the identity in $\mathcal{H}_j$ ($j = R, S$) and $H_{SR}$ is the system reservoir interaction term defined in the Hilbert space $\mathcal{H}$. Let $\rho_{SR}(t)$ be the density operator for system and reservoir degrees of freedom. The time evolution of the density operator is determined by the von Neumann equation [43]

$$\frac{\partial}{\partial t} \rho_{SR}(t) = -\frac{i}{\hbar} [H, \rho_{SR}(t)]$$

(1.43)

where $H$ is given by Eq.(1.42). Since we are interested only in the system evolution, we will define the reduced density operator for the system $\rho_S(t)$, which is obtained by tracing the density matrix $\rho_{SR}(t)$ over the reservoir degrees of freedom, and which is defined as

$$\rho_S(t) = \text{Tr}_R \{ \rho_{SR}(t) \}$$

(1.44)

where $\text{Tr}_R$ denotes the trace over the reservoir degrees of freedom. Correspondingly, we also define the reduced density operator of the reservoir

$^3$From now on we omit the $\hat{}$ symbol for the operators.
\[ \rho_R(t), \text{ obtained by tracing } \rho_{SR}(t) \text{ over the system degrees of freedom, as } \]

\[ \rho_R(t) = \text{Tr}_S \{ \rho_{SR}(t) \} \quad (1.45) \]

where Tr\_S denotes the trace over the system degrees of freedom. We now move to the interaction picture with respect to \( H_0 = H_S \otimes 1_R + 1_S \otimes H_R \). Accordingly, Eq.(1.43) transforms as

\[ \tilde{\rho}_{SR}(t) = e^{(i/\hbar)H_0 t} \rho_{SR} e^{-(i/\hbar)H_0 t} \quad (1.46) \]

and from Eq.(1.42) and Eq.(1.43) we obtain the evolution for the density matrix of the full system in the interaction picture as

\[ \dot{\tilde{\rho}}_{SR}(t) = -\frac{i}{\hbar} \left[ \tilde{H}_{SR}(t), \tilde{\rho}_{SR}(t) \right] \quad (1.47) \]

with \( \tilde{H}_{SR}(t) = e^{(i/\hbar)H_0 t} H_{SR} e^{-(i/\hbar)H_0 t} \). By formally integrating Eq.(1.47), we get

\[ \tilde{\rho}_{SR}(t) = \rho_{SR}(0) - \frac{i}{\hbar} \int_0^t dt' \left[ \tilde{H}_{SR}(t'), \tilde{\rho}_{SR}(t') \right] \quad (1.48) \]

and after inserting Eq.(1.48) into Eq.(1.47) we obtain

\[ \dot{\tilde{\rho}}_{SR}(t) = -\frac{i}{\hbar} \left[ \tilde{H}_{SR}(t), \rho_{SR}(0) \right] - \frac{1}{\hbar^2} \int_0^t dt' \left[ \tilde{H}_{SR}(t'), [\tilde{H}_{SR}(t'), \tilde{\rho}_{SR}(t')] \right] \equiv \mathcal{L}\rho \quad (1.49) \]

where \( \mathcal{L} \) is an operator defined over matrices (superoperator) or Lindbladian \([43, 42]\). Now we assume that initially, at \( t = 0 \), the system and the reservoir are uncorrelated, thus, the total density matrix is the product of the system and the reservoir density matrices, \( \rho_{SR}(0) = \rho_S(0) \otimes \rho_R(0) \), where \( \rho_S(t) \) and \( \rho_R(t) \) are defined in Eq.(1.44) and (1.45) respectively\(^4\). A master equation for the system can be derived by using a perturbative approach based on two assumptions. The first assumption is that the coupling is weak, and the reservoir is so large that its statistical properties will not be substantially affected by the interaction with the system. Therefore at time \( t \) the density

\[ \tilde{\rho}_S = \text{Tr}_R (\tilde{\rho}_{SR}) = e^{(i/\hbar)H_0 t} \rho_S e^{-(i/\hbar)H_0 t}. \quad (1.50) \]

\(^4\)Note that reduction of the density operator is preserved in the interaction picture i.e.

\[ \tilde{\rho}_S = \text{Tr}_R (\tilde{\rho}_{SR}) = e^{(i/\hbar)H_0 t} \rho_S e^{-(i/\hbar)H_0 t}. \]
matrix of the total system is given by
\[ \tilde{\rho}_{SR}(t) = \tilde{\rho}_S(t) \otimes \rho_R(0) + O(H_{SR}) \] (1.51)

where the second term on the right-hand side of this equation emerges due
to the coupling $H_{SR}$ and is a small term. We now use Eq.(1.51) in Eq.(1.49)
and trace over the external degrees of freedom. At second order perturbation
theory in $H_{SR}$ we obtain
\[
\dot{\tilde{\rho}}_S(t) = -\frac{i}{\hbar} \text{Tr}_R \left[ \tilde{H}_{SR}(t), \tilde{\rho}_S(0) \otimes \rho_R(0) \right] \\
- \frac{1}{\hbar^2} \text{Tr}_R \int_0^t dt' \left[ \tilde{H}_{SR}(t), \left[ \tilde{H}_{SR}(t'), \tilde{\rho}_S(t') \otimes \rho_R(0) \right] \right] (1.52)
\]

This master equation hence contains the initial state of the reservoir, and
correlations between systems and reservoir are neglected, as they are corrections
at higher order in the perturbative expansion (Born approximation).

In Eq. (1.52), $\tilde{\rho}_S$ depends of its past history, as one can see from the
term $\tilde{\rho}_S(t')$ of the integrand. In most quantum optical systems, however,
one can assume the Markov approximation by replacing $\tilde{\rho}_S(t')$ by $\tilde{\rho}_S(t)$ in
the integrand. The validity of the Markov approximation lies on the existence
of two well separated time scales $T_R$ and $T_S$ determining the reservoir
and system correlation function respectively, such that $T_R \ll T_S$. When
this is fulfilled, one can safely assume that the changes in the system can be
neglected over the time scales in which the reservoir reaches its stationary
state, which corresponds to evaluating the integral in Eq. (1.52) by neglecting
the time changes of $\tilde{\rho}_S$. The validity will be discussed case by case in the
following sections. By doing this, the master equation in the Born-Markov
approximation is obtained, and reads
\[
\frac{\partial}{\partial t} \tilde{\rho}_S = -\frac{i}{\hbar} \text{Tr}_R \left[ \tilde{H}_{SR}(t), \tilde{\rho}_S(0) \otimes \rho_R(0) \right] \\
- \frac{1}{\hbar^2} \text{Tr}_R \int_0^t dt' \left[ \tilde{H}_{SR}(t), \left[ \tilde{H}_{SR}(t'), \tilde{\rho}_S(t') \otimes \rho_R(0) \right] \right] (1.53)
\]

In this process the evolution of the reduced density matrix $\tilde{\rho}_S(t)$ is de-
scribed in Eq.(1.43). This evolution is Markovian but not unitary, and we
can describe it by Eq.(1.49) [42, 43]. This equation fulfills the Lindblad’s
theorem which warrants that positivity is preserved ($\mathcal{L}\rho > 0$) as well as
1.4 Master Equation

hermiticity ($\rho_S = \rho_S^\dagger$) of the density operator, and conservation of the trace ($\text{Tr}_S \{ \rho_S (t) \} = 1 \rightarrow \text{Tr}_S \{ \dot{\rho}_S \} = 0$).

1.4.1 Cavity field damping

Let us now discuss the generic derivation of the Born-Markov master equation, Eq. (1.53), for a specific system-reservoir model, namely a cavity mode in the optical regime, coupled to the external modes of the electromagnetic field by partially transmitting mirrors, as sketched in Fig. (1.5).

Figure 1.5: The cavity mode is coupled to the continuum of radiation modes outside the cavity via the finite transmittivity of the cavity mirrors. This introduces damping (leakage of cavity photons) and quantum fluctuations of the cavity mode. This is an example of an open system.

System, reservoir and coupling Hamiltonians now read

$$H_S = H_{\text{cav}}$$  \hspace{1cm} (1.54)  

$$H_R = H_f$$ \hspace{1cm} (1.55)  

$$H_{SR} = \hbar \sum_j \zeta_j \left( b_j^\dagger a + a^\dagger b_j \right)$$ \hspace{1cm} (1.56)

where the terms $H_{\text{cav}}$ and $H_f$ are defined in Eq.(1.17) and Eq.(1.4), respectively, and the interaction between the cavity mode and the external electromagnetic field $H_{SR}$ describes the coherent exchange of photons between the external electromagnetic field and the cavity mode, while the coefficient $\zeta_j$ gives the mode coupling. In the interaction picture with respect to $H_0 = H_S \otimes 1_R + 1_S \otimes H_R$ the interaction term transforms as

$$\tilde{H}_{SR} (t) = \hbar \left( \tilde{\Gamma}^\dagger (t) \tilde{a} (t) + \tilde{a}^\dagger (t) \tilde{\Gamma} (t) \right)$$ \hspace{1cm} (1.57)
where

\[ \tilde{a} (t) = ae^{-i\omega_c t} \tag{1.58a} \]
\[ \tilde{a}^\dagger (t) = a^\dagger e^{i\omega_c t} \tag{1.58b} \]

and

\[ \tilde{\Gamma} (t) = \sum_j \zeta_j b_j e^{-i\omega_j t} \tag{1.59a} \]
\[ \tilde{\Gamma}^\dagger (t) = \sum_j \zeta_j b_j^\dagger e^{i\omega_j t} \tag{1.59b} \]

Substituting Eq. (1.57) in Eq. (1.52), we find

\[
\dot{\rho}_S (t) = -i \left\langle \tilde{\Gamma}^\dagger (t) \right\rangle_R [a, \rho_S] e^{-i\omega_c t} - \int_0^t dt' \left\{ \right. \\
\left. [a a\tilde{\rho}_S (t') - a\tilde{\rho}_S (t') a] e^{-i\omega_c (t+t')} \left\langle \tilde{\Gamma}^\dagger (t) \tilde{\Gamma}^\dagger (t') \right\rangle_R \\
+ [a^\dagger a^\dagger \tilde{\rho}_S (t') - a^\dagger \tilde{\rho}_S (t') a^\dagger] e^{i\omega_c (t+t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma} (t') \right\rangle_R \\
+ [a a\tilde{\rho}_S (t') - a\tilde{\rho}_S (t') a] e^{-i\omega_c (t-t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma}^\dagger (t') \right\rangle_R \\
+ [a^\dagger a^\dagger \tilde{\rho}_S (t') - a^\dagger \tilde{\rho}_S (t') a^\dagger] e^{i\omega_c (t-t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma} (t') \right\rangle_R + H.c \right\} 
\]

Substituting Eq. (1.57) in Eq. (1.52), we find

\[
\dot{\rho}_S (t) = -i \left\langle \tilde{\Gamma}^\dagger (t) \right\rangle_R [a, \rho_S] e^{-i\omega_c t} - \int_0^t dt' \left\{ \right. \\
\left. [a a\tilde{\rho}_S (t') - a\tilde{\rho}_S (t') a] e^{-i\omega_c (t+t')} \left\langle \tilde{\Gamma}^\dagger (t) \tilde{\Gamma}^\dagger (t') \right\rangle_R \\
+ [a^\dagger a^\dagger \tilde{\rho}_S (t') - a^\dagger \tilde{\rho}_S (t') a^\dagger] e^{i\omega_c (t+t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma} (t') \right\rangle_R \\
+ [a a\tilde{\rho}_S (t') - a\tilde{\rho}_S (t') a] e^{-i\omega_c (t-t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma}^\dagger (t') \right\rangle_R \\
+ [a^\dagger a^\dagger \tilde{\rho}_S (t') - a^\dagger \tilde{\rho}_S (t') a^\dagger] e^{i\omega_c (t-t')} \left\langle \tilde{\Gamma} (t) \tilde{\Gamma} (t') \right\rangle_R + H.c \right\} 
\]

where we have used the cyclic properties of the trace and introduced the notation

\[
\left\langle \tilde{\Gamma} (t) \tilde{\Gamma}^\dagger (t') \right\rangle_R = \text{Tr}_R \left[ \rho_R \tilde{\Gamma} (t) \tilde{\Gamma}^\dagger (t') \right] 
\]

In order to evaluate the reservoir correlation functions, we now assume that the electromagnetic field is in thermal equilibrium at temperature T. Its density matrix is hence described by

\[
\rho_R = \prod_j \left[ 1 - e^{-\hbar\omega_j / k_B T} \right] e^{-\hbar\omega_j b_j^\dagger b_j / k_B T}, \tag{1.62} \]

where \( k_B \) is the Boltzmann constant. The reservoir correlation functions are
1.4. Master Equation

given by

\[ \langle \tilde{\Gamma}(t) \rangle_R = \langle \tilde{\Gamma}^\dagger(t) \rangle_R = 0 \]  
(1.63a)

\[ \langle \tilde{\Gamma}^\dagger(t) \tilde{\Gamma}^\dagger(t') \rangle_R = \langle \tilde{\Gamma}(t) \tilde{\Gamma}(t') \rangle_R = 0 \]  
(1.63b)

\[ \langle \tilde{\Gamma}^\dagger(t) \tilde{\Gamma}(t') \rangle_R = \sum_j |\zeta_j|^2 e^{i\omega_j (t-t')} \bar{n}_j \]  
(1.63c)

\[ \langle \tilde{\Gamma}(t) \tilde{\Gamma}^\dagger(t') \rangle_R = \sum_j |\zeta_j|^2 e^{-i\omega_j (t-t')} (\bar{n}_j + 1) \]  
(1.63d)

where

\[ \bar{n}_j = \frac{1}{e^{\hbar\omega_j/k_BT} - 1} \]  
(1.64)

is the thermal occupation of the mode at frequency \( \omega_j \). In free space the spectrum of modes is well approximated by a continuum. Hence, the sum over \( j \) can be replaced by an integral over the frequency, properly weighted by the density of states \( \rho_c(\omega) \). In the continuum limit the function \( \zeta_j \rightarrow \zeta(\omega) \) and \( \bar{n}_j \rightarrow \bar{n}(\omega) \). The nonzero correlation functions of the reservoir are rewritten as

\[ \langle \tilde{\Gamma}^\dagger(t) \tilde{\Gamma}(t') \rangle_R = \int_0^\infty d\omega e^{i\omega(t-t')} \rho_c(\omega) |\zeta(\omega)|^2 \bar{n}(\omega) \]  
(1.65a)

\[ \langle \tilde{\Gamma}(t) \tilde{\Gamma}^\dagger(t') \rangle_R = \int_0^\infty d\omega e^{-i\omega(t-t')} \rho_c(\omega) |\zeta(\omega)|^2 (\bar{n}(\omega) + 1) \]  
(1.65b)

showing that they depend on the times \( t \) and \( t' \) through the difference \( \tau = t - t' \). The fact that the density operator, in Eq. (1.60) depends not just on \( \tilde{\rho}_S(t) \) but also on \( \tilde{\rho}_S(t') \) is because the information can flow on two directions. Information can flow from the cavity mode (system) to the external electromagnetic field (reservoir), but it can also flow back from the reservoir to the system, which would result in a non-Markovian system. Let us now check whether we can apply the Markov approximation to Eq. (1.60), namely, whether we may replace \( \tilde{\rho}_S(t-\tau) \) by \( \tilde{\rho}_S(t) \) in the integrals of Eq. (1.60). This is valid provided that the correlation functions of the reservoir, Eqs. (1.65), decay rapidly on the time scale on which \( \tilde{\rho}_S(t) \) varies and may be approximated by delta functions in time. The key idea is the separation between the correlation time of the fluctuation, and the time scale of the density matrix evolution. The correlation time \( T_R \) is the time it takes for the reservoir to "forget" the information that gets from the system.
After this time $T_R$ we can think that this information is lost, and neglect the possibility for this information to flow back and influence the evolution of the system. The time scale of the dynamics, $T_S$, that we want to observe is given by the cavity decay rate, which is significantly much larger than $T_R$. In this limit, the Markovian approximation is valid. From Eqs. (1.65) we can see that the correlation time $T_R$ of the reservoir is determined by the inverse of the spectral width of $\bar{n}(\omega)$, which is given by $T_R = \frac{\hbar}{k_B T}$ [42]. At room temperature, $T_R \sim 10^{-13}$ s. The inverse of the characteristic spectral width of the system is given by the cavity decay rate, which we obtain by means of this theory. Anticipating the result, this is of the order of several $\mu$s, and it is hence significantly much longer than $T_R$. We may thus replace $\tilde{\rho}_S(t - \tau)$ by $\tilde{\rho}_S(t)$ in Eq. (1.60). Using relations (1.65) we obtain

$$\partial_t \tilde{\rho}_S = (\kappa + i\Delta) \left[ a\tilde{\rho}_Sa^\dagger - a^\dagger a\tilde{\rho}_S \right]$$

$$+ \left( \kappa\bar{n} + i\Delta' \right) \left[ a\tilde{\rho}_Sa^\dagger + a^\dagger a\tilde{\rho}_S - a^\dagger a\tilde{\rho}_S - \bar{n}a a^\dagger \right] + h.c.$$  

(1.66)

with

$$\Delta = P \int_0^\infty d\omega \frac{\rho_c(\omega) |\zeta(\omega)|^2}{\omega_c - \omega}$$  

(1.67)

$$\Delta' = P \int_0^\infty d\omega \frac{\rho_c(\omega) |\zeta(\omega)|^2}{\omega_c - \omega} \bar{n}$$  

(1.68)

$$\kappa = \pi \rho_c(\omega_c) |\zeta(\omega_c)|^2,$$  

(1.69)

where $P$ indicates the Cauchy principal value. In obtaining this expression we have used the relation

$$\lim_{t \to \infty} \int_0^t d\tau e^{-i(\omega - \omega_c)\tau} = \pi \delta(\omega - \omega_c) + \frac{iP}{\omega_c - \omega}$$  

(1.70)

in evaluating the time integrals. We now go back to the original reference frame. From Eq. (1.66), recollecting the terms we obtain

$$\partial_t \rho_S = -\frac{i}{\hbar} \left[ H_{cav}'(t), \rho_S \right] + \kappa(\bar{n} + 1) \left( 2a\rho_Sa^\dagger - a^\dagger a\rho_S - \rho_S a a^\dagger \right)$$

$$+ \kappa\bar{n} \left( 2a^\dagger \rho_S a - aa^\dagger \rho_S - \rho_S a a^\dagger \right)$$

(1.71)

with $H_{cav}' = \hbar \omega_c a^\dagger a$ and $\omega_c' = \omega_c + \Delta$ the renormalized cavity field frequency.
In particular, at room temperature and for optical modes we can set \( \bar{n} \approx 0 \), and the master equation then simplifies to the form

\[
\dot{\rho}_S = -\frac{i}{\hbar} \left[ H'_{\text{cav}}, \rho_S \right] + \kappa \left( 2a\rho_S a^\dagger - a^\dagger a\rho_S - \rho_S a^\dagger a \right) = -\frac{i}{\hbar} \left[ H'_{\text{cav}}, \rho_S \right] + \mathcal{L}_\kappa \rho_S \tag{1.72}
\]

where

\[
\mathcal{L}_\kappa \rho_S = \kappa \left( 2a\rho_S a^\dagger - a^\dagger a\rho_S - \rho_S a^\dagger a \right) \tag{1.73}
\]

denotes the superoperator that describes cavity decay at rate \( \kappa \). This term introduces exponential damping of the energy of the cavity field as a function of time, as one can see by evaluating the time evolution of the average number of photons. Dynamics in presence of this term will be evaluated in Chapter 3.

### 1.4.2 Atomic decay

In this section we sketch the basic steps which lead to the Master equation of spontaneous emission of an atomic dipole. Now, the system is the atomic dipole and the reservoir, the modes of the electromagnetic field.

The Hamiltonian terms are given by

\[
H_S = H_{at} \tag{1.74}
\]

\[
H_R = H_f \tag{1.75}
\]

\[
H_{SR} = H_{int} \tag{1.76}
\]

where \( H_{at} \), \( H_f \) and \( H_{int} \) are given in Eq.(1.1), Eq.(1.4) and Eq.(1.10), respectively. In the interaction picture

\[
\tilde{H}_{SR} (t) = \hbar \left( \tilde{\Gamma}^\dagger (t) \tilde{\sigma} (t) + \tilde{\sigma}^\dagger (t) \tilde{\Gamma} (t) \right) \tag{1.77}
\]
1. Atom-Photon Interactions: Basics

where

\[ \tilde{\sigma}(t) = \sigma e^{-i\omega_0 t} \quad (1.78a) \]
\[ \tilde{\sigma}^\dagger(t) = \sigma^\dagger e^{i\omega_0 t} \quad (1.78b) \]
\[ \tilde{\Gamma}(t) = \sum_{i,\epsilon} g_{i,\epsilon} b_i e^{-i\omega_i t} \quad (1.78c) \]
\[ \tilde{\Gamma}^\dagger(t) = \sum_{i,\epsilon} g_{i,\epsilon} b_i^\dagger e^{i\omega_i t} \quad (1.78d) \]

The situation is analogous to the one described in the previous section, where now the master equation for the dipole is obtained by substituting \( a \rightarrow \sigma \) and \( a^\dagger \rightarrow \sigma^\dagger \) in Eq. (1.66). The corresponding master equation then reads

\[
\frac{\partial}{\partial t} \rho_{at} = -\frac{i}{\hbar} [H'_{at}, \rho_{at}] + \frac{\gamma}{2} (\bar{n} + 1) \left( 2\sigma\rho_{at}\sigma^\dagger - \sigma^\dagger\sigma\rho_{at} - \rho_{at}\sigma^\dagger\sigma \right) \\
+ \frac{\gamma}{2} \bar{n} \left( 2\sigma^\dagger\rho_{at}\sigma - \sigma\sigma^\dagger\rho_{at} - \rho_{at}\sigma\sigma^\dagger \right) \quad (1.79)
\]

where \( H'_{at} = \hbar \omega'_0 \sigma^\dagger\sigma \), with \( \omega'_0 = \omega_0 + 2\Delta' + \Delta \) and

\[
\gamma = 2\pi \sum_{\vec{k},\vec{\epsilon}} \int d^3k \rho_{at}(\vec{k},\vec{\epsilon}) |g(\vec{k},\vec{\epsilon})|^2 \delta(kc - \omega_0) \quad (1.80)
\]
\[
\Delta = \sum_{\vec{k},\vec{\epsilon}} P \int d^3k \rho_{at}(\vec{k},\vec{\epsilon}) \frac{|g(\vec{k},\vec{\epsilon})|^2}{\omega_0 - kc} \quad (1.81)
\]
\[
\Delta' = \sum_{\vec{k},\vec{\epsilon}} P \int d^3k \rho_{at}(\vec{k},\vec{\epsilon}) \frac{|g(\vec{k},\vec{\epsilon})|^2}{\omega_0 - kc} \bar{n} \quad (1.82)
\]

Here, \( \rho_{at}(\vec{k},\vec{\epsilon}) \) is the density of states of the modes at wave vector \( \vec{k} \) coupling with the atomic transition, and \( \gamma \) gives the damping rate of the excited state and coincides with the value obtained with the Fermi Golden rule, see Eq.(1.13). In particular, for optical transitions at room temperature we can

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Note that we label by \( i \) the reservoir degrees of freedom that couple the dipole transition, while the reservoir degrees of freedom that couple the cavity mode by the mirror transmittivity in the previous section where labeled by \( j \)
24

1.5. Heisenberg-Langevin equations

set \( \bar{n} \approx 0 \), and the master equation can be written in the form

\[
\frac{\partial}{\partial t} \rho_{at} = -\frac{i}{\hbar} \left[ H_{at}', \rho_{at} \right] + \frac{\gamma}{2} \left( 2\sigma \rho_{at} \sigma^+ - \sigma^+ \sigma \rho_{at} - \rho_{at} \sigma^+ \sigma \right)
\]

(1.83)

where

\[
\mathcal{L}_{\gamma} \rho_{at} = \frac{\gamma}{2} \left( 2\sigma \rho_{at} \sigma^+ - \sigma^+ \sigma \rho_{at} - \rho_{at} \sigma^+ \sigma \right)
\]

(1.84)

is the superoperator that describes the atomic spontaneous emission at rate \( \gamma \).

1.5 Heisenberg-Langevin equations

In this section we will consider an operator approach for the description of the dynamics of a cavity mode and of a dipole coupled to the modes of the external electromagnetic field. This approach is alternative to the master equation, and the equations whose derivation we sketch here, are based on the same approximations, namely the Born and the Markov approximation. Hence, Born-Markov master equation and Heisenberg-Langevin equations are two alternative methods for describing the system’s dynamics.

We now focus on a single cavity mode coupled to the external electromagnetic field by the partially transmitting mirrors of the resonator. The total Hamiltonian is given by Eqs.(1.54), (1.55), (1.56). The Heisenberg equations of motion for the cavity-mode field operator \( a \), and of the reservoir’s operator \( b_j \) are given by

\[
\dot{a} = -i \omega_c a(t) - i \sum_j \zeta_j b_j(t), \quad (1.85)
\]

\[
\dot{b}_j = -i \omega_j b_j(t) - i \zeta_j a(t), \quad (1.86)
\]

where we have used the property by which the cavity and external field mode operators commute at the same instant of time. By formally integrating Eq.(1.86), we obtain

\[
b_j(t) = b_j(0) e^{-i \omega_j t} - i \zeta_j \int_0^t dt' a(t') e^{-i \omega_j (t-t')} \quad (1.87)
\]

The first term on the right-hand side of the equation describes the reservoir
free evolution, while the second term comes from the interaction with the single mode cavity field. By substituting Eq. (1.87) into Eq. (1.85), we find

$$\dot{a} = -\imath \omega_c a(t) - \sum_j \zeta_j^2 \int_0^t dt' a(t') e^{-\imath \omega_j (t-t')} + f(t)$$ (1.88)

with

$$f(t) = -\imath \sum_j \zeta_j b_j(0) e^{-\imath \omega_j t}$$ (1.89)

depending on the free-evolved reservoir operators. In the interaction picture with respect to the cavity and free-electromagnetic field energy, Eq. (1.88) is transformed as

$$\dot{\tilde{a}} = -\tilde{a}(t) \sum_j \zeta_j^2 \int_0^t dt' e^{-\imath (\omega_j - \omega_c) (t-t')} + \eta(t),$$ (1.90)

where we made the Markov approximation, hence neglecting the variation of the system’s operators with time in the integral, and we defined

$$\eta(t) = -\imath \sum_j \zeta_j b_j(0) e^{-\imath (\omega_j - \omega_c) t}$$ (1.91)

In the continuum limit we replace the sum in Eq. (1.90) with an integral, and obtain

$$\dot{\tilde{a}} \approx - (\kappa + \imath \Delta) \tilde{a}(t) + \eta(t)$$ (1.92)

with $\kappa$ and $\Delta$ defined in Eq. (1.69) and Eq. (1.81) respectively.

Let us now characterize the correlation functions of the operator $\eta(t)$, that depend on the reservoir variables and which are denoted by the noise operator. Assuming that the reservoir is in thermal equilibrium, we obtain

$$\langle \eta(t) \rangle_R = \langle \eta^\dagger(t) \rangle_R = 0$$ (1.93)

$$\langle \eta(t) \eta(t') \rangle_R = \langle \eta^\dagger(t) \eta^\dagger(t') \rangle_R = 0,$$ (1.94)

$$\langle \eta^\dagger(t) \eta(t') \rangle_R = \int_0^\infty \rho_c(\omega) |\zeta(\omega)|^2 \tilde{n}(\omega) e^{i(\omega - \omega_c)(t-t')} d\omega$$

$$= 2\kappa \tilde{n}(\omega_c) \delta(t-t'),$$ (1.95)

$$\langle \eta(t) \eta^\dagger(t') \rangle_R = \int_0^\infty \rho_c(\omega) |\zeta(\omega)|^2 (\tilde{n}(\omega) + 1) e^{i(\omega - \omega_c)(t-t')} d\omega$$

$$= \kappa (\tilde{n}(\omega_c) + 1) \delta(t-t'),$$ (1.96)
where we used the relations given in Eqs.(1.63a). Here, $\bar{n}(\omega_c)$ is defined in Eq.(1.64) and can be considered practically zero at room temperature. Hence, the noise operators have zero average and their two-time correlation functions are $\delta$-correlated in time. We will use this formalism in order to solve the field correlation functions in Sec.(3.1.1).

### 1.5.1 Input-output formalism

In experiments, the state of the cavity field can be characterized by measuring the field leaking from the mirrors (field at the cavity output). While classically the field at the output is calculated by multiplying the intracavity field by the mirror transmission coefficient, in quantum mechanics this is not as trivial, since we have to take special care of the commutation relations between the operators. In this section we establish a formal relationship between the intracavity field and the output field using the Heisenberg-Langevin equations introduced in Sec.(1.5).

The field at the cavity output is the external electromagnetic field, which couples to the intracavity field via the mirrors. The equations of motion are given in Eq.(1.86). When integrating them, the field at time $t$ can be written as a function of the operators at previous instant $t_0 < t$ or of the later instant $t_1 > t$. We can thus write the solution as

- For $t_0 < t$,
  \[ b_j(t) = e^{-i\omega_j(t-t_0)} b_j(t_0) - i\zeta_j \int_{t_0}^{t} e^{-i\omega_j(t'-t')} a(t') dt' \]  
  \[ (1.97) \]

- For $t_1 > t$
  \[ b_j(t) = e^{-i\omega_j(t-t_1)} b_j(t_1) + i\zeta_j \int_{t}^{t_1} e^{-i\omega_j(t'-t')} a(t') dt' \]  
  \[ (1.98) \]

For $t_0 = 0$, we obtain Eq. (1.92), which we can rewrite as

\[ \dot{a} = -\kappa a(t) + \sqrt{2\kappa} a_{in}(t) \]  
\[ (1.99) \]

with

\[ a_{in}(t) = \frac{-i}{\sqrt{2\pi}} \int d\omega_j e^{-i(\omega_j - \omega_c)(t-t_0)} b_j(t_0) \]  
\[ (1.100) \]
being the input field operator \([22]\), and using the convention that a leftward propagating field is negative and the opposite is positive. In Fig.(1.6) a schematic representation of this convention is plotted, where the input field \((a_{in})\) is taken negative, since it is propagating to the left, and the field that leaks out of the cavity \((a_{out})\) is taken positive since it is propagating to the right.

\[ a_{in} \quad \sim \quad \sim \quad a_{out} \]

Figure 1.6: Schematic representation of the input-output modes, where the input mode is leftward propagating, and the output is the opposite.

Analogously, when substituting the solution (1.98) in Eq. (1.92) we find

\[
\dot{a} = \kappa a(t) - \sqrt{2} \kappa a_{out}(t)
\]  

(1.101)

where

\[
a_{out} = \frac{i}{\sqrt{2\pi}} \int d\omega_j e^{-i(\omega_j - \omega_c)(t-t')} b_j(t_1)
\]

(1.102)

is the field at the cavity output. Equating Eq.(1.99) and Eq.(1.101), we obtain the “input-output” relation

\[
a_{out}(t) + a_{in}(t) = \sqrt{2} \kappa a(t).
\]

(1.103)
Non-linear optics is the branch that studies the propagation of light in media, where the polarization $P$ responds nonlinearly to the electric field of the light. Such nonlinearities are usually observed when the light fields are sufficiently intense, such as the light provided by lasers. In lossless and dispersionless materials, the medium polarization can be written in a power series of the electrical field $E$ as

$$P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \ldots$$  \hspace{1cm} (2.1)$$

where we considered the case in which the induced dipole moments of the material respond instantaneously to the electric field. Here, $\chi^{(1)}$ is the linear electric susceptibility, while $\chi^{(j)}$ is the nonlinear susceptibility of $j$th order ($j \geq 2$). Correspondingly, we denote by $P^{(j)} = \chi^{(j)}E^{(j)}$ the $j$th-order polarization.

The cases we will discuss in this thesis are those based on materials which exhibit second and third order nonlinearities. These are usually realized in nonlinear optics by means of crystals whose structure exhibits broken symmetry with respect to spatial inversion, while the atomic electronic transitions are only virtually excited, being the fields far-off resonance. Hence, in typical nonlinear crystals the excitation processes are parametric: the initial and final quantum-mechanical electronic states of the system are the same, while the atom can live in states different from the ground state only through virtual levels for small intervals of time of the order of $\frac{\hbar}{\Delta E}$, with $\Delta E$ being the energy difference between the ground and the excited states.
As a consequence, the parametric processes can be described with a real susceptibility, while the photon energy is always conserved [23].

In this chapter, we first review the basic quantum properties of a non-linear crystal, characterized by a second-order susceptibility, and then show how the corresponding effective Hamiltonian can be recovered in a microscopic system composed by two atoms inside a resonator.

### 2.1 Degenerate parametric amplification

In a parametric amplifier, a non-linear crystal with a second order nonlinear susceptibility $\chi^{(2)}$ is pumped by a laser at frequency $\omega_p$. The pump laser is coupled through the crystal with two modes, called signal and idler at frequencies $\omega_s$ and $\omega_i$, respectively, such that

$$\omega_p = \omega_s + \omega_i \quad (2.2)$$

The effective dynamics, obtained by eliminating the electronic degrees of freedom of the crystal and averaging over the crystal structure, is determined by the Hamiltonian [22]

$$\mathcal{H}_{int} = \hbar \lambda \left( a_s^\dagger a_i^\dagger b + a_s a_i b^\dagger \right) \quad (2.3)$$

with $b$, $a_s$ and $a_i$ being the annihilation operators of a photon of pump, signal, and idler mode, respectively. $\lambda$ is the coupling strength, on which the second-order susceptibility tensor depends. In the parametric approximation, the pumping laser is treated classically, since it is assumed to be in a coherent state of large amplitude, and Eq. (2.3) takes the form

$$\mathcal{H}_{int} = \hbar \lambda \epsilon \left( a_i^\dagger a_i e^{-i\phi} + a_s a_i e^{i\phi} \right) \quad (2.4)$$

where $\epsilon$ is the amplitude and $\phi$ the phase of the coherent pumping field. This approximation is valid in the regime where $\lambda t \to 0$, $\epsilon \to \infty$ and $\lambda \epsilon t = \text{constant}$ [36].

The degenerate parametric amplification (DPA) process is the particular case in which the signal and the idler are the same mode at frequency $\omega = \omega_s = \omega_i$, with $\omega_p = 2\omega$. The Hamiltonian for the degenerate parametric
amplification is
\[ \mathcal{H}_{\text{int}} = \hbar \lambda \epsilon \left( a^\dagger e^{-i\phi} + a e^{i\phi} \right) \] (2.5)

In this case, the mode at frequency \( \omega \) is amplified by pumping the \( \chi^{(2)} \)-
medium at frequency \( 2\omega \).

Now, we consider the mean values of the operators \( a \) and \( a^\dagger \) as a function
of time. By solving the Heisenberg equations of motion determined by the
Hamiltonian (2.5) we find
\[
\langle a(t) \rangle = \langle a(0) \rangle \cosh(2gt) - i \langle a^\dagger(0) \rangle \sinh(2gt) e^{-i\phi} \] (2.6)
\[
\langle a^\dagger(t) \rangle = \langle a^\dagger(0) \rangle \cosh(2gt) + i \langle a(0) \rangle \sinh(2gt) e^{i\phi} \] (2.7)

where \( g = \lambda \epsilon \). The variance of the two quadratures, \( X_1 = \frac{1}{2} (a + a^\dagger) \) and
\( X_2 = \frac{1}{2\pi} (a - a^\dagger) \), are given by
\[
(\Delta X_1)^2_t = \frac{1}{4} e^{-2r} \] (2.8)
\[
(\Delta X_2)^2_t = \frac{1}{4} e^{2r} \] (2.9)

where \( r = 2gt \) is the squeezing parameter. Taking that \( (\Delta X_1)^2_t \) becomes with
time smaller than \( \frac{1}{4} \), which means that the quantum fluctuation is reduced
below its value in a symmetric minimum uncertain state with the time,
and therefore we can say that the quadrature is squeezed. The amount of
squeezing is proportional to the strength of the nonlinearity, the amplitude
of the pumping laser, and the interaction time. More details on squeezed
states are given in Appendix B. This non-linear systems are frequently used
to obtain squeezed states and entangled states of light in the continuous
variable framework, which is useful for many quantum information protocols
[44, 45].

### 2.2 Quantum nonlinear optics with two atoms: The theoretical model

In this section we study a system composed by two atoms coupled to a res-
onator, and show that its dynamics reproduces in certain limits a degenerate parametric amplifier.
2.2. The theoretical model

We assume two identical atoms of mass $M$, which are confined inside a standing-wave cavity, and localized along the cavity axis at the positions $x_1$ and $x_2$, respectively. We denote by $p_1$ and $p_2$ the corresponding momenta, and by $H_{mec}$ the Hamiltonian determining the dynamics of the center of mass in absence of the coupling with the electromagnetic field, which has the form

$$H_{mec} = \frac{p_1^2}{2M} + \frac{p_2^2}{2M} + V(x_1, x_2)$$ (2.10)

with $V(x_1, x_2)$ being an external potential, which localizes the atoms at their equilibrium positions, such that they undergo small vibrations with respect to the cavity-mode wavelength. The relevant internal degrees of freedom of the atoms are the ground state $|g\rangle$ and the excited state $|e\rangle$ of a dipole transition with dipole moment $d$, which is at frequency $\omega_0$. The dipoles are driven by a transverse laser field at frequency $\omega_L$ and coupled to a resonator mode at frequency $\omega_c$ and wave vector $k$, as displayed in Fig. (1). A detecting apparatus measures the field at the cavity output.

2.2.1 Master Equation

In the reference frame rotating at the laser frequency, shown in more details in Appendix C, the coherent dynamics of the atoms and cavity mode is described by the Hamiltonian

$$H = H_{mec} + H_{at} + H_{cav} + H_{cav-at} + H_L.$$ (2.11)

The terms

$$H_{at} = -\hbar \Delta \sum_{j=1,2} \sigma_j^\dagger \sigma_j$$ (2.12)

$$H_{cav} = -\hbar \delta_c a^\dagger a$$ (2.13)

describe the system dynamics in absence of coupling with the electromagnetic field. Here $\Delta = \omega_L - \omega_0$ and $\delta_c = \omega_L - \omega_c$ are the detunings of the laser from the dipole and from the cavity frequency respectively. $\sigma_j = |g\rangle \langle e|$ is the lowering operator of the atom $j$, and $\sigma_j^\dagger$ its adjoint. $a$ and $a^\dagger$ are the
annihilation and creation operators of a cavity mode photon. The terms

\[ H_L = \hbar \Omega \sum_{j=1,2} \left( \sigma_j^\dagger + \sigma_j \right) \]

\[ H_{at\text{-}cav} = \hbar \sum_{j=1,2} g(x_j) \left( a^\dagger \sigma_j + \sigma_j^\dagger a \right) \]

describe the interaction of the dipoles with the cavity and laser fields, respectively, being \( \Omega \) the laser Rabi frequency and \( g(x_j) \) the cavity vacuum coupling strength at \( x_j \), with \( g(x_j) = g \cos(kx_j) \). In Eq. (2.14), the laser wave vector is orthogonal to the cavity axis.

Coupling to the external environment gives rise to dissipation and decoherence, which is described by spontaneous emission of the excited state at rate \( \gamma \) and by cavity decay at rate \( \kappa \). The dynamics of the density matrix \( \rho \), of the cavity and atomic degrees of freedom, is given by the master equation

\[ \frac{\partial}{\partial t} \rho = -i\hbar [H, \rho] + \mathcal{L}_\kappa \rho + \mathcal{L}_\gamma \rho \]

\[ \equiv \mathcal{L}_\rho \]  

(2.16)

where \( \mathcal{L}_\kappa \rho \), defined in Eq. (1.73), is the superoperator which describes noise due to cavity decay, and

\[ \mathcal{L}_\gamma \rho = \sum_{j=1,2} \frac{\gamma}{2} \left( 2\sigma_j \rho_j \sigma_j^\dagger - \sigma_j^\dagger \sigma_j \rho - \rho \sigma_j^\dagger \sigma_j \right) \]

(2.18)

is the superoperator which describes the quantum noise due to spontaneous emission.

### 2.2.2 Multi-photon processes and atomic patterns

It is instructive to consider the dynamics in terms of the dipole collective states. We denote by \(|+\rangle\) and \(|-\rangle\) the Dicke symmetric and antisymmetric states respectively, with \(|\pm\rangle = (|eg\rangle \pm |ge\rangle)/\sqrt{2} \), and rewrite the interaction of the atoms with laser and cavity mode in terms of the operators

\[ S_\pm = (\sigma_1 \pm \sigma_2)/\sqrt{2} \]

(2.19)
2.2. The theoretical model

In this representation, the laser-atom interaction, Eq. (2.14), is rewritten as

$$H_L = \hbar \sqrt{2} \Omega S_+ + \text{H.c.} \quad (2.20)$$

while the atom-cavity interaction term, Eq. (2.15), can be decomposed as

$$H_{at-cav} = H_+ + H_-, \text{ with}$$

$$H_\pm = \hbar g_\pm(x_1, x_2) \left( a_{S\pm}^\dagger + a_{S\pm}^\dagger \right) \quad (2.21)$$

and

$$g_\pm(x_1, x_2) = \frac{g}{\sqrt{2}} (\cos(kx_1) \pm \cos(kx_2)). \quad (2.22)$$

This decomposition highlights the relevant cavity-atom dynamics, which depend on the relative atomic position. The term $H_-$ describes the coupling of the cavity mode with the Dicke anti-symmetric state, and it vanishes when the interatomic distance $d = x_2 - x_1$ is an integer multiple of the cavity wavelength $\lambda = 2\pi/k$. We denote the corresponding atomic configuration as "$\lambda$-spaced pattern". The term $H_+$ describes the coupling of the cavity mode with the Dicke symmetric state, and it vanishes when $d$ is an odd multiple of $\lambda/2$. We denote the corresponding atomic configuration as "$\lambda/2$-spaced pattern". Below we discuss the corresponding dynamics in detail, and in Fig.(2.1) we sketch the corresponding $\lambda/2$ and $\lambda$-spaced pattern.

![Figure 2.1: Sketch of the $\lambda/2$ and $\lambda$-spaced pattern, where the red line represents the trapping potential. On the left picture, the interatomic distance is an odd multiple of $\lambda/2$, what we call "$\lambda/2$-pattern". On the right picture, the interatomic distance is an integer multiple of $\lambda$, giving rise to a pattern that we denote "$\lambda$-pattern".](image-url)
2. Non-linear optics with two trapped atoms

\(\lambda\)-spaced pattern.

We first consider the case in which the interatomic distance is an integer multiple of \(\lambda\). For this configuration, at steady state, and for large cooperativities, the atoms are in the ground state and the cavity mode is in a coherent state whose amplitude is determined by the laser intensity [46, 47, 48]. This behaviour can be understood in terms of the coherent buildup of a cavity field, such that its phase is opposite to the driving field. As a result the atomic dipole is not excited, even if the cavity mode is in a coherent state with a finite number of photons. When two or more atoms are present inside the resonator, this situation can be achieved when the atoms scatter in phase into the cavity modes, i.e., when they are arranged in a \(\lambda\)-spaced pattern.

The coherent scattering processes which two atoms undergo are sketched in Fig. 2.2 in the Dicke basis, showing that the antisymmetric state \(|-\rangle\) remains always decoupled from the coherent dynamics. Here, one identifies the suppression of excitation of the atoms at steady state, as due to interference between the excitation path \(|gg, n\rangle \rightarrow |+, n\rangle\), driven by the laser, and the excitation path \(|gg, n+1\rangle \rightarrow |+, n\rangle\), driven by the cavity. Figure 2.2 also displays the rest of higher-order processes. In particular, we note the processes which lead to the excitation of the state \(|ee, n\rangle\) by the absorption of two laser photons, followed by emission of pair of photons into the cavity. These processes are expected to give rise to squeezing of the coherent state of the cavity field. We note that squeezed-coherent radiation has been predicted in the resonance fluorescence of an atomic crystal, at wave vectors such that the Bragg condition of the atomic crystal is equivalent to the \(\lambda\)-spaced pattern here discussed [49]. Finally, we note that the formation of \(\lambda\)-patterns of laser-cooled atoms inside of resonators has been predicted as the result of a self-organizing process [50, 51]. Features of the field at the cavity output, associated with their formation, have been measured in [52, 53]. Theoretical works have shown that these patterns can be also stable in the strong coupling regime, under the condition, in which atomic excitation is suppressed and the cavity field is in a coherent state [46, 47, 54].

\(\lambda/2\)-spaced pattern.

We now analyze the case when the interatomic distance is an odd multiple of \(\lambda/2\), such that \(H_+ = 0\). In this case the atomic ground state couples
2.2. The theoretical model

Figure 2.2: Sketch of the coherent scattering processes between the collective states of two atomic dipoles driven by a laser and coupled to the cavity mode, when the interatomic distance $d$ is an integer multiple of the cavity-mode wavelength $\lambda$. The states $|J,n\rangle$ are the Dicke states of the two dipoles $|J\rangle$ at $n$ cavity photons, where $|J\rangle = |gg\rangle, |±\rangle, |ee\rangle$, and $|±\rangle = (|eg\rangle ± |ge\rangle)/\sqrt{2}$. The arrows labeled by $\Omega$ ($g_±$) indicate the transitions driven by the laser (the cavity mode).

via the laser to the Dicke symmetric state $|+\rangle$, and via the cavity to the antisymmetric state $|-\rangle$, as depicted in Fig. 2.3. Hence, when the laser drives the atoms well below saturation the cavity is empty [46, 47]. In fact, in this limit the two atoms scatter the laser photons with opposite phase into the cavity and the resulting field vanishes due to destructive interference. Figure 2.3 shows, however, that the cavity mode can be pumped by higher-order processes, which excite the state $|ee,0\rangle$. In this regime, the collective dipole can emit photons in pairs into the cavity mode. These processes are expected to give rise to squeezing of the cavity field state. We note that squeezed radiation has been predicted in the resonance fluorescence of an atomic crystal (at wave vectors such that the Bragg condition of the atomic crystal is equivalent to the $\lambda/2$-spaced pattern here discussed [49]). In our work we will investigate the quantum state of the light in presence of a high-finesse cavity when the atoms are initially in a $\lambda/2$ spaced pattern and determine the dynamics resulting from the competition between coherent processes and noise (such as cavity decay, spontaneous emission, and atomic vibrations at the equilibrium positions).
2.3 Non-linear response of two atoms confined in a cavity

In this section, starting from Eq. (2.16), we derive the equation that describes the effective dynamics of the cavity mode in the limit of large atom-laser detuning $|\Delta| \gg g, \Omega, |\delta_c|, \gamma, \kappa$. In this analysis, we neglect the effect of atomic motion, and identify the parameter regime in which the system operates as a Kerr medium or as a $\chi^{(2)}$-medium, defined in detail in Appendix A.

2.3.1 Effective Hamiltonian

We derive the effective Hamiltonian for the coherent cavity dynamics by eliminating the atomic degrees of freedom in fourth order perturbation theory with respect to the coupling with the laser and the cavity field. For later convenience we rewrite the total Hamiltonian given in Eq. (2.11) as

$$ H = H_0 + V $$

(2.23)
with $H_0 = H_{\text{cav}} + H_{\text{at}}$, and $V = H_L + H_{\text{at-cav}}$ the interaction to be treated in perturbation theory. Let us first consider the spectrum of $H_0$, $E_{n,\alpha}$, with $\alpha$ labeling the internal degrees of freedom, $\alpha = gg, \pm, ee$, and $n$ the number of photons. For $|\delta_c| \ll |\Delta|$ the inequality

$$|E_{n,\alpha} - E_{m,\alpha}| \ll |E_{n,\alpha} - E_{m,\alpha}'|$$

holds whenever $\alpha \neq \alpha'$. We hence derive an effective Hamiltonian defined on the manifold of states $|gg, n\rangle$ by eliminating the coupling to the rest of the levels. To accomplish this we proceed with a fourth-order perturbation expansion in the small parameters $g/|\Delta|$, $\Omega/|\Delta|$, which characterize the strength of the coupling $V$. The effective Hamiltonian $H'$ is related to the Hamiltonian $H$ by the Schiffer-Wolf transformation, defined with more details in Appendix D

$$H' = e^{iS}He^{-iS}$$

with $S = S^\dagger$ to be determined, imposing that the effective Hamiltonian has no terms which couple different manifolds, namely

$$P_\alpha H' P_\beta = 0$$

with $P_\alpha = |\alpha\rangle\langle\alpha|$ and $P_\beta = |\beta\rangle\langle\beta|$ with $\alpha, \beta = gg, \pm, ee$, and $\alpha \neq \beta$. Hence, $H'$ can be written as

$$H' = \sum_\alpha P_\alpha H_{\text{eff}}^\alpha$$

where as $H_{\text{eff}}^\alpha$ is the Hamiltonian acting only inside one manifold. We are interested in deriving the specific form of $H_{\text{eff}}$ inside the ground state manifold. Its non-vanishing matrix elements inside the manifold take the form

$$\langle gg, n | H_{\text{eff}} | gg, m \rangle = \langle gg, n | H_{\text{cav}} | gg, m \rangle + \sum_{k \neq gg} \sum_i \frac{\langle gg, n | V | k, i \rangle \langle k, i | V | gg, m \rangle}{(E_{gg, n} - E_{k, i})} + \sum_{k, \gamma, \nu \neq gg} \sum_{i, j, l} \frac{\langle gg, n | V | k, i \rangle \langle k, i | V | \gamma, j \rangle \langle \gamma, j | V | \nu, l \rangle \langle \nu, l | V | gg, m \rangle}{(E_{gg, n} - E_{k, i})(E_{\nu, l} - E_{\gamma, j})(E_{gg, n} - E_{\nu, l})}$$

(2.28)

where the sums over $k, \gamma$ and $\nu$ run over all the intermediate states in the different manifolds (i.e. $k, \gamma, \nu = \pm, ee$), while the sum over $i, j$ and $l$ runs
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over the levels of the same manifolds. By using the explicit form of $V$ given in Eq. (2.14) and in Eq. (2.15), and by using that the energies $E_{gg,n} = -\hbar \delta_c n$, $E_{\pm,n} = -\hbar \Delta - \hbar \delta_c n$ and $E_{ee,n} = -2\hbar \Delta - \hbar \delta_c n$, the resulting Hamiltonian that describes the coherent dynamics reads

$$H_{\text{eff}} = \left( \bar{\theta} - \delta_c \right) a^\dagger a + \beta \left( a^\dagger + a \right) + \bar{\chi} a^\dagger a^\dagger aa + \frac{\bar{\alpha}}{2} \left( a^\dagger a + a^2 \right),$$  \hspace{1cm} (2.29)

where

$$\bar{\theta} = \frac{g^2_+ (x_1, x_2) + g^2_- (x_1, x_2)}{\Delta} \hspace{1cm} (2.30)$$

$$\bar{\beta} = \frac{\sqrt{2} \Omega}{\Delta} g_+ (x_1, x_2) \hspace{1cm} (2.31)$$

$$\bar{\chi} = \frac{1}{\Delta^3} \left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right]^2 \hspace{1cm} (2.32)$$

$$\bar{\alpha} = \frac{2 \Omega^2}{\Delta^3} \left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right] \hspace{1cm} (2.33)$$

Here, $\bar{\theta}$ is the a.c.-Stark shift experienced by the cavity field due to the interaction with the atoms. The term $\bar{\beta}$ comes from the $H_+$ term, Eq. (2.21), and results from the two-photon transitions coupling the photon states $|n\rangle$ and $|n \pm 1\rangle$, see Fig. (2.2). The amplitude $\bar{\alpha}$ is the strength of the effective nonlinear pumping of the cavity field which gives rise to a $\chi^{(2)}$ nonlinearity, typical of a degenerate parametric amplifier [22]. This term is the sum of two contributions, which are weighted by $g_+$ and $g_-$ respectively. These terms represent the coherent sum of the four-photon processes coupling the states $|gg,n\rangle \rightarrow |gg,n \pm 2\rangle$ and depicted in Fig. (2.2) and Fig. (2.3). Finally, the amplitude $\bar{\chi}$ is the a.c.-Stark shift associated with four-photon processes, where two cavity photons are virtually absorbed and then emitted along the transition $|gg,n\rangle \rightarrow |ee,n - 2\rangle$. This term is present in both patterns, and gives rise to the $\chi^{(3)}$ nonlinearity typical of a Kerr medium.

The form of Hamiltonian (2.29) highlights how the two patterns we considered, $\lambda$- and $\lambda/2$-spaced, contribute to the various nonlinear processes. We first notice that in presence of only one atom (when, e.g., $g(x_2) = 0$) the terms $\bar{\alpha}$ and $\bar{\chi}$ trivially vanish. These types of nonlinearities can be clearly generated only when both atoms couple to the cavity mode. Then, one observes that the two patterns give rise to different nonlinear dynamics. In the $\lambda$-spaced pattern, for instance, all terms in Eq. (2.29) contribute to determine the coherent dynamics of the cavity mode. While the linear shift
2.3. Non-linear response of two atoms confined in a cavity

$\bar{\theta}$ can be set to zero by properly choosing the detuning $\delta_c$, on the other hand the linear term scaling with $\bar{\beta}$ is dominant, and one reasonably expects that it will determine the cavity steady state.

When the atoms are distributed in a $\lambda/2$-spaced pattern the linear drive in the Hamiltonian (2.29) vanishes, i.e., $\bar{\beta} = 0$, while the only terms which contribute to the coherent dynamics are at fourth order in the perturbative expansion. Two possible scenarios can be identified here. (i) When the laser drive is much weaker than the cavity coupling, $\Omega \ll g$, then $|\bar{\chi}| \gg |\bar{\alpha}|$ and the dynamics will be basically equivalent to a Kerr medium as in [55], whereby in our case the Kerr nonlinearity emerges from the interaction of the cavity field with the collective dipole of the atoms. (ii) When the laser drive is much stronger than the cavity coupling, $\Omega \gg g$, then $|\bar{\chi}| \ll |\bar{\alpha}|$ and the dynamics will be essentially equivalent to the one in a $\chi^{(2)}$-medium. This is the case on which we focus in the rest of this work.
Nonclassical radiation from two atoms

In this chapter we characterize the light at the cavity output, as it is generated by the interplay of the coherent dynamics of atoms and cavity field and of the incoherent dynamics due to spontaneous emission and cavity decay. In particular we study the system when the effective coherent dynamics is equivalent to a degenerate parametric amplifier.

In Sec.(3.1) we will focus on the realization of the $\chi^{(2)}$-medium with two atoms. In Sec.(3.2) the degree of squeezing of the light at the cavity output is investigated. The validity of our analytical predictions are verified using numerical simulations which take into account the internal dynamics of the atoms and their coupling with the quantized mode of the resonator. Finally, in Sec.(3.3), the effect of atomic vibrations on the field at the cavity output is estimated by using a semiclassical model for the atomic motion.

3.1 Realization of $\chi^{(2)}$-medium with two atoms

We now consider Hamiltonian (2.29) when the atoms are localized at the antinodes of the cavity modes in a $\lambda/2$-spaced pattern (the two atoms are coupled with the cavity mode with opposite phase so that $g_+ = 0$ and $g_- = \sqrt{2}g$). In this configuration the linear pump term plays no role ($\tilde{\beta} = 0$). In the regime where $\Omega \gg g$ (i.e., $|\tilde{\alpha}| \gg |\tilde{\chi}|$), and setting $\delta_c = \tilde{\theta}$, the effective coherent dynamics is described by Hamiltonian $H_{\text{eff}} \approx H'$, with

$$H' = \frac{\tilde{\alpha}}{2} \left( a^2 + a^\dagger a^2 \right)$$  \hspace{1cm} (3.1)
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3.1. Realization of $\chi^{(2)}$-medium with two atoms

and $\bar{\alpha} = \alpha$, where now

$$\alpha = -\frac{4\Omega^2g^2}{\Delta^2} \tag{3.2}$$

3.1.1 Squeezed light from two atomic dipoles

In the Hamiltonian derived in the previous section (Eq.(3.1)) the effective coherent dynamics of the cavity mode is analogous to the one obtained for a degenerate parametric amplification in the parametric approximation. We now consider the noise and dissipation effects in the dynamics, in this case the situation described in Eq.(3.1) would be analogous to an optical parametric oscillator. The signal field should include the losses from one end mirror, that we will consider to be partially transmitting. This source of noise is the cavity decay at rate $\kappa$. We consider also the spontaneous emission of the excited state at rate $\gamma$ as a source of noise. The master equation of the reduced density matrix $\rho$ of the cavity mode takes the form

$$\frac{\partial}{\partial t} \rho = -\frac{i}{\hbar} [H', \rho] + \mathcal{L}_\kappa \rho + \tilde{\mathcal{L}}_\gamma \rho \tag{3.3}$$

where $\mathcal{L}_\kappa \rho$ is defined in Eq.(1.73), and

$$\tilde{\mathcal{L}}_\gamma \rho = \frac{\gamma'}{2} \left(2a \rho a^\dagger - a^\dagger a \rho - \rho a^\dagger a\right) \tag{3.4}$$

describes the damping of the cavity mode via spontaneous emission. It is obtained at second order in the small parameters $\Omega/|\Delta|$, $g/|\Delta|$ and it is given by $\gamma' \approx \gamma \frac{g^2}{\Delta^2}$. We neglect higher order effects because we assume that coherent fourth order effects are of order of $\gamma'$ which imposes $\alpha \approx \gamma'$.

In the framework of an input output formalism the Heisenberg-Langevin equations for the field operators read

$$\dot{a} = -i\alpha a^\dagger - \kappa' a + \eta(t) \tag{3.5}$$

$$\dot{a}^\dagger = i\alpha a - \kappa' a^\dagger + \eta^\dagger(t) \tag{3.6}$$

where $\kappa' = \kappa + \gamma'$ is the cavity decay and $\eta(t)$ the associated noise which satisfy the relations given in Eq.(1.93). Since we wish to study the squeezing properties of the field in the steady state, the values of $\langle a \rangle_{sts}$, $\langle a^\dagger a \rangle_{sts}$ and $\langle a^2 \rangle_{sts}$
will be evaluated.

A solution of these equations, given in more detail in Appendix E, reads

\[ a(t) = e^{-\kappa' t} \left( a(0) \cosh(\alpha t) - i a^\dagger(0) \sinh(\alpha t) \right) \]
\[ + \frac{1}{2} \int_0^t \left[ e^{(\kappa' + \alpha)(\tau - t)} \left( \eta + i \eta^\dagger \right) + e^{(\kappa' - \alpha)(\tau - t)} \left( \eta - i \eta^\dagger \right) \right] d\tau \]
\[ (3.7) \]

\[ a^\dagger(t) = e^{-\kappa' t} \left( i a(0) \sinh(\alpha t) + a^\dagger(0) \cosh(\alpha t) \right) \]
\[ + \frac{1}{2} \int_0^t \left[ e^{(\kappa' + \alpha)(\tau - t)} \left( -i \eta + \eta^\dagger \right) + e^{(\kappa' - \alpha)(\tau - t)} \left( i \eta + \eta^\dagger \right) \right] d\tau' \]
\[ (3.8) \]

Note that considering the cavity decay \( \kappa' = 0 \), the squeezed state expressions for the optical parametric amplifier are recovered [37].

Now we have to obtain a solution for some quantities of interest \( \langle a^\dagger(t) a(t) \rangle \), \( \langle a^2(t) \rangle \) and \( \langle a^{12}(t) \rangle \). The average photon number is given by

\[ \langle a^\dagger(t) a(t) \rangle = e^{-2\kappa' t} \left\{ i \left( \langle a^2(0) \rangle - \langle a^{12}(0) \rangle \right) \cosh(\alpha t) \sinh(\alpha t) \right. \]
\[ + \left. \langle a(0) a^\dagger(0) \rangle \sinh^2(\alpha t) + \langle a^\dagger(0) a(0) \rangle \cosh^2(\alpha t) \right\} \]
\[ + \frac{1}{2} \alpha^2 + e^{-2\kappa' t} \left( \kappa'^2 - \alpha^2 - \kappa' \left( \kappa' \cosh(2\alpha t) + \alpha \sinh(2\alpha t) \right) \right) \frac{\kappa'^2 - \alpha^2}{\kappa'^2 - \alpha^2} \]
\[ (3.9) \]

which considering the case of a cavity without losses (i.e. \( \kappa' = 0 \)) becomes

\[ \langle a^\dagger(t) a(t) \rangle = i \left( \langle a^2(0) \rangle + \langle a^{12}(0) \rangle \right) \cosh(\alpha t) \sinh(\alpha t) \]
\[ + \langle a(0) a^\dagger(0) \rangle \sinh^2(\alpha t) + \langle a^\dagger(0) a(0) \rangle \cosh^2(\alpha t) \]
\[ (3.10) \]

Assuming that the cavity is initially in the vacuum state, we obtain the solution \( \langle a^\dagger(t) a(t) \rangle = \langle a(0) a^\dagger(0) \rangle \sinh^2(\alpha t) \).
3.1. Realization of $\chi^{(2)}$-medium with two atoms

We identify two regimes corresponding to $\alpha > \kappa'$ and $\kappa' > \alpha$. When $\alpha > \kappa'$ the energy of the cavity mode field amplitude increases exponentially as a function of time. Clearly, this exponential increase is a good approximation only for short times, when the number of photons inside the cavity mode still warrants the validity of the perturbative expansion, while for longer times the dynamics will be determined by competition with other processes which we neglected in the derivation.

When $\kappa' > \alpha$, a steady state solution exists. From the Eq.(3.7) and Eq.(3.8) and when the state is initially in vacuum, we can see that the expectation values of the field operators vanishes, $\langle a(t) \rangle_{sts} = \langle a^\dagger(t) \rangle_{sts} = 0$. The corresponding stationary average photon number is

$$n_0 \equiv \langle a^\dagger a \rangle_{sts} = \frac{1}{2} \frac{\alpha^2}{\kappa'^2 - \alpha^2}. \quad (3.11)$$

The mean values of $\langle a^2(t) \rangle$ and $\langle a^{1\dagger}(t) \rangle$ take the form

$$
\langle a^2(t) \rangle = \begin{aligned} 
e^{-\kappa't} & \left( a^2(0) \cosh^2 \alpha t - a^{1\dagger}(0) \sinh^2 \alpha t - i \left( a(0) a^{\dagger}(0) \right) \sinh \alpha t \cosh \alpha t \right) \\
+ & \frac{i}{2} \kappa' \left( -\frac{\alpha}{\kappa'^2 - \alpha^2} \right) + \frac{i}{2} \kappa e^{-2\kappa't} \left( \frac{e^{2\alpha t}}{2\kappa' - 2\alpha} - \frac{e^{-2\alpha t}}{2\kappa' + 2\alpha} \right) 
\end{aligned} \quad (3.12)
$$

At steady state it gives

$$\langle a^2(t) \rangle_{sts} = -\frac{i}{2} \frac{\kappa' \alpha}{(\kappa'^2 - \alpha^2)} \quad (3.13)$$

The steady-state variance of the field quadrature $X(t) = a(t)e^{-i\phi} + a^{\dagger}(t)e^{i\phi}$, takes the form of

$$\langle \Delta X^2 \rangle_{sts} = \frac{\kappa'^2 - \alpha \kappa' \sin (2\phi)}{\kappa'^2 - \alpha^2} \quad (3.14)$$

Optimum squeezing is obtained when $\phi = \frac{\pi}{4}$, with the variance that takes the value

$$\langle \Delta X^2_{\pi/4} \rangle_{sts} = \frac{\kappa'^2 - \kappa \alpha}{\kappa'^2 - \alpha^2} = \frac{\kappa'}{\kappa' + \alpha} \quad (3.15)$$
3. Nonclassical radiation from two atoms

For the orthogonal quadrature, at $\phi = -\pi/4$ one gets

$$\langle \Delta X^2_{-\pi/4} \rangle_{\text{sts}} = \frac{\kappa'}{\kappa' - \alpha}$$

(3.16)

A competition between the pumping parameter $\alpha$ and the dissipations $\kappa'$ is observed. The closer the value of $\alpha$ gets to $\kappa'$, the smaller the quadrature variance in Eq.(3.15) becomes.

3.1.2 Parameter regimes

We now identify parameter regimes in which these dynamics can be found. Master Equation (3.3) has been determined by evaluating the coherent processes up to fourth order, treating cavity decay at lowest order, and spontaneous emission at second order in the perturbative expansion. In particular, by deriving the superoperators in Eq. (1.73) and Eq. (3.4) we neglected dissipative scattering processes at higher order in the expansion in $\Omega/|\Delta|, g/|\Delta|$. This is valid provided that $g^2/|\Delta| > \kappa, \gamma$ and when $|\alpha| \gtrsim \gamma'$, which corresponds to the condition

$$\gamma \lesssim \frac{\Omega^2}{|\Delta|}$$

(3.17)

where we used Eq. (3.2). For a dipole transition with linewidth $\gamma/2\pi = 100$ kHz, in a cavity with $g/2\pi = 2.7$MHz, setting $\Omega/2\pi = 10$ MHz, $|\Delta|/2\pi = 100$ MHz, we find $|\alpha|/2\pi \approx 3$ kHz and a negligible rate of spontaneous decay. Appreciable squeezing could be observed for a cavity decay rate of few kHz, which is a demanding experimental condition. Later we will focus on this parameter regime and check numerically the correctness of the predictions of our analytical model.

3.2 Squeezing spectrum

The squeezing that we can achieve is $(\Delta X)_{\text{sts}} \gtrsim \frac{1}{2}$, and the best squeezing is in the limit of $\kappa' \to \alpha$. The reason of these result can be given to the vacuum fluctuations that comes from outside through the cavity mirror. The relation between the intracavity field and the cavity outside is not trivial when dealing with squeezing since we are working with the antinormal order of the expectation values. In a partial reflecting mirror, not just the cavity field can escape, but also the external field (vacuum field) can leak into the
cavity. Hence, the intracavity field and the input becomes correlated with time.

3.2.1 Squeezing spectrum of the field at the cavity output

Assuming that the system is in the regime where $\kappa' > \alpha$, we evaluate the spectrum of squeezing of the field at the cavity output, defined by the Fourier transform of the normally-ordered two time correlation function, given in more detail in Appendix F, $\langle : X_{\text{out}} (t'), X_{\text{out}} (t) : \rangle$ at steady state [22],

$$S_{\text{out}} (\omega) = 1 + \int_{-\infty}^{\infty} \langle : X_{\text{out}} (t'), X_{\text{out}} (t) : \rangle_{\text{sts}} e^{-i\omega t} dt$$

$$= 1 + 2\text{Re} \int_{0}^{\infty} \langle : X_{\text{out}} (t'), X_{\text{out}} (t) : \rangle_{\text{sts}} e^{-i\omega t} dt \quad (3.18)$$

where the quadratures of the output field can be expressed in terms of creation and annihilation operators of the output field $a_{\text{out}}^\dagger (t)$, $a_{\text{out}} (t)$ as

$$X_{\text{out},1}(t) = a_{\text{out}} (t)e^{-i\pi/4} + a_{\text{out}}^\dagger (t)e^{i\pi/4} \quad (3.19)$$

$$X_{\text{out},2}(t) = -i (a_{\text{out}} (t)e^{-i\pi/4} - a_{\text{out}}^\dagger (t)e^{i\pi/4}). \quad (3.20)$$

The two time correlation function of the output quadratures can be written, taking into account the input output formalism, and the phase dependent two time correlation function described above as

$$\langle X_{\text{out}} (t), X_{\text{out}} (0) \rangle = 2\kappa \langle a (\tau), a (\tau') \rangle e^{-i\pi/2} + \delta (t - 0) + 2\kappa \langle a^\dagger (0), a (t) \rangle + 2\kappa \langle a^\dagger (t), a (0) \rangle$$

$$+ 2\kappa \langle a^\dagger (\tau'), a^\dagger (\tau) \rangle e^{i\pi/2} \quad (3.21)$$

Therefore the spectrum of squeezing can be expressed in terms of correlation functions of the internal field as

$$S_{\text{out}} (\omega) = 1 + 4\text{Re} \int_{0}^{\infty} e^{-i\omega t} \left[ \langle a (t), a (0) \rangle_{\text{sts}} e^{-i\pi/2} + \langle a^\dagger (0), a^\dagger (t) \rangle_{\text{sts}} e^{i\pi/2} + \langle a^\dagger (t), a (0) \rangle_{\text{sts}} + \langle a^\dagger (0), a (t) \rangle_{\text{sts}} \right]. \quad (3.22)$$

By using the results obtained with the effective model developed in
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Eq. (3.3) we find an analytical solution for the squeezing spectrum written as

\[ S_{\text{out}}(\omega) = 1 - \frac{4\kappa |\alpha|}{(\kappa' + |\alpha|)^2 + \omega^2} \]  

(3.23)

showing that a large reduction of the quadrature fluctuations below the shot noise limit is achieved at \( \omega = 0 \) when \( \kappa' \approx \alpha \).

3.2.2 Numerical simulations

The squeezing spectrum is evaluated numerically by using the Liouvillian (2.16) defined in section (2.2.1).

Eq. (3.22) can be expressed in terms of averages performed over a density matrix. The expectation value of an operator \( A(t) \), over a state described by the density matrix \( \rho \) is

\[ \langle A(t) \rangle = \text{Tr} \{ A(t) \rho \} = \text{Tr} \{ A \rho(t) \} \]  

(3.24)

The evolution of the density matrix is defined by the Liouvillian \( \mathcal{L} \)

\[ \dot{\rho} = \mathcal{L} \rho \]  

(3.25)

whose formal solution is

\[ \rho(t) = e^{\mathcal{L}t} \rho(0) \]  

(3.26)

Inserting Eq. (3.26) into Eq. (3.24) we can rewrite the expectation value of the operator \( A \) as

\[ \text{Tr} \{ A(t) \rho \} = \text{Tr} \{ A e^{\mathcal{L}t} \rho(0) \} \]  

(3.27)

In particular, we will use the relations

\[ \langle A(t) A(0) \rangle_{\text{sts}} = \text{Tr} \{ A e^{\mathcal{L}t} (A \rho_{\text{sts}}) \} \]  

(3.28a)

\[ \langle A(0) A(t) \rangle_{\text{sts}} = \text{Tr} \{ A e^{\mathcal{L}t} (\rho_{\text{sts}} A) \} \]  

(3.28b)

where the cyclic property of the trace has been used.

The terms of the expression (3.22) can be written in terms of the averages over the density matrix by using relations (3.28) as
3.2. Squeezing spectrum

\[ \langle a(t), a(0) \rangle_{\text{sts}} = \text{Tr} \left\{ a e^{\mathcal{L}t} (a \rho_{\text{sts}}) \right\} - \left| \text{Tr} \left\{ a^\dagger \rho_{\text{sts}} \right\} \right|^2 \] (3.29)

\[ \langle a^\dagger (t), a^\dagger (0) \rangle_{\text{sts}} = \text{Tr} \left\{ a^\dagger e^{\mathcal{L}t} (a^\dagger \rho_{\text{sts}}) \right\} - \left| \text{Tr} \left\{ a^\dagger \rho_{\text{sts}} \right\} \right|^2 \] (3.30)

\[ \langle a^\dagger (t), a(0) \rangle_{\text{sts}} = \text{Tr} \left\{ a^\dagger e^{\mathcal{L}t} (a \rho_{\text{sts}}) \right\} - \left| \text{Tr} \left\{ a^\dagger \rho_{\text{sts}} \right\} \right|^2 \] (3.31)

\[ \langle a^\dagger (0), a (t) \rangle_{\text{sts}} = \text{Tr} \left\{ a e^{\mathcal{L}t} (\rho_{\text{sts}} a^\dagger) \right\} - \left| \text{Tr} \left\{ a \rho_{\text{sts}} \right\} \right|^2 \] (3.32)

Therefore the spectrum of squeezing can be rewritten as,

\[ S_{\text{out}}(\omega) = 1 - 4\kappa \text{Re} \left\{ \pi \delta(\omega) \text{Tr} \left\{ X^{\pi/4} \rho_{\text{sts}} \right\} \right\}^2 + \text{Tr} \left\{ X^{\pi/4} (\mathcal{L} - i\omega)^{-1} \left( a \rho_{\text{sts}} e^{-i\pi/4} + \rho_{\text{sts}} a^\dagger e^{i\pi/4} \right) \right\} \] (3.33)

where it has been used that \( \int_0^\infty dt e^{-i\omega t} = \pi \delta(\omega) \).

The numerical results are based on the evaluation of the spectrum of squeezing, as calculated from Eq. \( (3.33) \) by using the Liouvillian of Eq. \( (2.16) \).

Figure 3.1 displays the spectrum of squeezing, comparing the analytical prediction in Eq. \( (3.23) \) with the numerical result obtained using Eq. \( (2.16) \), hence including the full internal dynamics of cavity and atoms, as well as the incoherent processes due to cavity decay and spontaneous emission at all orders. The spectra are evaluated by setting \( \alpha = \kappa/2 \), and show that for this parameter regime the analytical model provides a good description of the dynamics. We note, as expected, that spontaneous emission tends to decrease the squeezing at the cavity output.

Figure 3.2 displays the spectra of squeezing for a larger value of the cavity coupling strength. Discrepancies between the analytical and the numerical model arise from the contribution of the Kerr non-linearity in Eq. \( (2.29) \), which is not negligible for this parameter regime, since the laser Rabi frequency \( \Omega \) and the cavity coupling strength \( g \) are of the same order of magnitude.

Figure 3.3 displays the value of the squeezing spectrum at \( \omega = 0 \) as a function of the cavity decay rate \( \kappa \). The spectrum is plotted for \( \kappa > \alpha \), when the analytical model described by Eqs. \( (3.3) \) allows for a steady state solution, and it clearly shows that squeezing at the cavity output is very sensitive to variations of \( \kappa \). On the other hand, the dependence on the
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Figure 3.1: Squeezing spectrum of the field at the cavity output, when the atoms are in a $\lambda/2$-pattern. The dashed lines correspond to the spectrum evaluated analytically from Eq. (3.23), the solid lines to the spectrum found from the numerical evaluation of the steady state of Eq. (2.16), see App. G. The frequency is in units of $\kappa_0 = \kappa$. The parameters are $\Delta = -1.25 \times 10^5 \kappa_0$, $\Omega = 1.25 \times 10^4 \kappa_0$, $g = 1.25 \times 10^3 \kappa_0$ and $\delta_c = -24 \kappa_0$ ($\delta_c$ is chosen so to compensate all a.c.-Stark shifts). For the choice of these parameters, $\alpha = \kappa/2$. The lower and upper curves have been evaluated for $\gamma = 0$ and $\gamma' = \kappa_0/2$ ($\gamma = 10^4 \kappa_0$), respectively. The average number of photons in the upper curve is $n_0 = \frac{1}{10}$, and $n_0 = \frac{1}{6}$ in the lower one.

Figure 3.2: Same as in Fig. 3.1, where now $\kappa = 100 \kappa_0$, $g = 1.25 \times 10^4 \kappa_0$, and $\delta_c = -24 \times 10^2 \kappa_0$. For the choice of these parameters, $\alpha = \kappa/2$. The discrepancy between analytical and numerical results is due to the contribution of the Kerr-nonlinearity, which is not accounted for in the analytical model.
3.2. Squeezing spectrum

Figure 3.3: Value of the squeezing spectrum $S_{\text{out}}(\omega)$ at $\omega = 0$, $S_{\text{out}}(0)$, as a function of the cavity decay rate $\kappa$ in units of $\kappa_0$. The dashed lines correspond to the value predicted from Eq. (3.23), the solid lines to the numerical result found from Eq. (2.16). The parameters are $g = 1.25 \times 10^3 \kappa_0$, $\Delta = -1.25 \times 10^5 \kappa_0$, $\Omega = 1.25 \times 10^4 \kappa_0$, and $\delta_c = -24 \kappa_0$. For these parameters $\alpha = \kappa_0/2$. The lower and upper curves have been evaluated for $\gamma = 0$ and $\gamma' = \kappa_0/2$ ($\gamma = 10^4 \kappa_0$), respectively.

Figure 3.4: $S_{\text{out}}(0)$ as a function of the atomic spontaneous emission rate $\gamma$ in units of $\kappa_0$. The spectra are plotted for two values of the cavity decay rate $\kappa = \kappa_0$ and $\kappa = \kappa_0/2$. The other parameters are as in Fig. 3.3.

atomic linewidth $\gamma$ is comparatively weak, as one can see from Fig. 3.4. The discrepancy between numerical and analytical model at lower values of $\gamma$ is due to the contribution of incoherent scattering processes at higher order, which are accounted for in the numerics and give rise to a very narrow peak at $\omega = 0$ in $S_{\text{out}}(\omega)$. This feature however does not appear for shorter
integration times, corresponding to the limit of validity of our perturbative treatment.

Figure 3.5: (a) $S_{\text{out}}(0)$ as a function of the total effective dissipation rate $\kappa' = \kappa + \gamma'$ in unit of $\kappa_0$ and (b) corresponding variance of the squeezed quadrature of the cavity field. The numerical results are displayed for $\kappa = \kappa'$, $\gamma = 0$ (circles) and $\kappa = \gamma' = \kappa'/2$ (crosses). The dashed lines are obtained from the analytical model. The other parameters are $g = 1.25 \times 10^3 \kappa_0$, $\delta_c = -24 \kappa_0$, $\Delta = -1.25 \times 10^5 \kappa_0$, $\Omega = 1.25 \times 10^4 \kappa_0$, and $\alpha = \kappa_0/2$.

Figures 3.5(a) and (b) display the spectrum of squeezing at $\omega = 0$ and the corresponding variance of the maximally squeezed quadrature of the cavity field as a functions of $\kappa' = \kappa + \gamma'$. In Fig. 3.5(a) the upper curves are obtained for $\kappa = \gamma' = \kappa'/2$, the lower curves correspond to $\gamma' = 0$, $\kappa' = \kappa$. Figure 3.5(b) shows that the variance of the quadrature is the same both for $\gamma' = 0$ and $\gamma' = \kappa$, showing that spontaneous emission in this regime only dissipates the squeezed field along other channels, as predicted from the analytical model of Eq. (3.3).
3.3 Effect of the atomic motion on the spectrum of squeezing

So far we have studied the dynamics of the cavity mode neglecting the atomic kinetic energy on the cavity-mode dynamics. In this section we study the effect of fluctuations in the atomic positions, when the system operates as an optical parametric amplifier. We assume that the atoms are confined by an external potential, which localize them at the antinodes of the cavity standing wave in a $\lambda/2$-spaced pattern, in the regime in which the mechanical effects of the cavity field on the atomic motion can be neglected. This situation could be realized experimentally with the technology developed for instance in [31, 56, 14, 57].

Denoting by $\bar{x}_j$ the atomic equilibrium positions, and by $q_j = x_j - \bar{x}_j$ the displacements, we write the external potential for small vibrations as

$$V(x_1, x_2) = \frac{1}{2} M \nu^2 \left( q_1^2 + q_2^2 \right).$$

(3.34)

where $\nu$ is the trapping frequency. The Heisenberg-Langevin equation of motion for the atomic displacement $q_j$ is given by [58]

$$\ddot{q}_j = -\nu^2 q_j - \frac{F_j}{M} + \xi(t)$$

(3.35)

where $\xi(t)$ is the quantum Langevin force, associated with the spontaneous emission and the cavity decay processes, and

$$F_j = \frac{\partial}{\partial x_j} H_{at-cav}$$

(3.36)

is the mechanical force operator arising from the spatial gradient of the atom-cavity interaction over the atomic wave packet. These equations have to be solved together with the Heisenberg-Langevin equations for the field, which depend on the atomic motion through the functions $\cos kx_j$. We assume that the atoms are well localized at the antinodes of the cavity mode, namely that $\delta q = \sqrt{\langle q_j^2 \rangle} \ll \lambda$, and make a perturbative expansion in the small parameter $k \delta q$. At second order, the equations for the fields
3. Nonclassical radiation from two atoms

\[ \dot{a}(t) = -\imath \alpha a(t) - \left[ \kappa + \imath \left( \theta - \delta_c \right) \right] a(t) + \eta(t) \]  
(3.37)

\[ \dot{a}^\dagger(t) = \imath \alpha a^\dagger(t) - \left[ \kappa' - \imath \left( \theta - \delta_c \right) \right] a^\dagger(t) + \eta(t) \]  
(3.38)

with \( \alpha \) defined in Eqs. (3.2), \( \beta = g\Omega/\Delta \), \( \theta = 2g^2\Delta \), and \( \eta(t) \) is the quantum Langevin term, \( \eta(t) = \sqrt{2\kappa a(t)} + \sqrt{2\gamma a(t)} \). Here \( a_{in}^\dagger(t) \) is the input noise term associated with atomic spontaneous emission, which satisfy the relation \( \langle a_{in}^\dagger(t) a_{in}^\dagger(t') \rangle = \delta(t - t') \), defined in Sec. (1.5).

Even when the atoms are well localized around the antinodes of the cavity mode, the systematic solution of these coupled equations is rather complex. Here, we assume that the external potential provides a steep confinement, such that the effect of the coupling with the cavity mode can be neglected in Eq. (3.35). In this limit the solution of Eq. (3.35) reads

\[ q_j(t) \simeq q_j^{(0)} \cos(\nu t + \phi_j), \]  
(3.39)

where \( q_j^{(0)} \) and \( \phi_j \) are determined by the initial conditions. When the trap frequency is much larger than the effective rates which determine the evolution of the field, \( \nu \gg \alpha, \kappa' \), we can derive a secular equation for the cavity field by averaging the equations for the cavity variables over a period \( T = 2\pi/\nu \) [59]. We insert Eq. (3.39) into the equations for the field variables, Eq. (3.37)-(3.38), and integrate them over the period \( T \). With this procedure we find equations for the operators \( \tilde{a}(t) \), \( \tilde{\eta}(t) \), defined as

\[ \tilde{a}(t) = \frac{1}{T} \int_t^{t+T} d\tau a(\tau), \quad \tilde{\eta}(t) = \frac{1}{T} \int_t^{t+T} d\tau \eta(\tau) \]  
(3.40)

Here, the new noise operators satisfy the equation \( \langle \tilde{\eta}(t) \tilde{\eta}^\dagger(t') \rangle \simeq 2\kappa' \delta(t - t') \), where the \( \delta \)-like correlation is to be interpreted for the coarse-grained time scale. The corresponding Heisenberg-Langevin equations read

\[ \dot{\tilde{a}}(t) = -\imath \alpha \tilde{a}^\dagger(t) - \left[ \kappa + \imath \left( \tilde{\theta} - \delta_c \right) \right] \tilde{a}(t) + \tilde{\eta}(t) \]  
(3.41)

\[ \dot{a}^\dagger(t) = \imath \alpha a^\dagger(t) - \left[ \kappa - \imath \left( \tilde{\theta} - \delta_c \right) \right] a^\dagger(t) + \tilde{\eta}^\dagger(t) \]  
(3.42)
3.3. Effect of the atomic motion on the spectrum of squeezing

while their derivation is discussed in App. G. Here,

\[ \tilde{\alpha} = \alpha(1 - k^2 \bar{q}^2 / 2) \]
\[ \tilde{\theta} = \theta(1 - k^2 \bar{q}^2 / 2). \]  

(3.43)

and we have assumed that the oscillation amplitudes of the two atoms are equal, \( q_1^{(0)} = q_2^{(0)} = \bar{q} \). The motion-induced a.c.-Stark shift can be compensated by properly tuning the laser frequency, \( \tilde{c} = \theta(1 - k^2 \bar{q}^2 / 2) \), and Eqs. (3.41)-(3.42) become

\[ \dot{\tilde{a}}(t) = -i \tilde{\alpha} \tilde{a}^\dagger(t) - \kappa' \tilde{a}(t) + \tilde{\eta}(t) \]
\[ \dot{\tilde{a}}(t) = i \tilde{\alpha} \tilde{a}(t) - \kappa' \tilde{a}^\dagger(t) + \tilde{\eta}^\dagger(t). \]  

(3.44)

Correspondingly, at lowest order in \( k\bar{q}_j \) the spectrum of squeezing is

\[ S_{\text{out}}(\omega) = 1 - \frac{4\kappa\alpha}{(\kappa' + \alpha)^2 + \omega^2} \times \left[ 1 + \left( \frac{\alpha^2 - \kappa'^2 - \omega^2}{(\kappa' + \alpha)^2 + \omega^2} \right) \frac{k^2 \bar{q}^2}{2} \right] \]  

(3.45)

where the term proportional to \( k^2 \bar{q}^2 \) is the correction to Eq. (3.23) due to small vibrations of the atoms at the equilibrium positions. Small fluctuations hence reduce the bandwidth of frequencies where the light is squeezed. The corresponding spectrum, Eq. (3.45), is displayed in Fig. 3.6 for \( k\bar{q} = 0.3 \) and compared to the one of Eq. (3.23), where atomic motion is neglected, showing that the modification of the spectrum of squeezing due to the motion is very small.
3. Nonclassical radiation from two atoms

Figure 3.6: Spectrum of squeezing of the field at the cavity output as a function of $\omega$ in units of $\kappa_0$, for the same parameters as in Fig. 3.1 and $\gamma = 0$. The solid curve corresponds to the spectrum of Eq. (3.44) for $kq = 0.3$. The dashed line corresponds to the spectrum of Eq. (3.23) when atomic vibrations are neglected.
Conclusions

In this part of the thesis, we have studied the dynamics and steady state of a medium composed by two atomic dipoles confined inside a resonator in an ordered structure.

Depending on the relative position of the atoms inside the cavity mode, the linear response can be suppressed, and by tuning the intensity of the laser, the system can operate as a Kerr medium or as an optical parametric amplifier. On that same relative position, the non-linear response emerges from the collective excitations of the atomic dipoles. It is essential to mention that in presence of a single atom, the non-linear response would vanish.

In this research, we have focused on the case in which the system operates as an optical parametric amplifier, and studied the degree of squeezing of the field at the cavity output as a function of the system parameters. Moreover we also considered the effects of atomic vibrations (in the squeezing spectrum at the cavity output), when the atoms are confined at the equilibrium positions of a steep external potential. This is a situation which can be experimentally accomplished as shown in the references [31, 56, 14, 57] for instance.

The results of the first part of the thesis provide an example of how non-linearities emerge from the microscopic dynamics of few simple quantum systems. In this respect, two atoms in a resonator can be considered to be the most basic realization of a non-linear crystal, with however limited efficiencies. We expect that the system response could improve, by scaling up the number of atoms given that the collective effects can enhance the non-linear properties.

Indeed, later works showed that strong nonlinearities can be achieved at the single photon level in atomic ensembles confined in structured photonic crystals [60], or optical nonlinear fibers [61, 62], undergoing dynamics
which may even lead to crystallization of photonic excitations [61]. In these systems, the non-linearity due to a single atom is enhanced by means of an atomic ensemble. In our work, instead, the nonlinearity emerges from the dipolar collective excitations, and it peculiarly depends on the atomic spatial ordering.

Periodic structures of atoms inside optical resonators have been realized in various experiments. One of the possible realization is by self-organisation of the atoms in the mechanical potential of the cavity field [53, 63]. The situations studied so far show ordering of the atoms into $\lambda$-spaced patterns. An open question is whether in absence of an external trapping potential, the atoms would evolve into a stable $\lambda/2$-spaced pattern. If this is accomplished, then we would certainly have a self-organized pattern, which sustains and is sustained by non-classical light. In this respect, in [54] it was shown, using a semi-classical model and a numerical analysis, that the $\lambda/2$-spaced pattern is expected to be stable for different parameter values, which are consistent with the operational regime in which squeezed light can be observed.

We conclude this part by remarking that so far we treated atomic motion classically. The effect of the quantum atomic motion on the cavity field is treated in the next part of this thesis, where we investigate the quantum ground state of atoms trapped by the potential arising from the intracavity field, which is itself affected by atomic ordering and by matter wave fluctuations. The problem is hence highly nonlinear, as the potential the atoms feel is determined by the atoms density at the quantum level.
Part II

Ultracold atoms in quantum light potentials
Introduction

Cavity quantum electrodynamics (CQEDs) [22, 64] has been a key area of quantum optics since its early days of optical instabilities, such as optical bistability [65, 66], up to the most recent CQED with single atoms interacting with single or few photons [67, 68, 69, 70, 71, 72, 73]. In recent years, considerable attention has been paid to a new regime of CQED, which we call CQED with many-body systems. These studies focus on the mechanical effects of the resonator field on the atomic motion, and on the non-linearity arising from the interdependence between the cavity field and the atoms dynamics. Following the theoretical prediction of [50], signatures of self-organization have been measured in the light scattered by laser-cooled atoms in a transversally-pumped cavity [53]. These selforganized structures and their properties have been theoretically studied in detail in [51, 46, 47, 54]. In different set-ups, Bragg scattering of atomic structures inside optical resonators has been experimentally investigated in [74]. While in all the cases mentioned so far the atomic motion is essentially classical, the stability and properties of these structures in the quantum regime are still largely unexplored. This question acquires a special relevance in view of the recent experimental progress of CQED with ultracold atoms. In fact, strong atom-field coupling between Bose-Einstein condensed (BEC) atoms, and the mode of a high-finesse optical cavity has been realized in the experiments reported in [75, 76, 77, 78]. Moreover, CQED techniques have been used to measure pair correlations in the atom laser [79, 80], and have been proposed for characterizing quantum states of ultracold matter [81, 82, 83, 84]. In [85, 86], the authors investigated the ground state of ultracold atoms in the optical lattice formed by the interaction with the cavity mode. This system combines CQED with the many-body physics of strongly correlated ultracold atoms. In particular, the non-linear dependence of the cavity field on the atomic mo-
tion opens novel perspectives to the rich scenario of ultracold atomic gases in optical lattices. In open space, in fact, these systems offer the possibility to realize paradigmatic systems of quantum many-body physics [87, 88], such as various versions of Hubbard models [89]. A prominent example is the Bose-Hubbard (BH) model [90], exhibiting the superfluid (SF)-Mott insulator (MI) quantum phase transition [91], whose realization with ultracold atoms was proposed in [92], and demonstrated in [93].

A relevant issue is how the MI-SF transition is modified when the atoms are inside a resonator, where the optical lattice, trapping the atoms, is due to the intracavity-field and in the strong-coupling regime depends on the atomic density. This is what we define a "quantum potential”, meaning by it the dependence of the potential on the matter wave properties of the atoms. Within this part of the thesis we investigate the quantum ground state of atoms trapped in the intracavity potential for two specific setups, corresponding to quantum potentials of different physical properties.

In one case, the action of the atoms on the cavity field is a perturbation, shifting the cavity frequency. Effectively, the atoms are a refractive index, hence affecting the condition at which the cavity field can be pumped at resonance. In this regime, we analyze the quantum ground state of the atoms and identify parameter regimes in which it is incompressible.

In the second case, the atoms are pumped and scatter photon into the cavity mode. The atoms are trapped by the field they scatter. In this case, the system state strongly depends on the amplitude of the driving field. The situation is the one of self-organization, as discussed in several theoretical works [50, 51, 94]. Within this thesis, we analyze whether incompressible states of the selforganized system exist, and for which experimental parameters they could be observed.

This part is organized as follows. In Chap. 4 we introduce the Bose-Hubbard model for ultracold atoms in optical lattices, with particular focus on the MI-SF quantum phase transition in these systems. In Chap. 5 and Chap. 6 the quantum ground state of ultracold atoms in optical resonators is analyzed, considering that the cavity and the atoms are pumped, respectively. Further outlooks of this work are discussed in the conclusions.
Experimental progress in laser cooling and trapping has reached in the last decades a high control of the atomic dynamics at the quantum level [95]. One remarkable example is the realization of conservative periodic potentials for cold atoms, the so-called optical lattices [96, 97]. Optical lattices emerge from a position-dependent dynamical Stark shift of the atomic ground state energy, due to the non-resonant interaction between laser fields and atoms. The basic physical concepts have been introduced in sections 1.2 and 1.3 for the interactions of an optical dipole transition with a quantum electric field. For a large number of photons, when the electric field amplitude can be treated as a scalar, one finds that the ground state of a dipolar transition experiences an energy shift which is proportional to the intensity $I(x)$ of the laser field in the regime in which atom-light interactions can be treated in perturbation theory,

$$\delta E_g(x) \propto \frac{I(x)}{\Delta_a}$$

where $\Delta_a = \omega_L - \omega_0$ is the detuning between laser and dipolar frequency.

The effect is represented in Fig. 4.1 for a dipolar transition with ground state $|g\rangle$ and excited state $|e\rangle$, coupled by a laser with Rabi frequency $\Omega$. When the laser field is a standing wave, the Rabi frequency, and hence the dynamical Stark shift, are periodically modulated. For a standing wave with wave vector $k$, the a.c.-Stark shift has a periodic modulation of the form $\cos^2(kx)$. In particular, when the atoms are sufficiently cold, this energy shift corresponds to a mechanical, periodic potential for the atomic
center-of-mass motion.

Figure 4.1: A dipolar transition with ground state $|g\rangle$ and excited state $|e\rangle$ is driven far-off resonance by a laser field at frequency $\omega$ and detuning $\Delta_a$ from resonance. As a result, the atomic ground-state energy is shifted by the quantity $I/\Delta_a$, with $I = \Omega^2$. The example refers to the case when the laser is red detuned from atomic resonance, $\Delta_a < 0$. In the opposite case, when $\Delta_a > 0$, the shift has opposite sign.

Thus, a spatially-dependent field induces a mechanical potential. Such field can be generated by overlapping two counterpropagating laser beams with the same frequency and polarization. A standing wave, with modulation along $x$ according to $\cos(kx)$, arises from the interference between the two laser beams at wave vector $k$, thereby creating a spatially oscillating potential with period $\lambda/2$ (with $\lambda = 2\pi/k$, the wavelength of the light field), as sketched in Fig. 4.2. In the rest of this thesis we will assume that the atoms are sufficiently cold to just feel a (quasi one-dimensional) periodic potential of the form

$$V_I(x) = V_0 \cos^2(kx) \quad (4.2)$$

with $V_0 = I_0/\Delta_a$ the potential depth, which results from Eq.(4.1) when taking $I(x) = I_0 \cos^2(kx)$. From Eq.(4.1) one can see that the sign of the detuning $\Delta_a$ determines the sign of the optical potential $V_0$. In particular, if the laser is blue detuned ($\Delta_a > 0$) the sign of the potential is positive and as a result its minima are found at the nodes of the standing wave. In this case, hence, the atoms tend to be confined where the intensity of the field is zero. On the other hand, when the laser is red detuned ($\Delta_a < 0$) the

---

1For simplicity we restrict the motion of the atoms to the $x$-direction, and assume a strong external potential which tightly confines the transverse motion, $V(y, z) = \frac{1}{2}m\omega_r^2(y^2 + z^2)$, being $\omega_r$ the frequency of the harmonic external potential.
atoms are attracted to the antinodes of the standing wave, namely, where the intensity of the field is maximal.

Figure 4.2: Sketch of a possible setup, realizing a periodic potential along one axis of periodicity $d = \lambda/2$. The potential is created by two-counterpropagating laser beams at the same wavelength $\lambda$ and polarization, coupling far-off resonance with an atomic dipolar transition.

The rest of this chapter is organized as follows. In Chapter 4.1, the dynamics of a single atom in an optical lattice is discussed. Chapter 4.2 introduces the formalism which will be used for the description of many bosonic atoms in an optical lattice potential, interacting via a contact potential. The Bose-Hubbard model is derived and the superfluid-Mott insulator quantum phase transition is shortly discussed.

4.1 Single particle in optical lattices

We now study the dynamics of a single atom of mass $m$, in the regime in which we can assume that the center of mass moves in the potential given in Eq. 4.2. The corresponding Hamiltonian reads

$$H_s = \frac{p^2}{2m} + V_i(x)$$

(4.3)

where $V_i(x+a) = V_i(x)$, with $a = \lambda/2$. For periodic boundary conditions, the system is invariant by displacements of $a$, and Bloch theorem holds [98, 99]. The eigenstates of Hamiltonian (4.3) then read $\phi_q^{(n)}(x) = e^{iqx}u_q^{(n)}(x)$, where $n$ labels the band, and $q$ is the quasi-momentum of the lattice, taking values within the Brillouin zone $[-\pi/a, \pi/a]$. Function $u_q^{(n)}(x)$ is periodic with period $a$, $u_q^{(n)}(x+a) = u_q^{(n)}(x)$. It fulfills the eigenvalue equation
4.1. Single particle in optical lattices

\[
\left[ \frac{(p + \hbar q)^2}{2m} + V_l(x) \right] u_q^{(n)}(x) = E_q^{(n)} u_q^{(n)}(x) \tag{4.4}
\]

with \( E_q^{(n)} \) the corresponding energy. In our specific case, the optical lattice creates a sinusoidal potential, and the band structure can be found analytically from the Mathieu equation \cite{100}

\[
- \frac{\partial^2}{\partial y^2} \phi_q^{(n)}(y) + \frac{V_0}{4E_r} (2 + 2 \cos(2y)) \phi_q^{(n)}(y) = \frac{E_q^{(n)}}{E_r} \phi_q^{(n)}(y) \tag{4.5}
\]

where \( y = kx \) and we rescaled the equation by dividing by the recoil energy \( E_r \), defined as

\[
E_r = \frac{\hbar^2 k^2}{2m} \tag{4.6}
\]

Figure 4.3 displays different band structures, obtained for increasing values of the potential depth \( V_0 \).

4.1.1 Wannier functions

A convenient basis for studying the dynamics in periodic potentials are the so called Wannier functions. Differing from the Bloch functions, which are completely delocalized eigenfunctions over the entire lattice, the Wannier functions are maximally localized around each optical lattice site, what makes them more intuitive. The Wannier functions are a set of orthonormal wave functions, and are obtained by the Bloch functions with a unitary transformation. In terms of Bloch functions, for a finite lattice with number of sites \( K \) and periodic boundary conditions they are defined as

\[
w_n(x - x_i) = \frac{1}{\sqrt{K}} \sum_q e^{-iqx_i} \phi_q^{(n)}(x) \tag{4.7}
\]

where the sum over \( q \) runs over the first Brillouin zone. Here, \( n \) is the band index, \( x_i \) the potential minimum (with \( i = 1, \ldots, K \)). Figure 4.4 displays the spatial dependence of the Wannier functions for different values of the lattice depth.
Figure 4.3: Band-structure of a 1D optical lattice with periodicity $a$: the Bloch-state energy (in units of $E_r$) is plotted versus the quasimomentum $q$ (in units of $a/\pi$) in the first Brillouin zone for increasing lattice depths $V_0$ (from left to right). The first plot displays the case $V_0 = 0$, where the atoms move freely. The spectrum is quadratic in $q$ and here folded in the first Brillouin zone. As $V_0$ increases, an increasing gap is created at the crossings between the energy curves. At the same time the band widths decreases.
Figure 4.4: Spatial dependence of the Wannier function (black line) for a) $V_0 = 0.5 E_r$, b) $V_0 = 7 E_r$ and c) $V_0 = 25 E_r$. The red line reports the corresponding spatial dependence of the optical lattice potential.

4.2 Ultracold atomic gas in an optical lattice

We now extend the previous model of a single-particle Hamiltonian to a gas of $N$ bosons at ultralow temperatures. Since we deal with a system of $N$ particles, the dynamics should now contain interactions, which are here considered to be two-body interactions. The Hamiltonian is obtained from the single-particle Hamiltonian and the two-body interaction term $V(x_i, x_i')$, and can be written as

$$H = \sum_i \left( \frac{p_i^2}{2m} + V_i(x_i) \right) + \frac{1}{2} \sum_{i \neq i'} V(x_i, x_i').$$  \hspace{1cm} (4.8)

For cold gases, in the ultra-low temperature regime we are interested in, the thermal de Broglie wavelength is much larger than the effective extension of the interaction potential. Thus, the only relevant scattering process is s-wave scattering, as the centrifugal barrier for other partial waves is much higher than the typical atoms kinetic energies. The interatomic potential can be replaced by an effective contact interaction [101]

$$V(x_j, x_{j'}) = \frac{\hbar^2 4 \pi a_s}{m} \delta(x - x').$$  \hspace{1cm} (4.9)
where $a_s$ is the scattering length and $m$ the mass of the atom.

### 4.2.1 Hamiltonian in second quantization

In order to describe the many-body system of identical bosons, prepared in the same spin state, we will use the Hamiltonian in second quantization. For this purpose we introduce the field operators $\Psi(x)$ and $\Psi^\dagger(x)$ which fulfill the commutation relations

$$\begin{align*}
[\Psi(x),\Psi^\dagger(x')] &= \delta(x-x') \\
[\Psi(x),\Psi(x')] &= \left[\Psi^\dagger(x),\Psi^\dagger(x')\right] = 0
\end{align*}$$

where $\Psi^\dagger(x)$ is the Hermitian conjugate of $\Psi(x)$ and $[A,B] = AB - BA$.

In addition, we define the number operator

$$N \equiv \int d^3x \Psi^\dagger(x) \Psi(x) \quad (4.11)$$

Using the commutation relations it is easily verified that $\Psi(x)$ and $\Psi^\dagger(x)$ annihilates and creates, respectively, an atom at position $x$. Within this treatment, we introduce the vacuum state $|0\rangle$, which is assumed to be unique and fulfilling the relations $\langle 0|0\rangle = 1$, $H|0\rangle = 0$, $N|0\rangle = 0$. The Hamiltonian in second-quantized form is found from Eq. (4.8) according to the procedure reported in App. (H), and it reads

$$H = \int d^3x \Psi^\dagger(x) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_l(x)\right) \Psi(x) + \frac{1}{2} \int d^3x \Psi^\dagger(x) \Psi^\dagger(x') V(x,x') \Psi(x) \Psi(x') \quad (4.12)$$

The second-quantized Hamiltonian (4.12), is the starting point for the derivation of the Bose Hubbard model that we introduce in the next section.

### 4.2.2 Bose-Hubbard Model

The ultracold atomic gas with repulsive interaction in a periodic potential, derived in the previous section, can be seen in a very simple picture as a bunch of atoms with no internal structure in an "egg-carton" potential, as
4.2. Ultracold atomic gas in an optical lattice

sketched in Fig. 4.6. These atoms in such "egg carton" potential can move by hopping (quantum tunneling) between sites, and interact by means of the repulsive on-site interaction (which penalizes multiple occupancy per site). In [92] Jaksch and coworkers showed that such systems can be well described by a Bose-Hubbard model [90]. This model is used in solid-state physics to describe, for instance, Josephson-junction arrays [102, 103] and it allows one to study the thermodynamic properties of a strongly interacting gas of bosons due to the competition between kinetic and interaction energy.

The Bose-Hubbard Hamiltonian can be derived from the second-quantized Hamiltonian (4.12). Assuming that the potential is deep, and the temperature is ultralow, we can assume that only the lowest band is occupied. In the tight-binding limit we then can expand bosonic field operators $\Psi(x)$ in terms of Wannier functions (defined in section 4.1.1) [92]

$$\Psi (x) = \sum_i w(x - x_i) b_i$$

where the operators $b_i^\dagger$ and $b_i$ are the bosonic creation and annihilation operators of an atom at the site centered in $x_i$. These operators satisfy the bosonic commutation relations

$$[b_i, b_j^\dagger] = \delta_{ij},$$

$$[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$$

which are found from the commutation relation of the field operators, Eqs. (4.10), and are a direct consequence of the orthonormality of the Wannier function. By inserting the Wannier decomposition (4.13) in Hamiltonian (4.12), we obtain the Bose-Hubbard Hamiltonian

$$H = -t \sum_{<i,j>} (b_i^\dagger b_j + b_i b_j^\dagger) + \frac{1}{2} U \sum_i n_i (n_i - 1) - \mu \sum_i n_i$$

where $n_i = b_i^\dagger b_i$ is the number of bosons at the site centered in $x_i$. The first term of Hamiltonian (4.16) is a hopping term that describes processes in which a particle is annihilated in one site and created in another one. The summation in this term is restricted to the nearest-neighbors sites, since next-to-nearest neighbors tunneling amplitudes are, in the regime of
the tight-binding approximation, typically two orders of magnitude smaller. The second term describes the interaction of each atom with the other atoms on the same lattice site. The third term enters within the grand-canonical description of the system, it is proportional to the total number of atoms and is multiplied by the chemical potential $\mu$. The coefficients $t$ and $U$, multiplying the hopping and the onsite interaction terms, respectively, are found from overlap integrals of Wannier functions. The strength of the tunnel coupling $t$ is given by the integral

$$t = -\int dx \, w^*(x-x_i) \left( \frac{-\hbar^2}{2m} \nabla^2 + V_l(x) \right) w(x-x_{i+1})$$

which is independent of the site, since the system is periodic.

The coupling element $U$ measures the repulsive interaction strength of two atoms at lattice site $i$ and reads

$$U = g_{1D} \int dx \, |w(x)|^4$$

The values of the on-site energy can be estimated analytically, by replacing the Wannier functions by Gaussian functions, since the integral (4.18) is not sensitive to the oscillatory tails of the Wannier functions. This approximation allows us to study the dependence of the integral (4.18) on the physical parameters. Under the Gaussian approximation, the Wannier function can be estimated to be the ground state of the harmonic oscillator, with frequency $\omega$. By using this ansatz, the Wannier function is approximated by the function

$$w(x_i) \approx \frac{1}{\sqrt{\pi \sigma^2}} e^{-\frac{(x_i)^2}{2\sigma^2}}$$

and the value of the onsite interaction is given by

$$U \approx \frac{g_{1D}k}{\sqrt{2\pi}} \left( \frac{V_0}{E_R} \right)^{1/4}$$

4.2.3 Superfluid-Mott insulator transition

The Bose Hubbard model provides one of the simplest realizations of a quantum phase transition: the Superfluid (SF)-Mott insulator (MI) transition. The superfluid regime can be described theoretically in the limit of vanish-
ing interaction (i.e. when $U$ is much smaller than $t$) when kinetic energy dominates. At $U = 0$, Hamiltonian (4.16) takes the form

$$H_t = -t \sum_j \left( b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1} \right) - \mu \sum_j n_j$$

(4.21)

The ground state is a coherent state with each atom delocalized over the entire lattice, and the many-body ground state can be described as

$$|\Phi_{SF}\rangle \propto \left( \sum_j b_j^\dagger \right)^N |0\rangle$$

(4.22)

being $N$ the number of bosons, $K$ the total lattice sites number, and $|0\rangle$ the vacuum state (for simplicity we have dropped the normalization factor).

This many-body state is a superposition of different independent atoms, therefore, for a large number of atoms $N$, the number of atoms at each site follows a Poisson distribution as exemplified in Fig. 4.5, and the fluctuations in the number of atoms per site is $\langle n_j^2 \rangle - \langle n_j \rangle^2 = \langle n_j \rangle$. The system is described by a macroscopic wave function with a well defined macroscopic phase.

Figure 4.5: Possonian atom-number statistics for an optical lattice with mean number of atoms per site $\bar{n} = 2$ for the superfluid ground state. At each lattice site there is a coherent state with a superposition of different atom numbers but a well defined phase. A measurement of the atom number per site would give a occupancy obeying the distribution $f(n)$ plotted in (a). (b) Possible outcome of a atomic number measurement.

For strong interactions (i.e. when $t \ll U$) the atoms localize at the
individual sites. Hamiltonian (4.16), for $t = 0$ reads now

$$H_U = \frac{U}{2} \sum_j n_j (n_j - 1) - \mu \sum_j n_j$$

(4.23)

whose ground state is

$$|\Phi_{MI}\rangle \propto \prod_j (b_j^\dagger)^{n_j} |0\rangle$$

(4.24)

The number of particles per site is therefore well determined and there is no macroscopic phase coherence.

If the strength of the interaction or the tunneling term is changed, the system undergoes a quantum phase transition between the two different phases: the SF-MI phase transition. This quantum phase transition occurs at some value of the ratio $t/U$ and is driven by quantum fluctuations (i.e. can occur also for $T = 0$). The regions in which the system is superfluid or insulator can be represented in a phase diagram in a plane, in which the Mott-insulator states are plotted as a function of the chemical potential $\mu$ and the tunneling strength $t$ [90, 104, 105]. This phase diagram exhibits a lobe-like MI phase in which inside each lobe, there is a fix number of particles per site, an example is shown Fig. (4.6).

In this chapter we sketch the derivation of the SF-MI phase diagram obtained from the strong-coupling expansion derived by Freericks and Monien [106, 107]. In this method, one starts from $t = 0$ and consider a perturbation expansion in the small parameter $t/U$ up to third order. We consider first the MI regime when $t = 0$ and every site is occupied by a fixed number of bosons. In the ground state, the number of bosons per site ($n_0$) is chosen to
minimize the on site energy. If the chemical potential is parametrized such that \( \mu = (n_0 + \delta) U \), then the on-site energy reads

\[
E(n_0) = -\delta U n_0 - \frac{1}{2} U n_0(n_0 - 1).
\]

The energy to add a boson into the system is

\[
E(n_0 + 1) - E(n_0) = -\delta U n_0
\]

Therefore, for \( \delta \neq 0 \) there is an energy gap that corresponds to the necessary energy to add an extra particle. Similarly, the energy for removing a particle (i.e. adding a hole) into the system is given by \( E(n_0 - 1) - E(n_0) = \delta U n_0 \). Thus, for nonzero \( \delta \), a finite amount of energy is required for moving a particle across the lattice. (Note that the difference between adding a particle or a hole is that \( \delta < 0 \) and \( \delta > 0 \) respectively). Starting from the MI phase and by increasing \( t \), the energy gap decreases until it disappear. Then, the bosons condense into the superfluid phase. When \( \delta = 0 \), \( E(n_0 + 1) = E(n_0) \) and there is no extra energy needed to add or extract a particle. In this regime the quantum ground state of the system is compressible.

Using the strong coupling expansion we calculate the free energy of the Mott-insulator state \( E_M(n_0) \) and the free energy of a defect state \( E_\pm(n_0) \) obtained by adding a particle or hole to the MI state defined in (4.24). The defect phases are characterized by adding or extracting an extra particle that moves coherently over the lattice. Its wave functions are determined by degenerate perturbation theory [107]

\[
|\Phi_+\rangle \propto \sum_i f_i b_i^\dagger |\Phi_{MI}\rangle,
\]

\[
|\Phi_-\rangle \propto \sum_i f_i b_i |\Phi_{MI}\rangle
\]

where \( f_i \) is the eigenvector of the tunneling matrix element \( t \) with the lowest eigenvalue. At third order in \( t/U \), the energy of the Mott-insulator state is given by

\[
E_M(n_0) = K \left[ -\delta U n_0 - \frac{1}{2} U n_0(n_0 + 1) - \frac{t^2}{U} n_0(n_0 + 1) \right]
\]
while the energy of the defect states read

\[
E_+(n_0) = -(Kn_0 + 1)\delta U - \frac{U}{2}Kn_0(n_0 + 1) - 2t(n_0 + 1) \\
- 2\frac{t^2}{U} \left[ K(n_0^2 + n_0) - \frac{1}{2}n_0 \right] + \frac{t^3}{U^2}n_0(n_0 + 1)(n_0 + 2) \tag{4.30}
\]

\[
E_-(n_0) = (1 - Kn_0)\delta U - \frac{U}{2}Kn_0(n_0 + 1) - 2tn_0 \\
+ \frac{t^2}{U} \left[ (n_0 + 1)^2 - 2Kn_0(n_0 + 1) \right] - \frac{t^3}{U^2}n_0(n_0 + 1)(n_0 - 1) \tag{4.31}
\]

The phase boundaries between the MI and the compressible phase occur when the energy difference between ground and defect states vanishes

\[
E_\pm(n_0) - E_M(n_0) = 0 \tag{4.32}
\]

The critical chemical potential \(\mu^+(n_0)\) at which the MI phase, with occupation \(n_0\), becomes unstable when adding an extra particle fulfills the following equation

\[
\mu^+(n_0) = Un_0 - 2t(n_0 + 1) + \frac{t^2}{U}n_0^2 \\
+ \frac{t^3}{U^2}n_0(n_0 + 1)(n_0 + 2) \tag{4.33}
\]

In the same way the critical chemical potential \(\mu^-(n_0)\) at which the MI phase becomes unstable when extracting a particle fulfills the following equation

\[
\mu^-(n_0) = Un_0 + 2tn_0 - \frac{t^2}{U}(n_0 + 1)^2 \\
- \frac{t^3}{U^2}n_0(n_0 + 1)(n_0 - 1) = 0 \tag{4.34}
\]

The upper and lower boundaries of the Mott lobes are given respectively by \(\mu^+(n_0)\) and \(\mu^-(n_0)\). When \(\mu^+(n_0) > \mu^-(n_0)\), the zone in between the values of these two chemical potentials corresponds to the Mott insulator state. When increasing \(t\), \(\mu^+(n_0) \leq \mu^-(n_0)\), and the equality gives the value of \(t\) where the lobes close.

The phase diagram plotted in Fig 4.7 shows the boundaries between the MI and SF phase as a function of \(\mu/U\) and \(t/U\). It exhibits a lobe-like MI...
4.2. Ultracold atomic gas in an optical lattice

Figure 4.7: Superfluid-mott insulator phase diagram at zero temperature of the one-dimensional Bose-Hubbard model. The solid lines give the phase boundaries between the Mott insulator and the superfluid state.

phase. At each lobe, there is a fixed integer density, i.e. a fixed number of particles per site.

The phase diagram can be experimentally explored by varying either $\mu$ or $t$. The chemical potential $\mu$ can be changed by shifting the potential with respect to a reservoir [92, 108], while the tunneling $t$ can be tuned by changing the laser intensity (i.e. the potential depth). Let us first fix $t$ at a certain value and increase or decrease $\mu$. There is going to be a point where the extra particle (hole) moves freely over the lattice and the system enters into the superfluid regime. By increasing (decreasing) $\mu$ the system can enter into a new Mott lobe with $(n_0 - 1)$ particle per site. On the other hand, one can fix the density and increase $t/U$, giving the bosons the possibility to overcome the on-site repulsion and get into the superfluid regime.
In this chapter, we investigate a paradigmatic example of cavity quantum electrodynamics with a many-body system: an ultracold atomic gas in the potential formed inside an optical resonator. As in open space, when the optical potential is deep enough, the atomic gas is in the Mott-insulator state. Inside the cavity, nevertheless, the potential is critically affected by the photon-mediated interaction between the atoms. The presence of the atoms determines the cavity resonance, and thus the intracavity field amplitude, which then determines itself atomic localization and the quantum state of the gas.

At ultralow temperatures we assume that the atoms occupy only states of the lowest band of the periodic optical potential. In this regime, we present the detailed derivation of the BH model for atoms in the one-dimensional (1D) potential of an optical resonator. Using this model we study the SF-MI crossover as a function of the system parameters: the chemical potential $\mu$, the pump strength, and the atomic density. Assuming the tight-binding regime, we may describe the MI states using Wannier functions [98], whose form is determined by the optical potential. The Wannier functions are then used to calculate the coefficients in the BH model, as in standard textbooks. We determine the boundaries of the MI states, using the strong coupling expansion of [107, 106], which is a quite accurate method for the calculation of the phase-diagram of the BH model in 1D [88]. It must be stressed that the derivation of the BH model in the cavity does involve certain novel aspects. Namely, the periodic optical potential depends functionally on the atomic density, and hence on the Wannier functions. The problem is therefore
5.1 The Model

We study a gas of ultracold atoms with mass $m$ and atomic dipole transition frequency $\omega_0$, between the ground state $|g\rangle$ and the excited state $|e\rangle$, that couples quasi-resonantly with a standing wave cavity mode at frequency $\omega_c$, and wave vector $k = 2\pi/\lambda$. The coupling strength, as defined in Eq.(1.20), is position-dependent

$$g(x) = g_0 \cos(kx)$$

(5.1)

where $g_0$ is the vacuum Rabi frequency.

The cavity is driven by a laser field with frequency $\omega_p$ through one of the cavity mirrors with amplitude $\eta$. On the other hand, the atoms are pumped by a classical field of amplitude $\Omega$ that oscillates at frequency $\omega_p$, as shown in Fig.5.1. We consider the atomic motion along the cavity axis,
which coincides here with the x-axis, and assume tight confinement in the radial plane so that the radial motion can be considered frozen out. Atomic center-of-mass position and momentum operators are \( x \) and \( p \), fulfilling the uncertainty relation \( [x, p] = i\hbar \).

Figure 5.1: A gas of ultracold atoms inside an optical resonator. The cavity is driven by an external laser through one of the partially transparent mirrors. The atoms are driven by a laser and couple to a mode of the cavity. The parameters are defined in section 5.1.1

5.1.1 Single Particle Hamiltonian

In order to give a first insight on the physics that lies behind this model, we will start by reducing the system to a single atom coupled to a cavity. The system is modeled by the Jaynes-Cummings Hamiltonian in the rotating wave and dipole approximation. In the reference frame oscillating at the laser frequency \( \omega_p \), the normally-ordered Hamiltonian describing the coherent dynamics of the atomic and cavity mode state reads

\[
H = H_{mec} + H_{at} + H_{cav} + H_{JC} + H_L + H_P
\]

(5.2)

where \( H_{mec} = \frac{p^2}{2m} \) describes the center of mass motion dynamics in absence of coupling with the electromagnetic field. The terms

\[
H_{at} = -\hbar \Delta_a \sigma^\dagger \sigma,
\]

(5.3)

\[
H_{cav} = -\hbar \Delta_c a^\dagger a
\]

(5.4)
are the free Hamiltonians of the atomic transition and the cavity field, respectively, in the reference frame rotating at the frequency $\omega_p$ of an external laser driving the system. Here, $\Delta_a = \omega_p - \omega_0$ is the detuning of the atom from the drive frequency, and $\Delta_c = \omega_p - \omega_c$ is the detuning of the cavity from the drive frequency. The operators $a$ and $a^\dagger$ are the annihilation and creation operators of a cavity photon at frequency $\omega_c$, that fulfill the commutation relation, $[a, a^\dagger] = 1$. $\sigma = |g\rangle \langle e|$, and $\sigma^\dagger = |e\rangle \langle g|$ are the dipole lowering and raising operators described in detail in section (1.2). The terms

$$H_{JC} = \hbar g(x) \left( \sigma^\dagger a + a^\dagger \sigma \right), \quad (5.5)$$

$$H_L = \hbar \Omega \left( \sigma^\dagger + \sigma \right), \quad (5.6)$$

$$H_P = \hbar \eta (a^\dagger + a) \quad (5.7)$$

describe the interaction of the dipole with the cavity field, Eq. (5.5), and with a laser, Eq. (5.6), driving the atoms with coupling strength $\Omega$. Equation (5.7) describes a laser pumping the cavity field with coupling strength $\eta$. Both laser fields are here assumed to be at the same frequency $\omega_p$.

Coupling to the external environment gives rise to dissipation and decoherence, which are described by spontaneous emission of the excited state at rate $\gamma$ (defined in Eq.(1.81)), and by cavity decay at rate $\kappa$ by means of the Langevin formalism. The Heisenberg-Langevin equations of motion for the dipole and field operators read [22]

$$\dot{\sigma}^\dagger = -i \frac{1}{\hbar} [\sigma^\dagger, H] - \frac{\gamma}{2} \sigma^\dagger + \xi^\dagger(t)$$

$$\dot{a} = -i \frac{1}{\hbar} [a, H] - \kappa a + \sqrt{2\kappa} a_{\text{in}}$$

where $\sigma_z = \sigma^\dagger \sigma - \sigma \sigma^\dagger$ and $f_{\text{in}}$ and $a_{\text{in}}$ are the input noise operators, whose mean values vanish and are $\delta$-correlated in time $\langle f_{\text{in}}(t) f_{\text{in}}(t')^\dagger \rangle = \delta(t - t')$, $\langle a_{\text{in}}(t) a_{\text{in}}(t')^\dagger \rangle = \delta(t - t')$.

Let us assume the regime in which the changes in the atomic position are negligible during the time scale in which the atom reaches its internal steady state, namely when $k_B T \ll \hbar |\Delta_a|$ (being $k_B$ the Boltzmann constant and $T$ the temperature). In this regime we can set the derivative of the
dipole equation of motion to zero. For low saturation, $|\Delta_a| \gg g_0, \gamma, |\Delta_c|$, we can adiabatically eliminate the excited atomic state and set $\sigma_z(t) \approx -1$ in Eq.(5.8). We thus obtain

$$\sigma^\dagger = \frac{g(x) a^\dagger + \Omega}{\Delta_a}$$

(5.9)

where we neglected the noise term since we assume the reservoir to be at zero temperature. By inserting the dipole steady state solution (5.9) into (5.2), the single-particle Hamiltonian for cavity and atomic center-of-mass degrees of freedom reads

$$H^\prime = \frac{p^2}{2m} + \hbar \left[ U_0 \cos^2(kx) - \Delta_c \right] a^\dagger a + \hbar S_0 \cos(kx) \left( a^\dagger + a \right)$$

$$+ \ \hbar \eta(a^\dagger + a) + \hbar \frac{\Omega^2}{\Delta_a}$$

(5.10)

where

$$U_0 = \frac{g_0^2}{\Delta_a}$$

(5.11)

is the depth of the single-photon dipole potential, and

$$S_0 = \frac{g_0 \Omega}{\Delta_a}$$

(5.12)

is the linear pump. The atom shifts the cavity resonance frequency by $U_0 \cos^2(kx)$, being maximum at the mode function antinodes. Although in this section we are describing the physics of a single particle, in which the atom shift can be small in comparison to the cavity decay rate $\kappa$, note that the strong collective coupling regime can be achieved by increasing the number of atoms.

From Eq. (5.10) we observe that the cavity potential, emerging from the a.c. Stark shift of the cavity mode on the atomic state, is spatially periodic with periodicity equal to half the wavelength $\lambda$. This term, in free space is the equivalent of the "optical lattice", with the difference here that its depth depends on the number of intracavity photons, which itself depends on the atomic density distribution. The potential due to light scattering by the atoms into the cavity mode, instead, is periodic with periodicity equal to the wavelength $\lambda$. 
5.2 Mott-insulator states of ultracold atoms in pumped optical resonators

Let us now consider the cavity to be pumped by a laser through one of the partially transparent mirrors, as shown in Fig. 5.2. The Jaynes-Cummings Hamiltonian in the rotating wave and dipole approximation reads now

\[ H = H_{mec} + H_{at} + H_{cav} + H_{JC} + H_P \] (5.13)

where \( H_{at} \), \( H_{cav} \), \( H_{JC} \), and \( H_P \) are defined in Eq. (5.3), Eq. (5.5) and Eq. (5.7) respectively. We assume the regime in which the changes in the atomic position are negligible during the time scale in which the atom reaches its internal steady state, i.e. \( k_B T \ll \hbar |\Delta_a| \), and the excited state is adiabatically eliminated as shown in section 5.1.1. The single-particle Hamiltonian for cavity and atomic center-of-mass degrees of freedom reads now

\[ H' = \frac{p^2}{2m} + \hbar \left[ U_0 \cos^2 (kx) - \Delta_c \right] a^\dagger a + \hbar \eta \left( a^\dagger + a \right) \] (5.14)

where \( U_0 \) is the depth of the single-photon dipole potential defined in (5.11).

---

Figure 5.2: A cavity driven by an external laser through one of the partially transparent mirrors.
5. Ultracold Atoms in Optical Cavities

5.2.1 Many-body dynamics

We now extend the previous model and derive the corresponding effective Hamiltonian for a gas of \(N\) bosons at ultralow temperatures. The particle interactions are modelled by \(s\)-wave scattering. We introduce the field operators \(\Psi_j(x), \Psi_j^\dagger(x)\), with \(j = g,e\) labeling the internal ground state, such that

\[
[\Psi_j(x), \Psi_j^\dagger(x')] = \delta_{jj'} \delta(x - x') \tag{5.15}
\]

\[
[\Psi_j(x), \Psi_i(x')] = [\Psi_j^\dagger(x), \Psi_i^\dagger(x')] = 0 \tag{5.16}
\]

Hamiltonian \((5.10)\) in second quantization is decomposed according to

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1,
\]

with \(\mathcal{H}_0\) defined in Sec. \((4.2.2)\), where the strength of the onsite interaction is integrated along the transverse directions, and

\[
\mathcal{H}_1 = -\hbar \Delta_a \int dx \left[ \Psi_e^\dagger(x) \Psi_e(x) \right] - \hbar \Delta_c a^\dagger a + \hbar \eta(a + a^\dagger)
\]

\[
+ \hbar g_0 \int dx \cos(kx) \left[ \Psi_g^\dagger(x) \Psi_g(x) a + a^\dagger \Psi_g^\dagger(x) \Psi_g(x) \right] \tag{5.18}
\]

where we have used \(g(x) = g_0 \cos(kx)\). In the above description we omit to write the Hamiltonian term describing the collisions between atoms in different internal states, as we will consider that the excited state is essentially empty in the parameter regime we choose. The quantum Heisenberg-Langevin equations for atomic and field operators read

\[
\dot{\Psi}_g(x) = -\frac{i}{\hbar} [\Psi_g(x), \mathcal{H}_0] - \frac{i}{\hbar} [\Psi_g(x), \mathcal{H}_1] - \sqrt{\gamma} f^{in} \Psi_e(x) \tag{5.19}
\]

\[
\dot{\Psi}_e(x) = -\frac{i}{\hbar} [\Psi_e(x), \mathcal{H}_0] - \frac{i}{\hbar} [\Psi_e(x), \mathcal{H}_1] - \frac{\gamma}{2} \Psi_e(x) + \sqrt{\gamma} \Psi_g(x) f^{in} \tag{5.20}
\]

\[
\dot{a} = (i \Delta_c - \kappa) a - i \eta + \sqrt{2 \kappa} a_r - ig_0 \int dx \cos(kx) \Psi_g^\dagger(x) \Psi_e(x) \tag{5.21}
\]
where $f^{in}(t)$ and $a_{in}(t)$ are the noise operators defined in the previous section, and the commutator with $\mathcal{H}_1$ can be found with

\begin{align*}
- \frac{i}{\hbar} [\Psi_g(x), \mathcal{H}_1] &= -i \hbar g_0 \int dx' \cos(kx') \left( a \Psi_g(x), \Psi_g^\dagger(x') \right) \\
&= -ig_0 \cos(kx) a \Psi_e(x) \tag{5.22}
\end{align*}

\begin{align*}
- \frac{i}{\hbar} [\Psi_e(x), \mathcal{H}_1] &= i \Delta_a \int dx' \left( \Psi_e(x), \Psi_e^\dagger(x') \right) \\
&- i g_0 \int dx' \cos(kx') \left( \Psi_e(x), \Psi_g^\dagger(x') \right) a \\
&= i \Delta_a \Psi_e(x) - ig_0 \cos(kx) \Psi_g(x) a \tag{5.23}
\end{align*}

Solving the equation for the stationary value of $\Psi_e(x, t)$ in the limit of large detuning, $|\Delta_a| \gg \gamma, g \sqrt{\langle n \rangle}$, we find

$$\Psi_e(x) \sim \frac{g \cos(kx)}{\Delta_a} \Psi_g(x) a \tag{5.24}$$

where the adiabatic approximation lies on the assumption that $|\Delta_a| \gg k_B T$, as in the single-particle case. Here we have neglected the input noise term, assuming the decay rate $\gamma \ll |\Delta_a|$. Substituting the result of Eq.(5.24) into Eq.(5.21), the Heisenberg-Langevin equation of motion for the field operator reads

$$\dot{a} = (i \Delta_c - \kappa) a - i \eta + \sqrt{2 \kappa a_{in}} - i \frac{g_0^2}{\Delta_a} \mathcal{Y} a \tag{5.25}$$

where

$$\mathcal{Y} = \int dx \cos^2(kx) \Psi_g^\dagger(x) \Psi_g(x) \tag{5.26}$$

is the integral of the density of atoms at position $x$ in the electronic ground state weighted by the cavity spatial-mode function squared. We now assume the bad-cavity limit, namely the cavity field relaxes to the steady state on a much faster time scale than the one in which the medium varies. This limit implies $\kappa \gg k_B T/\hbar$, and consistently with the previous assumption imposes that $|\Delta_a| \gg \kappa \gg k_B T/\hbar$. In this limit the dependence of the
field on the initial condition is negligible, and its solution is essentially the inhomogeneous one, that can be written as

\[ a \simeq \eta F(Y) \] (5.27)

Here, we have discarded the input noise term, as they are at higher-order in the perturbative expansion and we will be dealing with normally-ordered equations, so that two-time correlations of the noise operators vanish. We also introduced the operator

\[ F(Y) = \frac{1}{i\kappa + (\Delta_c - U_0 Y)} \] (5.28)

which is a function of the atomic density distribution in the ground state. Substituting Eq. (5.27) into the equation for the ground-state field operator we obtain

\[ \dot{\Psi}_g = -\frac{i}{\hbar}[\Psi_g(x), H_0] - i\mathcal{C}, \] (5.29)

where

\[ \mathcal{C} = iU_0\eta^2 \cos^2(kx) F^\dagger(Y) \Psi_g(x) F(Y) \]

### 5.2.2 Discussion

Equation (5.29) shows explicitly the effect of the coupling with the resonator on the atom dynamics: the coupling to the common cavity mode induces a nonlinear interaction, which enters in the equation through operator (5.28). It is useful to consider the average number of photons at steady state \( n_{\text{ph}} = \langle a^\dagger a \rangle_{\text{St}} \), which we obtain from Eq. (5.27) and reads

\[ n_{\text{ph}} = \left\langle \frac{\eta^2}{\kappa^2 + (\Delta_c - U_0 Y)^2} \right\rangle \] (5.30)

The average number of photons \( n_{\text{ph}} \) hence depends on the atomic density distribution. On the other hand, it determines the depth of the confining potential, \( V \approx |U_0| n_{\text{ph}} \), and thus the atomic density distribution. In particular, the confining potential reaches a maximum for the values at which the denominator of Eq. (5.30) is minimum. From the form of operator (5.27) one infers that \( n_{\text{ph}} \) can reach the maximum value when parameters \( \Delta_c \) and
$U_0$ have the same sign, being operator $\mathcal{Y}$ positive valued. From Eq. (5.11) this requires that detunings $\Delta_c$ and $\Delta_a$ have equal signs. This property highlights the role of the detuning in the dynamics as control parameters.

We now comment on the parameters required for accessing the regime in which the effect of the nonlinearity will be important, and its consistency with the derivation we performed. We first review the important assumptions on which our model is based. Spontaneous decay is neglected over the typical timescales of the system. This imposes that the effective spontaneous scattering rate $\gamma'$, due to off-resonant excitation of the dipole transition, fulfills the inequality $\gamma' \ll \kappa$. Using that $\gamma' \sim n_{ph} g_0^2 \gamma / \Delta_a^2$, where $n_{ph}$ is the mean value of intracavity photons (equation (5.30)) the spontaneous emission can be neglected provided that

$$n_{ph} \frac{g_0^2 \gamma}{\Delta_a^2} \ll \kappa$$

As our model is based on a single-mode cavity, we also require that the detuning between atom and cavity mode is smaller than the free spectral range $\delta \omega$. This reduces to the condition

$$|\Delta_a| \ll \delta \omega.$$ \hspace{1cm} (5.32)

A further important assumption relies on the relaxation time of the cavity field, which has to be much faster than the typical timescale of atomic motion. This can be estimated as $k_B T \ll \hbar \kappa$. Finally, in order to ensure that the non-linear effect on $n_{ph}$ is sufficiently large for a small number of atoms, we have required that $U_0 \sim \kappa$. This condition is however not strictly necessary: strong nonlinear effects can be observed for smaller values of $U_0$ when the number of atoms is sufficiently large [65, 66].

Let us now estimate the number of intracavity photons which are usually needed, in order to find the atoms in the MI state. We specifically consider the case in which overlap (bistability) regions between different Mott zones can be observed. In section 5.2.6, we find that this occurs at values of the pump amplitude $\eta \sim 20 \kappa$. This value was evaluated for 50–100 atoms in the resonator. Correspondingly, the number of intracavity photons is $n_{ph} \sim 100$. From condition (5.31) we find that $\gamma \ll 2|\Delta_a|/n_{ph}$, where we used $U_0 = \kappa$, and which is fulfilled for $\gamma = 2 \times 3$ MHz and $|\Delta_a| = 2 \times 10$ GHz.
Condition (5.32) is then satisfied when the free spectral range $\delta \omega$ is of the order of terahertz. Once $|\Delta_a|$ is fixed, we find that $g_0 \sim 2 \times 0.1 \sqrt{\kappa/2\pi} \text{MHz}$. Using the value $\kappa = 2 \times 53 \text{MHz}$ [76], this requires $g_0 \sim 2 \times 700 \text{ MHz}$, which is currently at the border of the experimental reach. However, for smaller values of $U_0$, say $U_0 \sim 0.1\kappa$, and for larger numbers of atoms, say $N \sim 1000$, the peculiar CQED effects on ultracold atoms we predict in this work, could be well observed for parameter regimes of present experiments, see for instance [82, 84].

5.2.3 The Bose-Hubbard Hamiltonian

Derivation of the Bose-Hubbard Model

In the following, we derive a Bose-Hubbard type of model for the atom dynamics in their self-sustained potential maintaining the regime in which the atoms are well localized in the minima of the potential itself. We notice that the nonlinear dependence of the potential on the atomic density distribution, gives rise to a nonlinear equation for the atomic wave-function, which has to be evaluated self-consistently. Starting from the assumption that the atoms are in a Mott-insulator type of state, we decompose the atomic field operator into operators $b_i, b_i^\dagger$, which create and respectively annihilate, atoms at lowest band of the potential site centered at $x = x_i$, according to

$$\Psi(x) = \sum_i \tilde{w}(x - x_i) b_i$$

(5.33)

whereby $\tilde{w}(x - x_i)$ are Wannier functions, which are to be determined by solving self-consistently the equations of motion. The operators $b_i, b_i^\dagger$ obey the bosonic commutation relations in the regular Bose-Hubbard model, where the potential is independent of the state of the atoms. We will show that in our case this is not a priori warranted, but the bosonic commutation relations are recovered in a properly defined thermodynamic limit, which we will identify. We now rewrite Eq. (5.29) within this Wannier decomposition,

$$\dot{b}_\ell = \frac{1}{i\hbar}[b_\ell, \mathcal{H}_0^{(BH)}] - iC$$

(5.34)
where $\mathcal{H}_0^{(BH)}$ and $C$ are obtained from $\mathcal{H}_0$ and $C$ respectively, by using the Bose-Hubbard decomposition. They read

$$\mathcal{H}_0^{(BH)} = E_0 N + E_1 B + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu N$$  \hspace{1cm} (5.35)

where we have introduced the chemical potential $\mu$, and

$$C = U_0 \eta^2 F^1(Y) \left[ J_0 b_\ell + J_1 (b_{\ell+1} + b_{\ell-1}) \right] F(Y)$$  \hspace{1cm} (5.36)

The coupling matrix elements in Eq. (5.35) read

$$E_l = -\frac{\hbar^2}{2m} \int dx \tilde{w}^* (x-x_i) \nabla^2 \tilde{w} (x-x_{i+l})$$

$$J_l = \int dx \tilde{w}^* (x-x_i) \cos^2(kx) \tilde{w} (x-x_{i+l})$$  \hspace{1cm} (5.37)

$$U = g_{1D} \int dx |\tilde{w}(x)|^4$$

with $l = 0, 1$, where we have kept on-site and nearest-neighbour couplings. In Eq.(5.36) we introduced the operator

$$F(\hat{Y}) = \frac{1}{\kappa - i(\Delta_c - U_0 Y)}$$  \hspace{1cm} (5.38)

where $Y = J_0 N + J_1 B$ is obtained from Eq. (5.28) making the Bose-Hubbard decomposition of operator $Y$, Eq. (5.26), after neglecting couplings beyond the nearest neighbors. In order to determine the Bose-Hubbard Hamiltonian, we now derive an effective Hamiltonian $\mathcal{H}_{BH}$ such that $C = [b_\ell, \mathcal{H}_{BH}] / \hbar$. This is performed in the limit in which we can expand operator $F$ in Eq. (5.38) in the small quantity $J_1$, assuming $J_1 \ll J_0$, as it is verified in the Mott-insulator state, using $[N, B] = 0$ and

$$F(J_0 N + J_1 B) \approx F(J_0 N) + J_1 BF'(J_0 N)$$  \hspace{1cm} (5.39)

where we have introduced the notation

$$F'(J_0 N) = \frac{\partial}{\partial y} F(y) \bigg|_{y=J_0 N}.$$  \hspace{1cm} (5.40)
At first order in $J_1$, we find

$$C = U_0 \eta^2 F^\dagger(J_0 N)[J_0 b_\ell + J_1(b_{\ell+1} + b_{\ell-1})]F(J_0 N) + U_0 \eta^2 F^\dagger(J_0 N)J_1 B J_0 b_\ell F(J_0 N) + U_0 \eta^2 F^\dagger(J_0 N)J_0 b_\ell J_1 BF'(J_0 N) + O(J_1^2)$$

Let us now consider the commutation relations between the various operators entering this expression. We note that

$$[b_\ell, F(J_0 N)] = (F(J_0 N + J_0) - F(J_0 N))b_\ell = F'(J_0 N)J_0 b_\ell + O(1/N^2)$$

and it is hence of order $1/N$. Similarly, the commutator $[b_\ell, B] = b_{\ell+1} + b_{\ell-1}$ is at higher order in the expansion in $1/N$. Henceforth, we can rewrite

$$C = U_0 \eta^2 F^\dagger(J_0 N)[J_0 b_\ell + J_1(b_{\ell+1} + b_{\ell-1})]F(J_0 N) + U_0 \eta^2 F^\dagger(J_0 N)J_0 b_\ell J_1 BF(J_0 N) + U_0 \eta^2 F^\dagger(J_0 N)J_0 b_\ell J_1 BF'(J_0 N)$$

$$\equiv [b_\ell, H_{BH}]$$

where

$$H_{BH} = \hbar U_0 \eta^2 F^\dagger(J_0 N)B F(J_0 N) + G(J_0 N)$$

and operator $G(J_0 N)$ has to be determined from the equation

$$[b_\ell, G(J_0 N)] + U_0 \eta^2 F^\dagger(J_0 N)J_0 b_\ell F(J_0 N) = 0$$

which is valid at the considered order in the expansion in $1/N$. At leading order in $1/N$, Eq. (5.43) is a differential equation, such that $G'(J_0 N) = -U_0 \eta^2 F^\dagger(J_0 N)F(J_0 N)$. Using the explicit form of operator $F(x)$, Eq. (5.38), we find

$$G'(x) = -\frac{U_0 \eta^2}{(\kappa^2 + (\Delta - U_0 x)^2)}$$

which gives

$$G(x) = \frac{\eta^2}{\kappa} \arctan \left[ (\Delta - U_0 x)/\kappa \right].$$

The Bose-Hubbard model is recovered for a large number of atoms, according to a properly defined thermodynamic limit. We define the ther-
modynamic by letting $N$ and the cavity volume go to infinity, keeping the number of atoms per potential site finite. This implies the scaling $U_0 \sim 1/N$. Additionally, we impose the scaling $\eta \sim \sqrt{N}$, which corresponds to keeping the potential depth constant as $N$ increases. This scaling corresponds to ramping up the pump intensity with $\sqrt{N}$. The Bose-Hubbard type of Hamiltonian $\mathcal{H}_{\text{eff}} = \mathcal{H}_0^{BH} + \mathcal{H}_{BH}$ is then

$$\mathcal{H}_{\text{eff}} = E_0 N + \frac{U}{2} \sum_i n_i(n_i - 1) - t(N)B + f(N) - \mu N \tag{5.46}$$

where

$$t(N) = -E_1 - \eta^2 U_0 J_1 F(J_0 N) F(J_0 N) \tag{5.47}$$

$$f(N) = \frac{\eta^2}{\kappa} \arctan \left( \frac{\Delta_c - U_0 J_0 N}{\kappa} \right) \tag{5.48}$$

We notice that the coefficients of Hamiltonian (5.46) are operator-valued, hence imposing a Wannier expansion such that the coefficients depend on the operator $N$, namely

$$w(x - x_1) = w_N (N, x - x_i)$$

In general, hence, the commutation relations between the operators $b_i$ are not the typical ones of bosonic operators as in the typical Bose-Hubbard model. Nevertheless, in the thermodynamic limit one finds

$$[b_i, b_j^\dagger] = \delta_{ij} + O(1/N) \tag{5.49}$$

We therefore perform the Wannier expansion in the thermodynamic limit, consistently with the assumptions made in order to obtain Hamiltonian (5.46).

The Bose-Hubbard Hamiltonian

We now rescale Hamiltonian (5.46) and obtain the Hamiltonian $\hat{H} = H/U$, where $U$ is the strength of the on-site interaction and

$$\hat{H} = -iB + \frac{1}{2} \sum_i n_i(n_i - 1) - \hat{\mu}N, \tag{5.50}$$
where

\[ \tilde{\mu} = \frac{\mu + E_0}{U} + \frac{f(N)}{NU} \] (5.51)

contains a rescaled chemical potential, while the tunnel parameter

\[ \tilde{t} = -\frac{E_1}{U} + \frac{\hbar \eta^2 U_0 J_1}{U (\kappa^2 + \zeta^2)} \] (5.52)

is expressed in terms of the coefficient

\[ \zeta = \Delta_c - U_0 J_0 N \] (5.53)

The higher order terms in \( J_1 B \), describing long-range interaction, have been neglected. Note, that in Eq. (5.50) the number of particles is conserved since \([N, \hat{H}] = 0\). We remark that the term \( f(N)/N \) tends to a constant and finite value in the thermodynamic limit.

An important physical quantity, which will be useful for the following study, is the cavity mode potential depth \( V = \hbar U_0 n_{ph} \), where \( n_{ph} \) is the number of photons in Eq. (5.30) in the Bose-Hubbard expansion. At leading order in the expansion \( J_1 \) it takes the form

\[ V = \frac{\hbar \eta^2 U_0}{\kappa^2 + \zeta^2} \] (5.54)

Hamiltonian (5.50) and potential (5.54) are the starting points of our analysis for the determination of the system’s ground state.

Let us now make some considerations about the system for a fixed number of atoms \( N \). From the form of the potential (5.54), and in particular from the form of the coefficient \( \zeta \), Eq. (5.53), we observe that the detunings \( \Delta_a \) and \( \Delta_c \) play a crucial role in the dynamics, as, for instance, for opposite signs of the detunings one can have the vanishing of the coefficient \( \zeta \). This case corresponds to driving the system on resonance, and gives a maximum of the cavity mode potential. This resonance situation occurs for atom numbers \( N \) that maximize the photon number, and gives rise to bistability \([65, 66]\), which modifies substantially the properties of the model with respect to the regular Bose-Hubbard one.
5.2.4 Ground state for a fixed number of particles

In this section we determine the ground state of the system for a fixed number of particles. Moreover, we discuss the situation when the number of atoms is fluctuating. Our purpose is to identify the parameter regime in which the atoms are in the MI state. Starting from the assumption that the system is in the Mott-insulator state, we use the strong coupling expansion by [107, 106] to verify its validity. In particular, we apply a standard degenerate perturbation calculation in the parameter \( \tilde{\mu} = \frac{\mu}{U} \), and determine the ground state energy \( E_M(n_0, \tilde{\mu}, \tilde{t}) \) for the Mott state with \( n_0 \) particles per site, and the ground state energies \( E_\pm(n_0, \tilde{\mu}, \tilde{t}) \) when one particle is added or subtracted to the \( n_0 \)th Mott state. The condition

\[
E_M(n_0, \tilde{\mu}, \tilde{t}) - E_\pm(n_0, \tilde{\mu}, \tilde{t}) = 0
\]

determines the boundaries \( \tilde{\mu}_\pm(n_0) \) of the \( n_0 \)th Mott phase as a function of the coupling parameter \( \tilde{t} \). As \( \tilde{t} \) is increased and \( \tilde{\mu}_+(n_0) = \tilde{\mu}_-(n_0) \), the Mott state gets unstable. In this section we determine the boundaries of the Mott state in a diagram, in which we plot \( \tilde{\mu} \) as a function of \( \tilde{t} \). We remark that, in the typical Bose-Hubbard model, when the system exits the Mott phase, then it is in a superfluid state. In our case, this is probably verified in most cases, which we will discuss individually.

Finally, the parameter \( \tilde{t} \) can be changed by varying the pump amplitude \( \eta \), which is straightforwardly related to the number of photons inside the cavity and hence to the height of the potential, or by varying the atom-pump detuning \( \Delta_a \) and the cavity-pump detuning \( \Delta_c \), which enter in the dynamics through the denominator (5.53) and correspond to changing the refractive index of the atomic medium.

Coefficients in the Gaussian approximation

In this subsection we determine analytically the integrals (5.37) by using the Gaussian approximation. This approximation is valid assuming the Mott insulator state, namely these states have to be well localized on the scale of the wavelenght \( (k\sigma \ll 1) \). The on-site and overlap integrals defined in Eqs. (5.37) are found by replacing the Wannier functions by Gaussian
functions,

\[ w(x - x_i) \approx \frac{1}{\sqrt{\pi \sigma^2}} e^{-\frac{(x-x_i)^2}{2\sigma^2}}. \]  

(5.55)

where \( \sigma \) is the Gaussian function width. This treatment allows us to identify the dependence of the coefficients on the physical parameters. For a sufficiently deep potential, the results obtained with the Gaussian functions are in good agreement with the results obtained with the Wannier functions. While for high enough potentials, the Gaussians are orthonormal, this is not the case for a lower potential. The Gaussians at different lattice sites have non-vanishing overlaps, giving small, but nonetheless, non-physical contributions. One overcomes this difficulty by modifying the Gaussian function, and imposing orthogonality. The overlap term is considered to be small

\[ \int w^*(x - x_i)w(x - x_{i \pm 1})dx = \delta \]  

and we modify the Gaussian functions such that

\[
\tilde{w}(x - x_i) = w(x - x_i) - \frac{\delta}{2}w(x - x_{i+1}) - \frac{\delta}{2}w(x - x_{i-1}).
\]  

(5.57)

We now need to determine the width \( \sigma \) of the Gaussian function. The starting point is to solve the Schrödinger equation

\[
\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \cos^2(kx) \right)w(x) = Ew(x)
\]  

(5.58)

The energy can be found by solving

\[
\int dx w(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \cos^2(kx) \right)w(x) = E \int dx |w(x)|^2
\]  

(5.59)

\[
E = \frac{\hbar^2}{4m\sigma^2} + \frac{1}{2} V \left( 1 + e^{-k^2\sigma^2} \right)
\]

\[
= \frac{E_r}{2k^2\sigma^2} + V \left( 1 - \frac{k^2\sigma^2}{2} \right)
\]  

(5.60)
where $E_r$ is the recoil Energy. Now, we minimize the energy as a function of the width

$$\frac{dE}{d\sigma} = -\frac{E_r}{k^3\sigma^3} - Vk\sigma = 0$$  \hspace{1cm} (5.61)$$

$$y = k^2\sigma^2 = \sqrt{\frac{E_r}{|V|}}$$  \hspace{1cm} (5.62)$$

In order to determine the boundaries of the Mott states in the diagram of $\tilde{\mu}$ as a function of $\eta$, we determine the coefficients for the three cases (1) $N = Kn_0 + 1$, (2) $N = Kn_0$ and (3) $N = Kn_0 - 1$, and introduce the subscript $(i)$ with $i = 1, 2, 3$ for the corresponding coefficient. We evaluate the integrals in Eqs. (5.37) for these three cases and express them as a function of the dimensionless parameter

$$y(i) = k^2\sigma(i)^2 = \sqrt{E_r/|V(i)|},$$  \hspace{1cm} (5.63)$$

where $E_r = \hbar^2/2m$ is the recoil energy. In term of $y(i)$, they read

$$E_{0(i)} = \frac{E_r}{2y(i)},$$  \hspace{1cm} (5.64)$$

$$J_{0(i)}^\pm = \frac{1}{2} \left[ 1 - \text{sign}(\Delta_a) \exp \left( -y(i) \right) \right],$$  \hspace{1cm} (5.65)$$

$$E_{1(i)} = -\frac{|V(i)|}{4} \exp \left( -\frac{\pi^2}{4y(i)} \right) \left( 2y(i) + \pi^2 \right),$$  \hspace{1cm} (5.66)$$

$$J_{1(i)}^\pm = \frac{\text{sign}(\Delta_a)}{2} \exp \left( -\frac{\pi^2}{4y(i)} - y(i) \right),$$  \hspace{1cm} (5.67)$$

$$U_{(i)} = \frac{4E_r a_s}{\sqrt{2\pi}\Delta yz} y(i),$$  \hspace{1cm} (5.68)$$

where $a_s$ is the scattering length, $\Delta yz$ is the atomic wave packet transverse width and the sign $\pm$ depends on the sign of $\Delta_a$. In the limit $J_{0(i)}^\pm \gg |J_{1(i)}^\pm|$ the potential amplitude according to (5.54) is given by

$$V(i) = \frac{\eta^2 h U_0}{k^2 + \left( \Delta_c - U_0 J_{0(i)}^\pm N \right)^2}.$$  \hspace{1cm} (5.69)$$

As $J_{0(i)}^\pm$ depends on $V(i)$ which, on the other hand, depends itself on $J_{0(i)}^\pm$, the above equations must be solved self-consistently. This is a consequence
of the atom-density dependence on the coupling parameters. In particular, for $\Delta_a > 0$ (atoms at the nodes), $J_{y(i)} \to 0$ in the strong pumping limit, $\eta \to \infty$, and the results become independent of the number of atoms. On the other hand, if $\Delta_a < 0$ (atoms at the antinodes) the parameter $J_{y(i)} \to 1$ for sufficiently large pumping, and the non-linearity is strongest.

Within this treatment we determine the nearest-neighbor tunneling parameter, which is given by

$$\tilde{t}(i) = \frac{E_r}{4\eta} y_{y(i)}^3 e^{-e_{y(i)}^2} \left(2y_{y(i)} + \pi^2 - 2e^{-y_{y(i)}}\right),$$

(5.70)

where $U = \frac{2\hbar^2 a_s k}{\sqrt{2\pi m} \Delta y z}$. For $\eta \to \infty$ the potential $|V_{y(i)}| \to \infty$ and consequently $y_{y(i)} \to 0$, and hence $\tilde{t} \to 0$.

### 5.2.5 Perturbative derivation of the zone boundaries

The starting Hamiltonian is of the form

$$H = -t(N) B + \frac{U(N)}{2} \sum_{i=1}^{K} n_i(n_i - 1) - \mu N,$$

(5.71)

where $t(N)$ is given by eq. (5.47). This Hamiltonian differs from the standard Bose-Hubbard Hamiltonian, as the coefficients depend on the operator $N$. We now apply the method of Ref. [107, 106] to Eq. (5.71), which allows to determine the stability region of the Mott-insulator states. The method consists in a perturbative expansion in the parameter $\tilde{t}$, which is assumed to be small within the parameter regime of interest. In this limit, for large onsite interaction strength $U$ (hard core limit), in the optical lattice the configuration which is energetically favorable has the smallest number of atoms per site. For a lattice of $K$ sites and $N = Kn_0 + j$ atoms, with $j < K$, there will be either $n_0$ or $n_0 + 1$ atoms per site. Clearly, when $N = Kn_0$ atoms ($j = 0$), there exists only one possible ground-state, while for $N > Kn_0$ several ground state configurations exist, and one has to apply degenerate perturbation theory.

The ground-state of Hamiltonian (5.71) is found after imposing periodic boundary conditions, and diagonalizing operator $B$ in the momentum

---

1In the opposite limit of small pumping we also have $\tilde{t} \to 0$, which, however, is within the regime where the Gaussian and the tight-binding approximations are not valid.
representation. At $t = 0$ the ground-state for $N = Kn_0$ is given by

$$|\Psi_0(n_0)\rangle = |n_0, n_0, ..., n_0\rangle,$$  \hspace{1cm} (5.72)

corresponding to $n_0$ atoms per site, while for $N = Kn_0 + j$, with $j > 0$, they are defined by the relation

$$|\Psi_j(n_0)\rangle = \hat{A}^{\dagger}_{k_j} |\Psi_{j-1}(n_0)\rangle,$$  \hspace{1cm} (5.73)

where

$$\hat{A}^{\dagger}_{k_j} = \frac{1}{\sqrt{K}} \sum_{n=1}^K e^{ink_j a} \hat{b}^{\dagger}_n \sqrt{n_n + 1}$$  \hspace{1cm} (5.74)

creates one particle in a site starting from the lowest energy states. There is an analogous state for one hole. Here, $a = \pi/k$ is the distance between neighboring sites, and the wave vector $k_j = 2\pi j/Ka$, with $j = -\frac{K}{2}, -\frac{K}{2} + 1, ..., \frac{K}{2} - 1$. Here we have assumed that $K$ is even, and it is understood that the operation of the creation operators $\hat{A}^{\dagger}_{k_j}$ is taken in such order that the lowest energy states ”fill” up first. Explicitly we have, for the $n_0$th Mott state and the SF states with $Kn_0 \pm 1$ atoms,

$$|\Psi_M(n_0)\rangle = |\Psi_0(n_0)\rangle,$$

$$|\Psi_+(n_0)\rangle = \frac{1}{\sqrt{K}} \frac{1}{\sqrt{n_n + 1}} \sum_{n=1}^K \hat{b}^{\dagger}_n |\Psi_M(n_0)\rangle,$$  \hspace{1cm} (5.75)

$$|\Psi_-(n_0)\rangle = \frac{1}{\sqrt{K}} \frac{1}{\sqrt{n_n + 1}} \sum_{n=1}^K \hat{b}_n |\Psi_M(n_0)\rangle.$$

The ground state energy is calculated applying perturbation theory in third-order in $\tilde{t}$ to this unperturbed basis. Due to symmetry, only zeroth and second-order in the perturbation of $t(\hat{N})\hat{B}$ contribute to the Mott-insulator ground-state energies. For $N = Kn_0$ one finds

$$E_M(n_0) = \frac{U(2)}{2} Kn_0(n_0 - 1) - \mu(2)Kn_0 - \frac{t^2(2)}{U(2)} 2Kn_0(n_0 + 1)$$  \hspace{1cm} (5.76)
while the SF energies for the added particle/hole energies are

\[
E_+(n_0) = \frac{U_{(1)}}{2} [K n_0(n_0 - 1) + 2 n_0 - \mu_{(1)}(K n_0 + 1)] \\
- t_{(1)} 2(n_0 + 1) - \frac{t_{(1)}^2}{U_{(1)}} [2K n_0(n_0 + 1) - n_0^2] \\
+ \frac{t_{(1)}^3}{U_{(1)}} n_0(n_0 + 1)(n_0 + 2),
\]

\[
E_-(n_0) = -\mu_{(3)}(K n_0 - 1) + \frac{U_{(3)}}{2} [K n_0(n_0 + 1) - n_0 + 1] \\
- t_{(3)} 2n_0 - \frac{t_{(3)}^2}{U_{(3)}} [2K n_0(n_0 + 1) - (n_0 + 1)^2] \\
- \frac{t_{(3)}^3}{U_{(3)}} n_0(n_0 + 1)(n_0 - 1).
\]

Here we have used the subscript \((i)\) corresponding to the three different cases, \(N = K n_0\) and \(N = K n_0 \pm 1\). The limit of stability of the Mott-insulator state is found when the states \(\ket{\Psi_M(n_0)}\) and \(\ket{\Psi_\pm(n_0)}\) are degenerated. The conditions \(E_M(n_0) - E_+(n_0) = 0\) and \(E_M(n_0) - E_-(n_0) = 0\) determine the boundaries \(\mu_{\pm}(n_0)\) of the Mott states in the phase diagram \(\tilde{\mu} - \tilde{t}\).

The third order result reads

\[
\tilde{\mu}_+(n_0) = n_0 + \frac{U_{(12)}}{2} K n_0(n_0 - 1) - t_{(1)} 2(n_0 + 1) \\
+ \frac{t_{(1)}^2}{U_{(1)}} n_0^2 - \left(\frac{t_{(1)}^2}{U_{(1)}} - \frac{t_{(2)}^2}{U_{(1)}} \frac{U_{(2)}}{U_{(1)}}\right) 2K n_0(n_0 + 1) \\
+ \frac{t_{(1)}^3}{U_{(1)}} n_0(n_0 + 1)(n_0 + 2),
\]

\[
\tilde{\mu}_-(n_0) = (n_0 - 1) - \frac{U_{(32)}}{2} K n_0(n_0 - 1) + t_{(3)} 2n_0 \\
- \frac{t_{(3)}^2}{U_{(3)}} (n_0 + 1)^2 - \left(\frac{t_{(3)}^2}{U_{(3)}} - \frac{t_{(2)}^2}{U_{(3)}} \frac{U_{(2)}}{U_{(3)}}\right) 2K n_0(n_0 + 1) \\
+ \frac{t_{(3)}^3}{U_{(3)}} n_0(n_0 + 1)(n_0 - 1).
\]

Here, \(U_{(i2)} = 1 - U_{(i)} / U_{(1)}\), \(\tilde{\mu}_+(n_0) = \mu_+(n_0) / U_{(1)}\) and \(\tilde{\mu}_-(n_0) = \mu_-(n_0) / U_{(3)}\).
5.2.6 Numerical results

In this section we study the regions of the Mott-insulator state as a function of the chemical potential and of the inverse pump amplitude $\eta^{-1}$. The boundaries are determined by numerical evaluation of Eqs. (5.37) using the modified Gaussian functions. The atomic parameters we choose correspond to $^{87}$Rb atoms with scattering length $a_s = 5.77$ nm, and atomic transition wavelength $\lambda = 830$ nm. The optical potential has $K$ lattice size and the transverse width of the atomic wave packet is $\Delta_y = \Delta_z = \sqrt{\Delta_y \Delta_z} = 30$ nm. We evaluate the "phase diagrams" for $K = 50 - 10000$ at fixed number of atoms $N$, scaling $N$ so to keep the atomic density constant. The results for the Mott zones agree over the whole range of values, so in the figures we report the ones obtained for $K = 50$ for different values of the detunings.

Figure 5.3 displays the first four Mott zones for (a) $\Delta_a < 0$ and $\Delta_c = \kappa$ and (b) $\Delta_a > 0$ and $\Delta_c = 0$, as a function of the dimensionless parameter $\kappa/\eta$. Interestingly, the extension of the Mott zones seems to decrease roughly as $n_0^{-1}$ in both cases. We first analyse the case displayed in Fig. 5.3(a). For $\Delta_a < 0$ the atoms are trapped at the maxima of the intracavity field. Hence, the coupling with the cavity mode is maximum when the confinement is very tight. Here, for large values of the pump intensity (i.e., for small values of $\kappa/\eta$) the Mott zones at different values of $n_0$ show some overlap. This overlap is a cavity QED effect, in fact Mott states with larger number of atoms per site are favored as they increase the coupling strength to the cavity mode, and thus the depth of the potential. The overlap is only at the border of the boundaries, as atom-atom collisions compete with this effect. In Fig. 5.3(b) the detuning $\Delta_a > 0$, and the atoms are hence trapped at the nodes (the zeroes) of the intracavity field. Hence, the coupling with the cavity mode is minimum when $\eta \to \infty$. Indeed, here we observe that for large values of $\eta$ (small values of $\kappa/\eta$), the Mott zones almost do not overlap. However, for smaller values of $\eta$ they exhibit an "exotic" behavior: overlap, disappear and reappear.

Further insight is gained in Fig. 5.4, where we study the depth of the cavity potential as a function of the pump parameters.

The curves displayed in Fig. 5.4(a) correspond to the parameters of the phase diagram in Fig. 5.3(a). Here, one observes that the potential amplitude increases monotonically as $V \sim \eta^2$ in the parameter regime where
Figure 5.3: Phase diagram, showing the Mott zones in the scaled chemical potential-cavity pump plane $\tilde{\mu}$-$\eta$. The parameters are (a) $U_0 = -5\kappa$ ($\Delta_a < 0$, atoms at the antinodes), $\Delta_c = 2\kappa$ and (b) $U_0 = 5\kappa$ ($\Delta_a > 0$, atoms at the nodes), $\Delta_c = 0$. The overlap and reappearance of the Mott zones originate from the non-linearity of the system. The dotted lines correspond to the boundaries of the covered zones.

the non-linearity is weak. Correspondingly, the width $\sigma_i$ of the Wannier functions, giving atomic localization at the minima of the potential, decreases smoothly as $\sigma_i \propto |V_i|^{-1/4} \sim 1/\sqrt{\eta}$, see Eq. (5.63). For larger pump strengths, when the non-linearity becomes important, the behaviour is slightly changed. The curves in Fig. 5.4(b) correspond to the parameters of the phase diagram in Fig. 5.3(b). Here, one finds that the potential depth increases rapidly where the corresponding Mott zones exhibit a minimum in the value of $\tilde{\mu}$. Correspondingly, the width $\sigma_i \propto |V_i|^{-1/4}$ diminishes rapidly. This behaviour changes at the value of $\eta$ where the potential gradient increases abruptly. In this regime $\sigma_i$ varies very slowly. This can be
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Figure 5.4: The potential amplitude $|V_{(i)}|$, in units of $E_r$ and in log-scale, as a function of the inverse pumping $\kappa/\eta$, where the curves in (a) and (b) have been evaluated in the parameter regimes of Figs 5.3(a) and 5.3(b), respectively. When the non-linearity is strong the potential amplitudes differ from the linear situation where $|V| \sim \eta^2$. The average number of cavity photons is found by multiplying the rescaled potential depths in the plots by the factor $f_n = E_r/|\hbar U_0|$, which here is $f_n \approx 0.006$.

understood as a competition between the cavity field, which tends to localize the atoms at the minima, and the atomic quantum fluctuations: When the potential is sufficiently high to trap the atoms within a small fraction of the wavelength, the cavity field is pumped more effectively.

We now consider the situation in which the detunings $\Delta_a$ and $\Delta_c$ have the same sign. In this case the parameter $\zeta(N)$ in Eq. (5.53) vanishes when the condition $J_{0(i)}^{\pm} = \Delta_c/U_0N$ is fulfilled, whereby $0 < J_{0(i)}^{+} < 1/2$ and $1/2 < J_{0(i)}^{-} < 1$, see Eq. (5.65). This resonance condition gives rise to bistability, leading to an abrupt change of the potential depth. As a consequence, the Mott state may become unstable. The upper plot of Fig. 5.5 displays the potential amplitudes $V_{(i)}/E_r$ for one atom per site as function of $\eta/\kappa$
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Figure 5.5: The bistability behaviour of the potential amplitudes $V_{(i)}$ as a function of $\kappa/\eta$ (upper plot) and corresponding phase diagram $\tilde{\mu} - \eta^{-1}$ (lower plot) for $\Delta_c = -45\kappa, U_0 = -\kappa$. At $n_0 = 1$ the Mott region suddenly ends for $\eta \sim \kappa$, where the corresponding potential $V_{(i)}$ jumps to a lower value. Here, the system most likely is in a state where higher Bloch bands are populated, due to non-adiabatic effects and the small potential depth of this solution.

for $U_0 = -\kappa$ and $\Delta_c = -45\kappa$, exhibiting the typical functional behavior of bistability. The lower plot displays the corresponding phase diagram. For the case of one atom per site, the Mott ground-state will suddenly disappear for $\eta \sim \kappa$ when the pumping is adiabatically lowered. Clearly the first "jump" occurs in the potential $V_{(i)}$ (corresponding to the lowest atom density), and comparing the two plots one finds that this takes place exactly when the first Mott zone suddenly ends. The system most likely jumps into a state where higher Bloch bands are populated. In this case the single-band and Gaussian approximations break down.

The overlapping of the Mott zones and the bistability, which we observe in the phase diagram, are novel features when compared with the typical scenario of cold atomic gases trapped by an external potential. Let us first discuss on the existence and uniqueness of the ground-state. When the Mott-insulator state is stable, given the number of atoms $N$, the ground state is fully determined once the atomic density $\rho = N/K$ is fixed. Outside of the Mott zones we expect superfluidity in the parameter regimes in which there cannot be optical bistability (detunings with opposite signs). In the situation of multiple solutions of the Eqs. (5.64)-(5.68), the system will most likely be found in the one solution which minimizes the energy.

A more complete picture of the phase diagram can be obtained by con-
5.2. Mott-Insulator states of ultracold atoms in optical ...
Figure 5.7: Phase diagram on the $\tilde{\mu} - \eta^{-1}$ plane, reporting the first four Mott zones. The Mott states with higher energy are plotted on top of the ones with lower energy. Typically, for large pumping the Mott zones with a large number of atoms $n_0$ per site have the highest energy. For moderate pumping this is not necessarily true as seen by comparing for example the third and fourth Mott zones at around $\kappa/\eta \approx 0.05$. The relevant parameters are reported in the inset.

the $\tilde{\mu} - \eta^{-1}$ plane, whereby the Mott states with higher energy are plotted on top of the ones with lower energy. We observe that for large pumping strengths the Mott states with a higher number of atoms $n_0$ have in general a greater energy, while for lower or moderate pumping strengths this is not necessary true. For example, the end of the Mott zone with $n_0 = 4$ has smaller energy than the corresponding one for the $n_0 = 3$. This is a pure CQED effect.

**Validity of the approximations**

We now discuss the regime of validity of the calculations, from which we extracted the phase diagrams presented in this section. The derivation of the system coupling parameters relies on the assumption $J_0 \gg |J_1^\pm|$. The maximum value of the ratio $|J_1^\pm|/J_0 \approx 0.056$ occurs at $|V| \approx E_r/2$, hence the nearest-neighbor coupling is at least 17 times smaller than the on site coupling. The expansion to first order in $J_1B$ of Eq. (5.38) is motivated for any number of atoms since the perturbative parameter $\lambda \equiv J_1B/J_0\tilde{N} \sim J_1/J_0$ is strictly smaller than unity.
The values of the chemical potential, as in Eq. (5.78), are derived from a third-order perturbation expansion in the parameter \( \tilde{t} = t/U \) and it is expected to break down for large \( \tilde{t} \). We verified that in general \( \tilde{t} < 0.25 \). Moreover, we compared the phase diagrams with the ones obtained by truncating at the second order in \( \tilde{t} \), and could verify that they do not differ substantially one from the others. We remark that the perturbation calculations are carried out assuming periodic boundary conditions, while the system here studied has a fixed number of sites, \( K = 50 \). We checked the validity of the assumption by comparing the results obtained for different lattice sites, up to 10000, keeping the density fixed.

![Figure 5.8](image)

Figure 5.8: Check of the validity of the involved approximations. The upper figure shows the difference \( \Delta - \Delta_{TBA} \), in units of \( E_R \), as a function of \( y^{-1} \), where \( \Delta \) is the width of the first energy band and \( \Delta_{TBA} = 2t_W \), with \( t_W \) the coupling element obtained from the corresponding Wannier functions in the tight-binding approximation. The lower figure displays \( t_W - t_G \) as a function of \( y^{-1} \), where \( t_G \) is the coupling element given by the Gaussian approximation. The quantities are numerically derived from Hamiltonian (5.10), where, in scaled units, there is only a single parameter of interest, namely the dimensionless potential amplitude or equivalently \( y \).

As it concerns the tight-binding approximation (i.e., only including nearest neighbor couplings), the single-band approximation (i.e., expanding the field operators \( \Psi(\hat{x}) \) and \( \Psi(\hat{x}') \) using only the lowest band Wannier functions), these are both related to the regime of validity of the Gaussian approximation. Within this approximation one finds \( |J_1/J_n| = \exp \left[ (n^2 - 1)\frac{\sigma^2}{y} \right] \gg \)

\[ \]
1, also indicating validity of the tight-binding approximation in this regime. Figure 5.8(a) displays the difference $\Delta - \Delta_{TBA}$ between the width $\Delta$ of the first Bloch band, obtained from diagonalization of the single-particle Hamiltonian in Eq. (5.10), and the width $\Delta_{TBA}$ evaluated with the tight-binding approximation, as a function of $y^{-1}$. Figure 5.8(b) displays the difference between the coupling parameters obtained by using the Wannier functions and the modified Gaussian functions as a function of $y^{-1}$. We note that for values $y^{-1} < 1$ the validity of both the tight binding and Gaussian approximation visibly breaks down. This has also been verified by recalculting some of the above phase-diagram using the Wannier functions.

5.3 Discussion

We have shown that ultracold bosonic atoms inside a resonator may form stable insulator-like states, and thus enter the Mott phase, which is sustained by and sustains the cavity potential. The low temperature properties of the system are determined by the competition between the quantum electrodynamical effects and the quantum fluctuations of the atomic matter waves. This competition gives rise to a non-trivial dependence of the regions of stability and of the collective atomic states on the system parameters. Since the cavity potential depends on the state of the atoms, the behavior of the ultracold atomic gas in the cavity hence differs significantly from the one which is encountered in open space. We have derived the BH Hamiltonian for the cavity confined system, and have shown that the coefficients of this Hamiltonian depend explicitly on the number of atoms. We have determined regions of parameters where the atomic insulator states are stable, predicting the existence of overlapping stability regions for competing Mott states. Bistable behavior is encountered in the vicinity of the shifted cavity resonance, controlled by the pump parameters.

Our theory allows us to determine the state of the atoms when their number is fixed, while for fluctuating, non-fixed atom number, in general, the system will choose the state of minimum energy. This will also take place when an external inhomogeneous potential, such as a harmonic trap potential, is additionally applied to the atoms. In such a case we envision the possibility of hysteresis effects in the harmonic potential, when the frequency of this potential is slowly increased and, subsequently, slowly decreased.
However, the question, how the presence of an inhomogeneous potential will modify the insulator-like states, requires further careful studies, since the state of the system depends in a highly non-trivial way on global parameters, which in turn determine the local density of the atoms and the intracavity field. The condition that atoms may locally affect the potential, hence giving rise to phonon-like features ([109] and references therein), may be reached in multi-mode resonators, allowing for localized polaritonic excitations [110, 111]. First studies in this direction have been presented in [112]. Further novel features are expected when fermions are considered instead of bosons.
Mott-insulator states in a quantum potential

Self-organization in systems of atoms and light has been observed in numerous experiments, some of which are reported in Refs. [113, 114, 115, 116, 117, 118, 119, 120, 53, 63]. Several experimental realizations show the formation of spatially-ordered atomic structures, which organize in the potential they form [113, 114, 115, 53, 63]. The basic mechanism behind the observed dynamics can be summarized by considering that the refractive index of the atomic medium, which is related to the atomic spatial density, is itself determined by the light fields via the mechanical effects of atom-photon interactions. Hence, the effective dynamics the atomic center of mass undergoes is determined by potentials and/or forces, which in return depend on the atom position and velocity distributions [121].

In this context, one remarkable example is the formation of regular patterns of atoms in the standing wave of a high-finesse optical cavity, arising when the atoms are transversally driven by lasers. Experimental signatures are the phase-locking between the field at the cavity output and the driving laser phase, according to two possible values with difference equal to \( \pi \). This occurs when the laser frequency is smaller than the cavity-mode frequency and its intensity exceeds a threshold value [53]. The phenomenon, first predicted by numerical simulations according to a semiclassical model for atoms and light [50], can be understood in terms of the atoms being trapped in the potential which originates from the light coherently scattered from the laser into the cavity mode. The largest intracavity amplitude is supported by the atomic configurations in which all atoms scatter in phase into the resonator, corresponding to the patterns where the interatomic distance is a multiple
of the wavelength of the cavity field. Since the possible configurations which fulfill this condition in a standing-wave cavity are two, one shifted with respect to the other by half a wavelength, the difference between the possible phases of the emitted field is exactly $\pi$. A further theoretical study discussed the phenomenon in terms of second-order phase transition and determined the pump threshold within a semiclassical, mean-field model [51].

Additional novel phenomena arise in this system when the quantum mechanical properties of light and matter are relevant. Theoretical works studied the dynamics of entanglement between atoms and fields during self-organization in a similar setup [122, 123, 124]. In Ref. [94] the pump threshold for self-organization at $T = 0$ was determined when the atoms are assumed to be forming a Bose-Einstein condensate. Most recently, the onset of selforganization has been experimentally observed in a Bose-Einstein condensate coupled to an optical resonator [63]. In such situation, an open question regards the nature of the quantum state of the system when the pump intensity is increased well above the self-organization threshold value. In this regime, in fact, the height of the potential increases, and one would expect localization of the atoms at the potential minima when the atom number is increased and hence the field in the cavity is larger. On the other hand, interparticle interactions due to s-wave collisions compete with such dynamics, favoring situations in which the number of atoms per site is small. This framework is reminiscent of the paradigmatic Mottinsulator / superfluid quantum phase transition [90], and in particular its realization with ultracold atoms in optical lattices [97]. In the case here considered, however, the dependence of the potential on the atomic distribution (and in particular, the expectation that its depth increases with the atomic density) makes it a priori unclear whether incompressible states can exist at large laser intensities.

In this chapter we study the quantum ground state of this self-organized system, in the setup sketched in Fig. 6.1. In particular, we determine under which conditions incompressible states exist at large pump intensities. This study finds particular motivation from experimental progress, which achieved the coupling of ultracold atoms with the optical mode of high-finesse cavities [63, 76, 77, 125, 126, 78, 127]. Indeed, we will argue that incompressible self-organized states could be observed in the setups of existing experiments [63, 128].
This chapter is organized as follows. The equations at the basis of the physical model are introduced in section 6.1, and the relevant approximations leading to the derivation of the effective atomic dynamics in the light potential are extensively discussed. In section 6.2 we assume that the atoms are tightly bound at the minima of the cavity potential inside the cavity, and derive an effective Bose-Hubbard model, whose coefficients are analytically determined within a modified Gaussian ansatz. The parameter regimes, where incompressible states of the self-organized atomic gas are found, are derived in section 6.3 within the strong coupling expansion method [106, 107]. Finally, a brief discussion of the results is presented in section 6.4.

### 6.1 The model

Identical bosonic atoms, with mass $m$, are confined inside an optical resonator, which is assumed to be a high-finesse cavity sustaining well resolved modes. The atoms are prepared at ultralow temperature $T$ and interact with each other by means of $s$-wave scattering. Furthermore, the atoms couple to light via a dipolar transition between the electronic ground and excited state $|g\rangle$ and $|e\rangle$ at the optical frequency $\omega_0$. In particular, the atomic dipole
is simultaneously driven by a laser and by the field of one cavity mode, both linearly polarized and whose wave vectors are perpendicular to one another, according to the geometry of the setup sketched in Fig. 6.1. We assume the atoms to be strongly confined in the plane perpendicular to the cavity axis, here chosen to be the x-axis, so that the motion is essentially along x. In absence of the resonator, the atomic dynamics for the atoms in states $|g\rangle$ and $|e\rangle$ are governed by the Hamiltonian $\mathcal{H}_0 + \mathcal{H}_{eg}$, where

$$\mathcal{H}_0 = \sum_{j=g,e} \int dx \Psi_j^\dagger(x) \left( \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{g_j}{2} \Psi_j^\dagger(x) \Psi_j(x) \right) \Psi_j(x),$$

with $g_j$ the strength of the state-dependent collisional interaction, and where $\mathcal{H}_{eg}$ describes s-wave scattering between atoms in different atomic states. The Hamiltonian in Eq. (6.1) is written in second quantization, where operators $\Psi_i(x)$ and $\Psi_i^\dagger(x)$ annihilate and create an atom at the position $x$ and in the electronic state $i = g, e$. The atomic field operators obey the bosonic commutation relations $[\Psi_i(x), \Psi_j^\dagger(x')] = \delta_{ij} \delta(x-x')$ and $[\Psi_i(x), \Psi_j(x')] = 0$.

The cavity is assumed to be a high-finesse resonator sustaining well-resolved modes, of which the mode at frequency $\omega_c$ is (quasi) resonant with the atomic transition. We denote by $a$ and $a^\dagger$ the annihilation and creation operators of a cavity photon at frequency $\omega_c$. The coherent coupling between atoms and light is described by a Hamiltonian in the Rotating-Wave approximation, which reads

$$\mathcal{H}_1 = -\hbar \Delta_a \int dx \Psi_e^\dagger(x) \Psi_e(x) - \hbar \Delta_c a^\dagger a$$

$$+ \left( \hbar \int dx \left( g_0 \cos(kx) a + \Omega(x) \right) \Psi_e^\dagger(x) \Psi_g(x) + \text{H.c.} \right),$$

and which is here reported in the reference frame rotating at the laser frequency $\omega_p$. Here, $\Omega(x)$ denotes the strength of the coupling to the laser field (Rabi frequency), $g_0$ is the cavity-mode vacuum Rabi frequency, $\cos(kx)$ gives the spatial dependence of the cavity-mode function with wave vector $k$, while $\Delta_a = \omega_p - \omega_0$ and $\Delta_c = \omega_p - \omega_c$ denote the detuning of the laser frequency from the atom and from the cavity-mode frequencies, respectively.
The coherent dynamics of coupled atoms and electromagnetic field are then governed by the full Hamiltonian

\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1. \]

This far we just considered Hamiltonian dynamics. We now introduce the sources of noise and dissipation, which in the present model are spontaneous radiative decay of the the electronic excited state \( |e \rangle \) at the lifetime \( \gamma \) and cavity losses at rate \( 2\kappa \) due to the finite transmittivity of the mirrors. By following the same procedure developed in 5.2.1, noise is here described within the Heisenberg-Langevin formalism. The Heisenberg-Langevin equations for the atomic and field operators read

\[
\dot{\Psi}_g(x) = -\frac{i}{\hbar} [\Psi_g(x), \mathcal{H}_0] - i \left( g_0 \cos (kx) a^\dagger + \Omega(x) \right) \Psi_e(x) - \sqrt{\gamma} f^\dagger_{\text{in}}(t) \Psi_e(x), \tag{6.3}
\]

\[
\dot{\Psi}_e(x) = -\frac{i}{\hbar} [\Psi_e(x), \mathcal{H}_0] + \left( i\Delta_a - \frac{\gamma}{2} \right) \Psi_e(x), \tag{6.4}
\]

\[
\dot{\Psi}_f(x) = \sqrt{\gamma} \Psi_g(x) (g_0 \cos (kx) a + \Omega(x)) - g_0 \int dx \cos (kx) \Psi_g^\dagger(x) \Psi_e(x) + \sqrt{2\kappa a_{\text{in}}(t)}. \tag{6.5}
\]

Here, the noise operators \( f^\dagger_{\text{in}}(t) \) and \( a_{\text{in}}(t) \) are the Langevin forces, with vanishing mean value and \( \langle f^\dagger_{\text{in}}(t) f_{\text{in}}(t') \rangle = \langle a_{\text{in}}^\dagger(t) a_{\text{in}}(t') \rangle = 0 \), while \( \langle f_{\text{in}}(t) f_{\text{in}}^\dagger(t') \rangle = \langle a_{\text{in}}^\dagger(t) a_{\text{in}}(t') \rangle = \delta(t - t') \), see for instance Ref. [42].

### 6.1.1 Effective dynamics

We now assume a time-scale separation, such that the electronic variables relax to a local steady state on a much shorter time scale than the one characterizing the dynamics of external and cavity degrees of freedom. This regime for the cavity degrees of freedom requires that the parameters satisfy \( |\Delta_a + i\gamma/2| \gg |\Omega|, g_0 \sqrt{N}, |\Delta_c|, \kappa \). Moreover, a change in the external degrees of freedom can be neglected over the typical time scale of the internal degrees of freedom provided that \( |\Delta_a + i\gamma/2| \gg \kappa_B T/\hbar \), with \( \kappa_B \) Boltzmann’s constant. In addition, we assume \( |\Delta_a| \gg |\Omega(x)|, g_0 \sqrt{N} \gg \gamma/2 \), so that we can identify a time scale in which coherent evolution is taking
place while dissipation due to spontaneous decay can be discarded. In these limits Eq. (6.4) can be set to zero and at leading order gives

\[ \Psi_e(x) \sim \Psi_g(x) \left[ a g_0 \cos(kx) + \Omega(x) \right] / \Delta_a, \]  

(6.6)

such that Eq. (6.5) takes the form

\[ \dot{a} = -\kappa a + i \left[ \Delta_c - U_0 \mathcal{Y} \right] a - i S_0 \mathcal{Z} + \sqrt{2} \kappa a_{in}, \]  

(6.7)

where \( U_0 \), defined in Eq. (5.11), is the maximal depth of the single-photon potential and \( S_0 \), defined in Eq. (5.12), is the maximal amplitude of scattering a laser photon into the cavity mode by a single atom. In writing Eq. (6.7) we have assumed, moreover, that \( \Omega(x) = \Omega f(x) \), with \( |f(x)| \leq 1 \).

The spatial distribution of atoms and fields is now contained in the operators \( \mathcal{Y} \) and \( \mathcal{Z} \), which read

\[ \mathcal{Y} = \int dx \cos^2(kx) \Psi_g^\dagger(x) \Psi_g(x), \]  

(6.8)

\[ \mathcal{Z} = \int dx f(x) \cos(kx) \Psi_g^\dagger(x) \Psi_g(x), \]  

(6.9)

and act on the Hilbert space of the atoms. The operators \( \mathcal{Y} \) and \( \mathcal{Z} \) are Hermitian and commute, \([\mathcal{Y}, \mathcal{Z}] = 0\), as they both depend solely on the atomic density. They are the quantum analogous of the semiclassical “bunching parameter” \( B = \sum_j \cos^2(kx_j)/N \) and of the “spatial order parameter” \( \Theta = \sum_j \cos(kx_j)/N \), respectively, which are defined for an ensemble of \( N \) atoms at the positions \( x_1, \ldots, x_N \), see for example [51]. These parameters characterize a semiclassical mean-field description of self-organization of the atoms in the cavity field, such that for \( \Theta \to \pm 1 \) the atoms are in a self-organized state at the even or odd antinodes of the cavity standing wave, while \( B \) provides their degree of localization about these points.

The cavity field can be eliminated from the matter-wave equations assuming a second characteristic time scale determined by the rate \( |\Delta_c + i\kappa| \), in which the cavity field approaches a local steady state. This requires that the effective coupling strength between matter waves and cavity field is smaller

\[ \text{1} \text{A uniform distribution of atoms along the cavity axis corresponds instead to } B \sim 1/2, \text{ and correspondingly } \Theta \approx 0. \text{ On the other hand, one could also have the situation in which } \Theta \approx 0 \text{ while } B \ll 1, \text{ corresponding to the atoms localized at both even and odd antinodes of the cavity standing wave potential.} \]
than this rate, namely $|\Delta_c + i\kappa| \gg |S_0|\sqrt{N}|U_0|N$, and that the uncoupled matter wave dynamics is slower, $|\Delta_c + i\kappa| \gg \kappa_B T/\hbar$. In this limit, one finds $a \sim a^{(0)}$, with

$$a^{(0)} = \frac{S_0 Z + i\sqrt{2}\kappa a(t)}{(\Delta_c - U_0 Y) + i\kappa},$$

(6.10)

where we have used that the operators in the numerator commute with the operators in the denominator. Using in Eq. (6.3) the solutions for $\Psi_e(x)$ and $a$, Eq. (6.6) and Eq. (6.10), at lowest order in perturbation theory we find

$$\dot{\Psi}_g(x) = \frac{i}{\hbar} [\Psi_g(x), H_0] - iU_0 \cos^2(kx) a^{(0)\dagger} \Psi_g a^{(0)}$$

$$-iS_0 f(x) \cos(kx) a^{(0)\dagger} \Psi_g - iS_0 f(x) \cos(kx) \Psi_g a^{(0)}$$

$$-i\frac{\Omega^2}{\Delta_a} f(x)^2 \Psi_g.$$ (6.11)

Here $a^{(0)}$ is now a function of the atomic density and hence does not commute with the field operator $\Psi_g(x)$.

### 6.1.2 Mechanical effects of the cavity field

Equation (6.10) for the cavity-field operator $a^{(0)}$ gives the field state at leading order in a perturbative expansion, in which it is assumed that the cavity field follows adiabatically the matter-wave dynamics. Furthermore, it is seen that it is a function of the atomic density, which enters both in the numerator and in the denominator of the expression. In this work we will be interested in determining the atomic quantum ground state, which emerges from a coupled dynamics between cavity field and atoms, giving rise to the mechanical potential sustaining such state.

In order to gain further insight into the effect of the cavity potential on the atoms, we consider the semiclassical limit, which can be found from Eq. (6.11). In this limit, we identify the terms which explicitly depend on the atomic position with mechanical forces. The corresponding potential takes the form

$$V(x) = V_1 \cos^2(kx) + V_2 \cos(kx) + \frac{\hbar^2 f(x)^2}{\Delta_a},$$

(6.12)

with $V_1 = \hbar U_0 \langle a^{(0)\dagger} a^{(0)} \rangle$ and $V_2 = 2\hbar S_0 \text{Re}\{\langle a^{(0)} \rangle\}$. The third term on the
6.1. The model

right-hand-side of Eq. (6.12) is the a.c.-Stark shift due to the laser field. In the following we assume that the external laser field drives the atoms uniformly and the Rabi frequency $\Omega$ does not depend on the position $x$ (i.e. $f(x) = 1$). The Fourier transform of the potential is hence composed by a term at wavevector $2k$ whose amplitude is proportional to the number of photons, and which is due to the dispersive coupling between photons and atoms. This term corresponds to a potential with periodicity $\lambda/2$, analogous to an optical lattice in free space. Differing from an optical lattice in free space, the number of photons depends on the atomic density via the "bunching parameter". The second component is at wave vector $k$ and thus oscillates with periodicity $\lambda$. It originates from coherent Raman scattering of laser photons into the cavity field and its amplitude is hence proportional to the cavity electric field amplitude, but it also depends on the positions of the scatterers through the "spatial order parameter" $\Theta$. The two Fourier components give rise to an effective potential with spatial periodicity $\lambda$ as displayed in Fig. 6.1. We remind that potential (6.12) is found in a semiclassical limit. In this limit, the expression we find agrees with the ones derived in [51, 54] within a semiclassical model.

The model of a semiclassical potential for the atoms does not take into account dissipative effects, which may be due for instance to cavity decay (while dissipation due to back-action of the resonator over the atoms is here $a$ priori neglected as we assume the adiabatic limit). Indeed, in the dynamics of the atoms we find non-hermitian terms, which are characterized by the position-dependent coefficient

$$\gamma'(x) = \text{Im}\{S_0 a^{(0)}\} \cos(kx),$$

scaling with the linewidth $\kappa$ of the resonator. Correspondingly, input noise gives rise to fluctuations in the height of the potential, which are described by the operator $a_{in}(t)$ in Eq. (6.10). The effect of cavity quantum noise will be here discarded, assuming that the detuning $|\Delta_c| \gg \kappa$ (more precisely, $|\Delta_c| \gg \kappa, |U_0 Y|$, which is consistent with the assumption of adiabatic elimination of the cavity degrees of freedom). In this regime, the atoms move in a dispersive potential, which is produced by the dynamical Stark coupling with the cavity mode photons and by the Raman-scattered field of the laser.
6.1.3 Tight-binding limit

The motion and steady state of the semiclassical model discussed in the previous section has been studied in several theoretical works. Numerical simulations demonstrated that the system self-organizes, such that the atoms localize at the antinodes of the cavity field, where their coupling is maximum, according to an array with periodicity \( \lambda \) \([50]\). This behavior appears when the laser intensity exceeds a critical value \([50, 51]\), and has been confirmed experimentally \([53]\). Localization of the atoms may take place around two possible set of minima, one centered at the positions \( x_{2j}^{(0)} = j \lambda \) (where \( \cos(kx^{(0)}_{2j}) = +1 \)), with \( j \) integer, and the other at the positions \( x_{2j+1}^{(0)} = (2j + 1)\lambda/2 \) (where \( \cos(kx^{(0)}_{2j+1}) = -1 \)), while the cavity field is a coherent state with amplitude proportional to the pump \([46, 47]\). In the limit in which the atoms are well localized at the minima one can expand potential \((6.12)\) till second order in the fluctuations of the particles position. For a particle localized at \( x_j^{(0)} \) the potential takes the form

\[
V(x) \approx V^{(0)} + V^{(2)} x^2
\]  

(6.13)

where \( x = x_j - x_j^{(0)} \) and \( V^{(0)} = V(x_j^{(0)}) \), while

\[
V^{(2)} = -\frac{\hbar k^2 S_0^2 \langle Z \rangle}{(\Delta_c - U_0 \langle Y \rangle)^2 + \kappa^2} \left( U_0 \langle Z \rangle + (-1)^j (\Delta_c - U_0 \langle Y \rangle) \right)
\]  

(6.14)

where the potential due to the other particles enters in a mean-field approach through the mean value of operators \( Z \) and \( Y \). Note that when the atoms are self-organized at the set of positions \( \{x_{2j}^{(0)}\} \) (respectively, \( \{x_{2j+1}^{(0)}\} \)), then the sign of \( \langle Z \rangle \) is positive (respectively, negative).

Consistently with the approximations made so far, the dynamics can be characterized by the dispersive dipolar potential provided that

\[ |U_0 \langle Y \rangle|, |U_0 \langle Z \rangle| \ll |\Delta_c|, \]

which allows for the adiabatic elimination of the cavity field from the matter-wave equations. This implies that, for the regime we consider, the sign of this term of the potential is solely determined by the sign of the detuning between cavity and pump. One hence finds that the position \( x_j^{(0)} \) are minima provided that \( \Delta_c < 0 \). This behavior can be understood in terms of positive feedback of the system, which is warranted whenever the sign of \( \langle Z \rangle \) is opposite to the one of the harmonic potential \( V^{(2)} \), and hence when \( \Delta_c < 0 \). This latter condition leads to the property
that the conservative force, due to the potential, is attractive \[54\]. It is a sufficient condition, provided that the detuning \(\Delta_a\) between atom and laser is negative, \(\Delta_a < 0\) (and consequently \(U_0\) is negative), as it is visible from the numerator of Eq. \((6.14)\) (note that for the situations here considered, \(\langle Z\rangle > \langle Y\rangle\), see also Ref. \([94]\)). Indeed, in this regime the minima of the potential, formed by light scattering of the atoms, are also minima of the standing-wave potential of the cavity field, so that the attractive forces of both contributions add up to confine the atoms. On the contrary, when \(\Delta_a > 0\) the opposite situation is realized: the minima of the potential due to light scattering are now maxima of the cavity standing-wave potential: the term proportional to \(U_0\) in the numerator of Eq. \((6.14)\) has opposite sign than the detuning \(\Delta_c\), and the overall effect is to make the effective potential, resulting from the two contributions, shallower. An extensive discussion on the semiclassical forces as a function of the detunings can be found in Refs. \([54, 51]\).

Finally, the amplitude of the semiclassical detuning depends nonlinearly on the atomic density through quantity \(\Delta_c - U_0\langle Y\rangle\) in the denominator. Bistability effects due to this nonlinearity have been discussed for the situation, in which the cavity is pumped by a laser \([85, 129, 130, 125, 127, 128]\). In this article we will focus on the regime where \(|\Delta_c - U_0\langle Y\rangle| \gg \kappa\), when the potential is conservative and dissipative effects can be neglected. This parameter regime is far away from the bistability region. Correspondingly, this term will be treated as a small correction of the semiclassical potential in the framework of perturbation theory.

### 6.2 Effective dynamics in the cavity potential

#### 6.2.1 Derivation of the effective Hamiltonian

We now assume that the atoms are tightly confined in one set of minima of potential \((6.12)\), say, at the position \(x_{2j} = j\lambda\). This assumption is clearly based on the semiclassical dynamics, as a potential cannot be simply singled out from Eq. \((6.11)\). Our aim is to identify the quantum ground state by considering the full quantum dynamics. For this purpose, starting from the assumption of tight confinement, we perform a Wannier decomposition of
the atomic field operator,

$$\Psi_g(x) = \sum_j w_j(x)b_j,$$

(6.15)

where operator $b_j$ annihilates a particle at the site centered in $x_j^{(0)}$, and $w_j(x)$ is the Wannier function, taken to be real valued and with center in $x_j^{(0)}$. This decomposition is based on the assumption that the atoms are in the lowest band of the semiclassical potential, which is justified at ultralow temperatures. Within the decomposition of Eq. (6.15), Hamiltonian (6.1) takes the form $H_0 \simeq H_0^{BH}$, with

$$H_0^{BH} = E_0 N + E_1 B + \frac{1}{2} U L \sum_i n_i (n_i - 1) - \mu_0 N,$$

(6.16)

where $N = \sum_j b_j^{\dagger}b_j$ is the atom number operator, and $B = \sum_j \left( b_j^{\dagger}b_{j+1} + \text{H.c.} \right)$ is the hopping operator, while the coefficients read

$$E_\ell = \int dx w_\ell(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) w_{i+\ell}(x)$$

(6.17)

$$U = g_{1D} \int dx w_1(x)^4,$$

(6.18)

and $g_{1D} = g_g$ is the scattering strength in one dimension. In writing Eq. (6.16) we made the nearest-neighbor approximation, and introduced the chemical potential $\mu$, assuming a grand-canonical ensemble. We remark that the Bose-Hubbard expansion of Hamiltonian (6.16) relies on localization of the atoms at the minima of the potential inside the cavity.

We now use Eq. (6.15) in Eq. (6.11), and determine the equations of motion for the operators $b_j$ by multiplying with $w_1(x)$ and integrating over the position. We find

$$\dot{b}_l = -i \hbar \left[ b_l, H_0^{BH} \right] - i U_0 A^{(0)} \left[ J_0 b_l + J_1 B_l \right] A^{(0)}$$

$$- i S_0 A^{(0)} \left[ Z_0 b_l + Z_1 B_l \right] - i S_0 \left[ Z_0 b_l + Z_1 B_l \right] A^{(0)}$$

$$- \frac{\Omega^2}{\Delta_s} b_l,$$

(6.19)

which is written in the regime in which $|\Delta_s| \gg |U_0\mathcal{Y}|$. Here, $B_l = b_{l+1} +$
6.2. Effective dynamics in the cavity potential

\[ b_{l-1} = [b_l, B], \] and \( A^{(0)} \simeq a^{(0)} \), such that

\[
A^{(0)} = \frac{S_0(Z_0 N + Z_1 B)}{\Delta_c + i \kappa} \left( 1 + \frac{U_0}{\Delta_c + i \kappa} (J_0 N + J_1 B) \right),
\]

which considers only nearest-neighbor coupling and where we used

\[
Z \simeq Z_0 N + Z_1 B,
\]

\[
Y \simeq J_0 N + J_1 B,
\]

with

\[
Z_\ell = \int dx w_i(x) \cos (kx) w_{i+\ell}(x),
\]

\[
J_\ell = \int dx w_i(x) \cos^2 (kx) w_{i+\ell}(x),
\]

and \( \ell = 0, 1 \). At first order in the expansion in the small parameter \( U_0 / |\Delta_c| \), Eq. (6.19) can be exactly cast in the form

\[
\dot{b}_l = -\frac{i}{\hbar} \left[ b_l, H_{\text{BH}}^{\text{CQED}} \right],
\]

with

\[
H_{\text{CQED}}^{\text{BH}} = \frac{\hbar S_0^2}{\Delta_c} \left[ (Z_0 N + Z_1 B)^2 + \frac{U_0}{\Delta_c} Z_0 \right.
\]

\[
\times \left. (Z_0 J_0 N^3 + Z_0 J_1 N^2 B N + J_0 Z_1 (N^2 B + B N^2) + o(Z_1^2)) \right],
\]

where we consider \( \kappa \ll |\Delta_c| \) and we truncated the second term in an expansion at first order in \( |Z_1 U_0 N/\Delta_c| \) and \( |J_1 U_0 N/\Delta_c| \). Note that in expression (6.26) the operators are symmetrically ordered, so to obtain Eq. (6.19).

The total dynamics of the system is now rendered by the Hamiltonian

\[
H_{\text{eff}} = H_0^{\text{BH}} + H_{\text{CQED}}^{\text{BH}},
\]

where the first term of the right-hand-side, defined in Eq. (6.16), describes the hopping between sites, due to the quantum fluctuations, and the on-site interaction emerging from s-wave scattering, while the second term contains the contributions due to the mechanical effects of the laser and cavity potential, which determine and sustain the atomic pattern. We note that
6. Mott-insulator states in a quantum potential

Hamiltonian (6.26) is similar to the Bose-Hubbard Hamiltonian, however, its terms are nonlinear in the number and hopping operators. Moreover, it differs also from the usual Bose-Hubbard model due to the appearance of a term proportional to the squared of the hopping operator, $B^2$.

The nonlinearity in Eq. (6.26) is due to the coupling with the cavity field, which scales with the number of atoms and which determines the confining potential: the larger is the atomic number the stronger is the coupling. This effect is exquisitely due to cavity quantum electrodynamics, and originates from the constructive interference with which the atoms scatter the laser photons into the cavity mode. We also note that, when considering higher order terms in $U_0/\Delta_c$, an exact effective Hamiltonian -which is a function solely of operators $N$ and $B$ fulfills Eq. (6.19)- cannot be found unless one resorts to a suitable thermodynamic limit [86]. In fact, these terms emerge from the nonlinear coupling between photons and atoms inside the resonator, in which the atoms act as a refractive index. The effect is hence highly nonlocal, and it is significant when the strong coupling regime is warranted. An immediate consequence is that Wannier functions will depend on the particle number. Most remarkable is the fact that the Hamiltonian is quadratic in the hopping operator, even when the nonlinearity deriving from the atomic refractive index, $U_0\gamma$, is negligible. This property is due to the collective scattering of the atoms into the resonator. Nevertheless, it does not affect substantially the property of the ground state at large potential depth (small tunneling rates) as we will show.

6.2.2 Mapping to a Bose-Hubbard model

For the purpose of studying the quantum phases of the many-body system, we define a thermodynamic limit. This is here so defined, that the density of the atoms is kept fixed as the particle number $N$ and the cavity-mode volume go to infinity. Denoting by $2K$ the total number of sites of the lattice, such that in the considered configuration there are $K$ lattice cells, the cavity coupling strength is inversely proportional to the squared root of the cavity mode volume, and thus scales as $g_0 \propto 1/\sqrt{K}$. The other parameters in Eq. (6.27) scale as $U_0 = u_0/K$ and $S_0 = s_0/\sqrt{K}$, where $u_0$ and $s_0$ are constants, while the number operator is now $N = Kn_0$, with $n_0$ the density operator, giving the number of atoms per site. This scaling is such that, as $K \to \infty$, the parameters in Hamiltonian (6.27) depend only on the atomic
density. We also note that in this thermodynamic limit a Bose-Hubbard form can be also derived when the terms scaling with $U_0$ are taken into account, see for instance chapter 5 for a discussion. In this thermodynamic limit we rewrite Hamiltonian (6.27) in the Bose-Hubbard-like form,

$$H = -t_1[n_0]B + t_2[n_0]B^2 + \frac{U[n_0]}{2} \sum n_i(n_i - 1) - \mu[n_0]N, \quad (6.28)$$

where

$$t_1[n_0] = -E_1 - n_0 \hbar \frac{s_0^2}{\Delta_c} \left[ 2Z_0Z_1 + n_0 \frac{u_0}{\Delta_c} (Z_0^2J_1 + 2J_0Z_0Z_1) \right], \quad (6.29)$$

$$t_2[n_0] = \frac{\hbar s_0^2}{\Delta_c} Z_1^2 \left[ 1 + O(u_0/\Delta_c) \right], \quad (6.30)$$

$$\mu[n_0] = \mu_0 - E_0 - n_0 \hbar \frac{s_0^2}{\Delta_c} Z_0^2 \left( 1 + n_0 \frac{u_0}{\Delta_c} J_0 \right), \quad (6.31)$$

and where $U$, $Z_j$, and $J_j$ are functions of $n_0$ through the Wannier functions. Insight into the dependence of the coefficients on the density can be gained using a (modified) Gaussian ansatz in place of the Wannier functions, as reported in next section 6.2.3.

Differing from the ordinary Bose-Hubbard model [90], in the case of self-organized atomic patterns the coefficients entering the effective BH Hamiltonian do depend on the atomic density. This property implies that the atomic density is not solely determined by the chemical potential [85, 86]. We also observe that, in addition to the nearest-neighbor hopping arising from the kinetic energy, there is a hopping term due to the cavity potential which contains a term proportional to $B^2$. This latter contribution describes long-range correlations among the atoms mediated by the scattered photons. Close inspection shows that, in the tight-binding regime, its coefficient is of higher order with respect to the coefficient multiplying $B$, see section 6.2.3. Within the considered thermodynamic limit, this term gives rise to a small correction to the spectrum of the lowest excitations and corresponding eigenstates of the Mott-insulator states, which must, however, be taken into account when determining the ground state of the system for larger values of the coefficient $Z_1$, scaling the tunneling coefficient $t_2$ and some terms of $t_1$. 

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6.2.3 Coefficients in the Gaussian Approximation

The solution of the Bose-Hubbard model requires the evaluation of the coefficients, which are integrals containing Wannier functions. The Wannier functions are solutions of the Schrödinger equation for a single particle in presence of the potential in Eq. (6.12), which itself depends on the spatial distribution of the atoms inside the cavity. The problem is hence nonlinear. We solve it by combining an analytical and a numerical approach. In first instance, we replace the Wannier functions by modified Gaussian functions, \( w_i(x) \rightarrow \tilde{w}_i(x) \), with

\[
\tilde{w}_i(x) = \left(1 + \frac{3\delta^2}{4}\right) g_i(x) - \frac{\delta}{2} \left(1 + \frac{3}{2}\delta^2\right) (g_{i+1}(x) + g_{i-1}(x))
\]

(6.32)

and

\[
g_i(x) = \frac{1}{\sqrt{\pi}\sigma^2} e^{-\frac{(x-x_i)^2}{2\sigma^2}}
\]

(6.33)

is a normalized Gaussian function of width \( \sigma \). The form of the modified Gaussian function in Eq. (6.32) warrants orthonormality up to second order in \( \delta \), where \( \delta = \int dx g_i(x) g_{i+1}(x) = e^{-\pi^2/(k^2\sigma^2)} \) and where the overlap between second neighbors is of the order \( O(\delta^4) \). We remark that the coefficient in (6.32) at second order in \( \delta \) warrants the correct normalization.

The width \( \sigma \) of the Gaussian function \( g_i(x) \) is found by minimizing the single-particle energy \( E \), for the Schrödinger equation in presence of potential (6.12). For later convenience we introduce the dimensionless parameter

\[
y = k^2\sigma^2
\]

(6.34)

which is \( y \ll 1 \), consistently with our assumptions. In terms of the parameter \( y \) this consists in finding the minimum of the equation

\[
E(y) = \frac{E_R}{2y} + F(y) - \frac{G(y)}{2} y
\]

(6.35)

where \( E_R = \hbar^2 k^2/2m \) is the recoil energy and we introduced the functions

\[
F(y) = \tilde{V}_1 + \tilde{V}_2
\]

(6.36)

\[
G(y) = \tilde{V}_1 + \tilde{V}_2/2
\]

(6.37)
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where $\tilde{V}_1$ and $\tilde{V}_2$ are

$$
\tilde{V}_1 = \frac{\hbar U_0 S_0^2 \mathcal{Z}(y)^2}{\kappa^2 + (\Delta_c - U_0 \mathcal{Y}(y))^2} \quad (6.38)
$$

$$
\tilde{V}_2 = \frac{2\hbar S_0^2 \mathcal{Z}(y)(\Delta_c - U_0 \mathcal{Y}(y))}{\kappa^2 + (\Delta_c - U_0 \mathcal{Y}(y))^2} \quad (6.39)
$$

Note that the cos-functions in Eq. (6.12) have been expanded up to second order in the displacement from the minima. Minimization with respect to $y$ leads to the nonlinear equation

$$
y^2 = \frac{E_R}{2F'(y) - yG'(y) - G(y)} \quad (6.40)
$$

with $F'(y) = dF(y)/dy$ and $G'(y) = dG(y)/dy$.

Using the value which minimizes the single-particle energy, $y := y_{\text{min}}$, we evaluate the coefficients we need in order to study the problem. They are reported below as a function of $y$,

$$
E_0 = \frac{E_R}{2y} \left( 1 + \delta^2 \frac{4\pi^2}{y} \right) \quad (6.41)
$$

$$
J_0 = \frac{1 + e^{-y}}{2} \quad (6.42)
$$

$$
Z_0 = (1 + 4\delta^2)e^{-y/4} \quad (6.43)
$$

$$
E_1 = -\frac{E_R\delta\pi^2}{y^2} \left( 1 + \frac{9}{4}\delta^2 \right) \quad (6.44)
$$

$$
J_1 = 0 \quad (6.45)
$$

$$
Z_1 = -2\delta e^{-y/4} \left( 1 + \frac{9}{4}\delta^2 \right) \quad (6.46)
$$

$$
U = g_1 D \kappa \frac{1 + 3\delta^2 - 4\delta^2}{\sqrt{2\pi y}} \quad (6.47)
$$

where $E_R = \hbar^2 k^2/2m$ is the recoil energy and we discarded terms of higher order than $\delta^2$. Note that the coefficients $Z_j$ are here reported for the pattern localized at the positions $x_{2j}^{(0)} = j\lambda$, nevertheless the coefficients are independent of the pattern considered, as one can easily verify since terms appear always in pairs ($Z_0^2$, $Z_0 Z_1$, $Z_1^2$).
6.3 Incompressible phase of self-organized atomic patterns

We now study whether the self-organized atomic pattern exhibits an incompressible ground state. Therefore, we focus onto the regime in which self-organization has set in, namely, when the laser amplitude exceeds the threshold value \[51, 94\] and the laser frequency is smaller than the cavity-mode frequency, \(\Delta_c < 0\). The atoms are assumed to be localized at the set of minima \(\{x_{2j} = j\lambda\}\), such that \(Z_0 > 0\).

In order to display the phase diagram for this system, we consider the chemical potential and the amplitude of the pump field \(s_0\), which indirectly determines the tunneling coefficients. In fact, for \(s_0 \to \infty\) the intracavity field potential is deepest and tightly localizes the atoms at their minima, and the tunneling parameters \(t_1\) and \(t_2\), Eqs. (6.29) and (6.30), vanish correspondingly (as one can check by considering the dependence of the coefficients \(Z_j\) and \(J_j\) on \(s_0\), see section 6.2.3).

We apply the strong coupling expansion developed in Ref. [107, 106] in order to determine the size of the incompressible states as a function of the pump amplitude and of the chemical potential. For this purpose we start by considering the limit \(s_0 \to \infty\), assuming the system to be in a Mott-insulator state with an integer occupation per site \(n_0\). We calculate the free energy of the Mott-insulator state \(E_M(n_0)\) and of the defect states \(E_{\pm}(n_0)\), which are obtained by adding or removing a particle to the Mott-insulator state. The energy of the defect state is found by means of degenerate perturbation theory, expanding in power of the small parameter \(t_1/U\) up to third order. In the parameter regime we consider, this expansion corresponds also to a first-order expansion in the parameter \(t_2\). The phase boundaries between the Mott-insulator and the compressible phase correspond to the situation where the energy difference between the defect state and the Mott-insulator state vanishes, namely, when

\[E_{\pm}(n_0) - E_M(n_0) = 0.\]  \hfill (6.48)

The values of the chemical potentials \(\mu_{\pm}(n_0)\) and \(\mu_{\pm}(n_0)\), at which the Mott-insulator phase with integer occupation \(n_0\) becomes unstable when adding
and removing a particle, respectively, fulfill the equations

\[
E_+(n_0) - E_M(n_0) = -\mu_{(n_0)}^+ + Un_0 - 2t_1(n_0 + 1) + \frac{t_1^2}{U}n_0^2
\]
\[
+ \frac{t_1^3}{U^2}n_0(n_0 + 1)(n_0 + 2)
\]
\[
+ t_22(2n_0 + 1)(n_0 + 2) = 0, \quad (6.49)
\]
\[
E_-(n_0) - E_M(n_0) = \mu_{(n_0)}^- - Un_0 - 2t_1n_0
\]
\[
+ \frac{t_1^2}{U}(n_0 + 1)^2 + \frac{t_1^3}{U^2}n_0(n_0 + 1)(n_0 - 1)
\]
\[
+ t_22(2n_0 + 1)(n_0 - 1) = 0. \quad (6.50)
\]

When \(\mu_{(n_0)}^+ > \mu_{(n_0)}^-\), then \(\mu_{(n_0)}^+\) and \(\mu_{(n_0)}^-\) determine the upper and lower boundaries of the parameter region where the system is in the Mott-insulator state. The phase diagrams reported afterwards are computed using the analytical formulae of the strong coupling expansion, Eqs. (6.49) and (6.50) in the thermodynamic limit, fixing the values of the parameters \(u_0\) and \(s_0\).

The coefficients are evaluated in section 6.2.3 by using a modified Gaussian ansatz in place of the Wannier functions.

Figure 6.2 displays the phase diagram for the considered system, showing three incompressible, Mott-insulator phase regions with \(n_0 = 1, 2, 3\), for \(\Delta_c = -50\kappa\) and \(u_0 = -0.1\kappa\). When plotted as a function of \(1/s_0\), the Mott-insulator regions become larger as a function of the laser amplitude as the number of atoms increases. This result can be understood with simple arguments, in fact the trapping potential is constituted of the light coherently scattered by the atoms: As the number of atoms increases, the cavity-field intensity, for a given pump amplitude, is larger, thus the potential becomes deeper and the configuration more stable. Another remarkable property is the appearance of gaps between the Mott-insulator lobes. In the limit of vanishing tunneling coefficients \(t_{1,2} \to 0\) (corresponding to \(s_0 \to \infty\)), this behavior implies that the degeneracy among states with different densities, found in the ordinary BH model, is here removed. This behaviour results from the dependence of the single-particle, on-site energy on the average density. In particular, while inside the lobes the density per site \(n_0\) takes integer values, in the gap between the lobes the density changes continuously in the interval \(r < n_0 < r + 1\) (with \(r = 1, 2, 3, \ldots\) integer number), as shown in Fig. 6.3. The region outside the Mott-insulator lobes is presumably
6. Mott-insulator states in a quantum potential

a peculiar superfluid state, which entails photonic excitations. A study of its properties close to the self-organization threshold has been presented in Refs. [94, 50]. The appearance of the gap is understood, when one considers the dependence of the coefficients on the density. In fact, at $s_0 \to \infty$ (corresponding to putting the tunneling elements to zero), the Mott-insulator region with $n_0 = 1$ is found for values of $\mu$ such that $0 < \mu_1 < U_1$, where $\mu_1 = \mu[n_0 = 1]$ and $U_1 = U[n_0 = 1]$ (see Eq. (6.18)). Similarly, the region at $n_0 = 2$ is found for $U_2 < \mu_2 < 2U_2$ (with $U_2 = U[n_0 = 2]$). The relation $U_1 < U_2$ ($U_j < U_{j+1}$) leads to the appearance of parameter regions where the system is compressible even at zero tunneling. This relation is a consequence of the fact that, for a fixed amplitude of the laser field, the intracavity field becomes larger as the number of atoms (scatterers) is increased.

Figure 6.4 displays different phase diagrams, obtained for various values and signs of the detuning $\Delta_a$, keeping $\Delta_c$ fixed. We first focus on the case in which $\Delta_a < 0$, when the potential due to the dynamical a.c.-Stark shift, induced by the coupling with the cavity mode, adds up to the potential due to light scattering, giving rise to a stronger attractive dipole force. In this case, we observe that for larger values of $u_0$ the gap between the chemical potentials of Mott-insulator states at different densities increases. Moreover, the larger is $n_0$, the larger is the area covered by Mott-insulator states at larger densities: incompressible states are found at smaller values of the laser amplitude. The opposite tendency is found when $\Delta_a > 0$, and hence when the potential due to the a.c.-Stark shift competes with the scattering potential. In this case, as $|u_0|$ is increased, the gap between the Mott-insulator lobes becomes smaller, while the area covered by Mott-insulator states with larger densities decreases. In particular, incompressible states are observed at larger values of the laser pump amplitude. This behavior can be understood from the dependence of the tunneling coefficient, Eq. (6.29), on the various terms: The term proportional to $u_0$ scales with the onsite density, and it hence becomes more important as $n_0$ is increased. For values of the detuning, such that the cavity potential adds up to the scattering potential ($\Delta_a < 0$), at a fixed laser intensity the confinement is larger for a larger density of atoms. Correspondingly, the parameter region where the system is compressible becomes larger. On the contrary, for $\Delta_a > 0$ the cavity potential tends to make the scattering potential shallower, the confinement tends to depend less strongly on the density and the gap between the Mott-
insulator lobes is smaller.

Figure 6.2: Phase diagram, showing the Mott-insulator states at different densities \( n_0 = 1, 2, 3 \) in the plane reporting the chemical potential \( \tilde{\mu} = \mu / U_1 \), Eq. (6.31), and the inverse of the laser amplitude, \( 1/s_0 \) (in units of cavity loss rate \( \kappa \)). The parameters are \( \Delta_c = -50\kappa \) and \( u_0 = -0.1\kappa \). The arrow indicates the threshold value of the laser amplitude, for which the system self-organizes [94]. The chemical potential is here reported in units of the on-site energy \( U_1 \), corresponding to the value of Eq. (6.18) for the density of one atom per site, with \( g_{1D}/(E_R\lambda) = 3.74 \cdot 10^{-4} \) and \( E_R \) the recoil energy, considering a gas of \(^{87}\text{Rb} \) atoms whose dipole-transition, at wavelength \( \lambda = 830 \text{ nm} \), is coupled to the cavity mode.

We remark that, while in this model atom-atom interaction is essentially \( s \)-wave scattering, it should be considered that, when the atomic occupation of each site exceeds unity, then dipole-dipole interaction, including superfluorescence, will be relevant. In our model we neglect collective effects in the spontaneous decay outside of the cavity. In particular, for the parameter regime we consider, incoherent processes are suppressed for the large atomic detunings we choose. On the other hand, one can identify parameter regimes where coherent coupling between the atoms at a site may be relevant, and which should be included in an effective onsite interaction term.

We finally estimate the parameter regime required for observing our predictions, considering the setup reported in Ref. [128]. Here, ultracold \(^{87}\text{Rb} \) atoms are loaded inside a resonator, where a mode couples quasi-resonantly with the transition at wave length \( \lambda = 780 \text{ nm} \). The parameters are \( g_0/\pi = 14.1 \text{ MHz} \), \( \kappa/2\pi = 1.3 \text{ MHz} \) and \( \gamma/2\pi = 3 \text{ MHz} \). Taking \( |\Delta_a|/2\pi = 60 \text{ GHz} \), \( \Omega/2\pi = 60 \text{ MHz} \), we find \( U_0/2\pi \sim 0.03 \text{ MHz} \) and \( S_0/2\pi = 0.1 \text{ MHz} \), while the effective rate of spontaneous emission is of the order of few KHz. For a number of atoms \( N \sim 10^4 \), the relation \( S_0\sqrt{N} \gg \kappa \).
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Figure 6.3: On-site density $n_0$ as a function of the chemical potential $\tilde{\mu}$ (in units of the on-site energy $U_1$) for $s_0 \to \infty$ (corresponding to $t_1, t_2 \to 0$). Same parameters as in Fig. 6.2.

Figure 6.4: Mott-insulator states at $n_0 = 1, 2$ in the plane $\tilde{\mu}/U_1 - \kappa/s_0$ for $\Delta_c = -50\kappa$ and (i) $u_0 = -2\kappa$ (red solid line), (ii) $u_0 = 0.1\kappa$ (green dashed line), and (iii) $u_0 = 10\kappa$ (blue dotted line). The other parameters are the same as in Fig. 6.2.
is fulfilled, warranting the existence of a time-scale in which the atoms may experience a conservative potential formed by their scattered photons. The relation $|\Delta_c| \gg |U_0|N, \kappa$ is satisfied taking $|\Delta_c|/2\pi = 100 \text{ MHz}$. For these parameters, the value $s_0/\kappa = 10$ at which incompressible phases are found in Figs. 6.2 and 6.4, corresponds to $S_0\sqrt{N} \sim 10\kappa$. This latter value corresponds to the one found for the experimental parameters in [128], showing that the regime, where quantum effects in self-organized atomic patterns are visible, can be accessed with existing experimental setups.

6.4 Discussion

The quantum ground state of a self-organized atomic pattern, confined by the potential of the field scattered into the cavity mode, can be incompressible provided that the laser intensity exceeds a certain critical value, which is found above the threshold value at which the system self-organizes. In addition, intervals of values of the chemical potential are identified, in which the state is compressible even when the tunneling vanishes. These appears as gaps between the Mott-insulator lobes in a phase diagram we derive, and their origin can be understood from the competition between confinement, which is steeper at large atomic density for a given laser intensity, and interparticle collisions, whose effective strength also depends on the density via the localization of the atomic wave function in the intra-cavity field potential. Our analysis is based on an effective Bose-Hubbard model, according to the assumption that the atoms are tightly bound at the minima of the intra-cavity field potential. Since the height of such potential depends on the atomic density, the coefficients of the model depend on the atomic density giving rise to the peculiarities encountered in the phase diagram. Comparison with typical parameters of experimental setups, dealing with ultracold atoms inside of optical cavities, shows that the prediction here made could be experimentally tested in existing setups. Detection of the quantum properties of the system may be performed by measuring the light using a probe field [63, 82, 81], in a direction of emission corresponding to a Bragg scattering angle. A spectral analysis of the probe intensity will provide information on the state of the system, which can be studied as a function of the laser pump intensity, and hence of the tunneling rate [131, 132]. Sweeping the phase diagram in the direction $\mu$ may be performed
in various ways. One possibility is to implement a shift of the atomic ground state by means of a magnetic field or by off-resonant coupling with a third electronic state. In this chapter we focused on the quantum ground state of the self-organized structure, arising by driving the atoms with a strong, transversal laser field. The mechanical potential results from the scattering potential, with periodicity equal to the wavelength, and from the potential due to the cavity field mode, with periodicity equal to the wavelength /2. The regime we considered is the one in which the scattering potential is the strongest. In this regime, it is expected that the light at the cavity output is coherent, while the intensity is independent on the number of atoms when the strong-coupling regime is warranted [46, 47]. An interesting question is what are the properties of the emitted light when the cavity-field mode potential dominates. In this regime, in the first part of this thesis we showed that the light at the cavity output can be squeezed, and in general anti-bunched [133, 134]. An intriguing question is whether and how these properties are modified, when the atomic quantum statistics is relevant to the dynamics of atom-photon interactions.
Conclusions

The work presented in this thesis discusses on many body effects in cavity quantum electrodynamics. In the first part, we have used collective properties of atomic systems in order to create quantum light sources. In the second part we focused on the quantum state of the atoms, confined in the cavity potential. In the individual chapters we provided frameworks and outlooks for the work there presented.

In this chapter we provide some general outlook to the work of this thesis. One of the interesting perspectives that "ultracold atoms inside cavities" may open is the possibility to nondestructively monitor the atomic quantum state by measuring the light that leaks out of the cavity. In this context, there are several proposals for determining the quantum state of an atomic gas by measuring the photons scattered by the atoms. For instance, in [81, 82] it is discussed how a cavity QED setup can give access to the quantum state of ultracold atoms interacting with the cavity field. In [131, 132], the authors showed how by using the Bragg spectroscopy one could measure the phase diagram of Mott-insulator/superfluid phase transition. An interesting question is whether this possibility could be used in order to implement feedback mechanisms on the atomic gas, so to realize, for instance, novel quantum states of the many-body systems.

Another perspective that these combinations of Cavity QED with many-body systems open, is the possibility to explore phases, appearing for instance by generating a disordered potential inside of the cavity. Indeed, throughout this work we always assumed that the potential the atoms experience is periodic. On the other hand, aperiodicity can emerge due to an incommensurable ratio between the period of the cavity potential and the one of the laser phase, driving the atoms, when for instance the laser is not perpendicular to the cavity axis [47]. In this context it is interesting to
consider which kind of ground state the atomic system may possess.
A

Non-linear Optics

A.1 Second harmonic generation

The simplest case we introduce is a crystal with a non zero second order
susceptibility (only the media that have no spatial symmetry inversion have
non zero $\chi^{(2)}$) pumped by an electric field

$$E(t) = \frac{1}{2} E_0 e^{-i\omega t} + c.c. \quad \text{(A.1)}$$

The nonlinear polarization created inside the crystal reads

$$P^2(t) = \frac{1}{2} \chi^{(2)} E_0 E_0^* + \frac{1}{4} \left( \chi^{(2)} E_0^2 e^{-2i\omega t} + c.c. \right) \quad \text{(A.2)}$$

This expression shows that the second order polarization depends on the
first term with zero frequency, while the second term doubles the frequency.
The first term of the last equation gives rise to the effect known as optical
rectification, in which a static electric field is generated inside the crystal.
The second term generates radiation at the frequency of the second harmonic
($2\omega$). The phase matching condition is fulfilled when the wave vector of the
oscillating second order polarization, that radiates at angular frequency $2\omega$,
is $k_{2\omega} = k_{\omega} + k_{\omega}$. Under this condition of phase matching (usually with
crystals being strongly birefringent), the radiation interfere constructively
and in phase, and almost all the incident power is converted in radiation
with double frequency. Thus, a $\chi^{(2)}$-medium generates radiation of double
frequency. Second harmonic generation can be visualized also as a quantum
mechanical process, as depicted in Fig.(A.1), where the photons interacting
with the $\chi^{(2)}$-medium became new photons with twice the energy.
A.1. Second harmonic generation

Figure A.1: a) Sketch of the nonlinear crystal with sum-frequency generation. b) Energy-level of the sum-frequency generation

A.1.1 Difference-Frequency Generation and Optical Parametric Amplification

When the incident field is bichromatic

\[ E(t) = \frac{1}{2} \left( E_1 e^{-i\omega_1 t} + E_2 e^{-i\omega_2 t} + \text{c.c.} \right) \quad (A.3) \]

the second order nonlinear polarization is written as

\[ P^{(2)}(t) = \chi^{(2)} \left[ \frac{1}{4} E_1^2 e^{-2i\omega_1 t} + \frac{1}{4} E_2^2 e^{-2i\omega_2 t} + \frac{1}{2} E_1 E_2 e^{-i(\omega_1 + \omega_2) t} + \frac{1}{2} E_1^* E_2 e^{-i(\omega_1 - \omega_2) t} + \text{c.c.} \right] + \frac{1}{2} \chi^{(2)} [E_1 E_2^* + E_2 E_1^*] \quad (A.4) \]

The generation of difference frequencies process is better understood by writing the last equation as

\[ P^{(2)}(t) = \frac{1}{2} \sum_n P^{(2)}(\omega_n) e^{-i\omega_n t} \quad (A.5) \]

and the complex amplitude we will be interested in is

\[ P^{(2)}(\omega_1 - \omega_2) = \chi^{(2)} E_1 E_2^* \quad (A.6) \]

Now, the frequency of the generated radiation is the frequency difference of the two input frequencies. Commonly the field with frequency \( \omega_1 \) is an intense pump field while \( \omega_2 \) is a weak signal one. This process amplifies the \( \omega_2 \) field by generating another field at frequency \( \omega_3 \) usually called idler. This process is known as optical parametric amplification (OPA). When \( \omega_2 = \omega_3 \) the system is called Degenerate Parametric Amplifier (DPA). When the crystal is placed in a cavity resonant with \( \omega_2 \), as depicted in Fig. A.2, we will obtain an optical parametric oscillator (OPO). The cavity may have also modes resonant at both frequencies \( \omega_2 \) and \( \omega_3 \). When \( \omega_2 = \omega_3 \) we obtain a
A. Non-linear Optics

Degenerate OPO. Both, the OPA and OPO will be discussed in more detail in Sec. 2.1.

\[ \omega_p = \omega_s + \omega_i \]

Figure A.2: Sketch of the optical parametric oscillator. The nonlinear crystal is inside a resonator and is pumped by a laser at frequency \( \omega_p \). The pump laser is coupled through the crystal with two modes at frequency \( \omega_s \) and \( \omega_i \).

A.2 Third harmonic generation and Kerr medium

The Kerr effect is a change of the refractive index of the material due to presence of the electric field of the light. In a Kerr medium the change in the refractive index is proportional to the square of the electric field. This effect is produced when light goes through a nonzero \( \chi^{(3)} \)-medium, and is responsible of effects such as self-focusing.

Let us consider the third-order component of the polarization, Eq (2.1), driven by a monochromatic input field at frequency \( \omega \) given in Eq (A.1). Following the procedure showed above, and taking into account that \( \cos^2 \omega t = \frac{1}{4} \cos 3\omega t + \frac{3}{4} \cos \omega t \), we rewrite the third-order polarization as

\[ P^{(3)}(t) = \frac{1}{4} \chi^{(3)} E_0^3 \cos 3\omega t + \frac{3}{4} \chi^{(3)} E_0^3 \cos \omega t. \]  

(A.7)

The first term is responsible of the generation of the third harmonic: the medium radiates at frequency \( 3\omega \). Here, the typical quantum process is the absorption of three photons at frequency \( \omega \) and emission of a photon at frequency \( 3\omega \). The second term gives rise to a change in the refractive index of the medium with the electric field intensity \( I \). In particular, the refractive index takes the form

\[ n = n_0 + n_2 I \]  

(A.8)

where \( n_0 = \left(1 + \chi^{(1)} \right)^{1/2} \) and \( n_2 = \left( \frac{3\chi^{(3)}}{8n_0} \right) \).
A.2. Third harmonic generation and Kerr medium

Figure A.3: a) Sketch of the third harmonic generation, where the non-linear crystal is pumped by a field at frequencies $\omega_1, \omega_2$, and $\omega_3$ and the emitted field is at frequency $\omega_4 = \omega_1 + \omega_2 + \omega_3$. b) Energy-level description of one of the possible mixing processes: An absorption of two photons and emission of two photons.
In a squeezed state, the quantum fluctuations in one variable are reduced below their value in a symmetric minimum uncertainty state. The Heisenberg uncertainty relation should not be violated, therefore fluctuations in the corresponding conjugate variable are increased. Consider two Hermitian operators $A$ and $B$ defined on a quantum system, with the correspondent commutation relation $[A, B] = iC$. Their Heisenberg uncertainty relation reads $\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|$, where $(\Delta \zeta)^2 = \langle \zeta^2 \rangle - \langle \zeta \rangle^2$, and $\langle \zeta \rangle$ is the mean value of the operator on the system, $\zeta = A, B, C$. A state is squeezed if

$$(\Delta A)^2 < \frac{1}{2} |\langle C \rangle|.$$  \hfill (B.1)

An ideal squeezed state satisfies, in addition to the above condition, the minimum-uncertainty relation

$$\Delta A \Delta B = \frac{1}{2} |\langle C \rangle|.$$  \hfill (B.2)

Let us now consider a harmonic oscillator, with annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ fulfilling the commutation relation $[a, a^\dagger] = 1$. We define the quadratures $X_1, X_2$, such that

$$X_1 = \frac{1}{2} \left( a + a^\dagger \right)$$
$$X_2 = \frac{1}{2i} \left( a - a^\dagger \right),$$  \hfill (B.3)

fulfilling $[X_1, X_2] = i/2$. 

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The uncertainty relation for the two amplitudes is

\[ \Delta X_1 \Delta X_2 \geq \frac{1}{4} \]  \hspace{1cm} \text{(B.4)}

The harmonic oscillator is in a squeezed state if \((\Delta X_i)^2 < \frac{1}{4}\).
Rotating reference frame

In this appendix we shortly describe the transformation of a time dependent Hamiltonian into the reference frame rotating at the laser frequency. The coherent dynamics of our model is described by the Hamiltonian $H' = H'_{at} + H'_{cav} + H'_{at-cav} + H'_L$, where the terms are defined as

\begin{align}
H'_{at} &= -\hbar \omega_0 \sum_{j=1,2} \sigma_j^\dagger \sigma_j \\
H'_{cav} &= -\hbar \omega_c a^\dagger a \\
H'_{at-cav} &= \hbar \sum_{j=1,2} g(x_j) \left( a^\dagger \sigma_j + \sigma_j^\dagger a \right)
\end{align}

which describe the interaction of the dipoles with the modes of the quantized field, where $\omega_0$ and $\omega_c$ are the frequencies of the dipole and the cavity. The term

\begin{equation}
H'_L = \hbar \Omega \sum_{j=1,2} \left( e^{-i\omega_L t} \sigma_j^\dagger + e^{i\omega_L t} \sigma_j \right),
\end{equation}

describe the interaction of the dipoles with the laser field. The Hamiltonian is time dependent, but this time dependence can be transformed by means of the unitary operator

\begin{equation}
U = \exp \left[ i\hbar \omega_L t \left( a^\dagger a + \sum_{j=1,2} \sigma_j^\dagger \sigma_j \right) \right]
\end{equation}
which makes a transformation to the reference frame rotating at the laser frequency $\omega_L$ to obtain the Hamiltonian (2.11) with

\[
H_{at} = -\hbar \Delta \sum_{j=1,2} \sigma_j^\dagger \sigma_j \tag{C.6}
\]

\[
H_{cav} = -\hbar \delta_c a^\dagger a \tag{C.7}
\]

\[
H_{at-cav} = \hbar \sum_{j=1,2} g(x_j) \left( a^\dagger \sigma_j + \sigma_j^\dagger a \right) \tag{C.8}
\]

\[
H_L = \hbar \Omega \sum_{j=1,2} \left( \sigma_j^\dagger + \sigma_j \right) , \tag{C.9}
\]

being $\Delta = \omega_L - \omega_0$ and $\delta_c = \omega_L - \omega_c$ the detunings of the laser from the dipole and from the cavity frequency respectively.
Derivation of the effective Hamiltonian

We consider $H_0 = H_{\text{cav}} + H_{\text{at}}$ with energy levels $E_{i\alpha}$ grouped in subspaces $\mathcal{E}_\alpha, \mathcal{E}_\beta$ well separated. The index $i$ denotes the different levels of the same manifold $|i, \alpha\rangle$, and $P_\alpha$ the projector over the manifold $\mathcal{E}_\alpha$ with

$$ H_0 |i, \alpha\rangle = E_{i,\alpha} |i, \alpha\rangle \rightarrow H_0 |gg, n\rangle = -\hbar \delta_n$$

$$P_\alpha = \sum_i |i, \alpha\rangle \langle i, \alpha| \rightarrow P_{gg} = \sum_n |gg, n\rangle \langle gg, n|$$

In order to assume that the manifolds are well separated, we have to require the energy difference between levels of the same manifolds to be

$$|\delta_c|$$

while the difference energy between different manifolds is $|\Delta|$. 

In each manifold the different levels, which corresponds to different number of photons are plotted. The energy difference between levels of the same manifold is $|\delta_c|$ while the difference energy between different manifolds is $|\Delta|$. 

Figure D.1: Manifolds $|gg\rangle, |+\rangle, |-\rangle$ and $|ee\rangle$. In each manifold the different levels, which corresponds to different number of photons are plotted. The energy difference between levels of the same manifold is $|\delta_c|$ while the difference energy between different manifolds is $|\Delta|$. 

In order to assume that the manifolds are well separated, we have to require the energy difference between levels of the same manifolds to be
smaller than energy difference between different manifolds, i.e.

\[ |E_{gg,n} - E_{gg,n+1}| \ll |E_{gg,n} - E_{+,n+1}| \]
\[ |\delta_c| \ll |\Delta - \delta_c| \]
\[ |\delta_c| \ll |\Delta| \] (D.3)

The different manifolds and its internal energy levels are sketched in Fig. (D.1). There are two degrees of freedom; the fast degrees of freedom that we characterize by Greek index (the atomic internal ones) and the slow degrees of freedom characterized by the Roman index (the modes of the cavity). The total Hamiltonian is given by the unperturbed Hamiltonian \( H_0 \) and the coupling \( V \) that will be treated as a small perturbation

\[ H = H_0 + V \] (D.4)

The matrix elements of the operator \( V = H_L + H_{cav-at} \) are between manifolds, thus \( V \) is not diagonal. The effective Hamiltonian is derived by applying a unitary transformation \( S \) to the total Hamiltonian

\[ H' = e^{iS}He^{-iS} \] with \( S^\dagger = S \) (D.5)

such that \( P_\alpha H'P_\beta = 0, \alpha \neq 0 \), (D.6)

where we require that

- \( H'^\dagger = H' \), i.e., it is hermitian

- \( H' \) has the same eigenvalues as \( H \) with the same degeneracy.

- \( H' \) does not have matrix elements between the unperturbed manifolds.

In the basis \( |i, \alpha\rangle \), \( H' \) can be written as

\[ H' = \sum_\alpha P_\alpha H_{\alpha eff} = P_{gg}H_{g eff}^{gg} + P_+H_{+ eff}^+ + P_-H_{- eff}^- + P_{ee}H_{e eff}^{ee} \] (D.7)

with + and −, the symmetric and antisymmetric Dicke states. In particular we are interested in finding the expression for the ground atomic state
D. Derivation of the effective Hamiltonian

manifold (i.e. $H_{e\text{ff}}^{gg} = H_{e\text{ff}}$). In the transformation we will assume

$$P_{gg}S P_{gg} = 0 \quad (D.8)$$

We can expand $S$

$$S = S_1 + S_2 + S_3 \ldots + S_n + \ldots \quad (D.9)$$

where $S$ has no matrix elements inside the manifold. We can expand Eq.(D.5)

$$H' = H + [iS, H] + \frac{1}{2!} [iS [iS, H]] + \ldots \quad (D.10)$$

and, by inserting Eq.(D.9)

$$H' = H_0 + H'_1 + H'_2 + \ldots + H'_p + \ldots \quad (D.11)$$

Each term $H'_p$ can be written in terms of $S_n$, $H_0$ and $V$. We will rewrite Eq.(D.10) by using the expansion Eq.(D.9), and use Eq.(D.4) up to fourth order.

Equating Eq. (D.10) and Eq. (D.11) one finds for the first order term reads

$$H'_1 = [iS_1, H_0] + V \quad (D.12)$$

By using that the matrix elements of $H'_1$ between different manifolds are zero, we obtain

$$\langle i, \alpha | H'_1 | j, \beta \rangle = \langle i, \alpha | iS_1 | j, \beta \rangle \left(E_{j\beta} - E_{i\alpha}\right) + \langle i, \alpha | V | j, \beta \rangle = 0 \quad (D.13)$$

deeply obtaining the relation

$$[iS_1, H_0] = -V \quad (D.14)$$

The second term is given by

$$H'_2 = [iS_2, H_0] + [iS_1, V] + \frac{1}{2} [iS_1, [iS_1, H_0]] \quad (D.15)$$
The third term is given by

\[ H'_3 = [iS_3, H_0] + [iS_2, V] + \frac{1}{2} [iS_1, [iS_1, V]] + \frac{1}{2} [iS_1, [iS_2, H_0]] + \frac{1}{2} [iS_1, [iS_1, H_0]] + \frac{1}{6} [iS_1, [iS_1, [iS_1, H_0]]] \]  \tag{D.16} \]

And finally the fourth term

\[ H'_4 = [iS_4, H_0] + [iS_3, V] + \frac{1}{2} [iS_1, [iS_2, V]] + \frac{1}{2} [iS_2, [iS_1, V]] + \frac{1}{6} [iS_1, [iS_3, H_0]] + \frac{1}{2} [iS_1, [iS_1, H_0]] + \frac{1}{2} [iS_2, [iS_1, H_0]] + \frac{1}{6} [iS_1, [iS_1, [iS_2, H_0]]] + \frac{1}{6} [iS_2, [iS_1, [iS_1, H_0]]] + \frac{1}{24} [iS_1, [iS_1, [iS_1, [iS_1, H_0]]]] \]  \tag{D.17} \]

From the equations (D.12) (D.15) (D.16) and (D.17) we can derive the relations

\[
\begin{align*}
[iS_1, H_0] &= -V & \text{(D.18)} \\
[iS_2, H_0] &= -\frac{1}{2} [iS_1, V] & \text{(D.19)} \\
[iS_3, H_0] &= -\frac{1}{2} [iS_2, V] - \frac{1}{12} [iS_1, [iS_1, V]] & \text{(D.20)} \\
[iS_4, H_0] &= -\frac{1}{2} [iS_3, V] - \frac{1}{12} [iS_1, [iS_2, V]] - \frac{1}{12} [iS_2, [iS_1, V]] & \text{(D.21)}
\end{align*}
\]

Inside the ground state manifold, we can calculate the coupling between
D. Derivation of the effective Hamiltonian

the states $|gg,n\rangle$ and $|gg\rangle$ as

$$
\langle gg,n | H_{\text{eff}} | gg,n \rangle = \langle gg,n | H_0 | gg,n \rangle 
+ \sum_{k \neq gg} \sum_i \frac{\langle gg,n | V | k,i \rangle \langle k,i | V | gg,n \rangle}{(E_{gg,n} - E_{k,i})} 
+ \sum_{k,\gamma,\nu \neq gg} \sum_{i,j,l} \frac{\langle gg,n | V | k,i \rangle \langle k,i | V | \gamma,j \rangle \langle \gamma,j | V | \nu,l \rangle \langle \nu,l | V | gg,n \rangle}{(E_{gg,n} - E_{k,i}) (E_{\nu,l} - E_{\gamma,j}) (E_{gg,n} - E_{\nu,l})}
$$

(D.22)

And the coupling between the states $|gg,n\rangle$ and $|gg,n + 1\rangle$ as

$$
\langle gg,n + 1 | H_{\text{eff}} | gg,n \rangle = \sum_{k \neq gg} \sum_i \frac{\langle gg,n + 1 | V | k,i \rangle \langle k,i | V | gg,n \rangle}{(E_{gg,n} - E_{k,i})}
$$

(D.23)

Finally the coupling between the states $|gg,n\rangle$ and $|gg,n + 2\rangle$ are written as

$$
\langle gg,n + 2 | H_{\text{eff}} | gg,n \rangle = \sum_{k,\gamma,\nu \neq gg} \sum_{i,j,l} \frac{\langle gg,n + 2 | V | k,i \rangle \langle k,i | V | \gamma,j \rangle \langle \gamma,j | V | \nu,l \rangle \langle \nu,l | V | gg,n \rangle}{(E_{gg,n} - E_{k,i}) (E_{\nu,l} - E_{\gamma,j}) (E_{gg,n} - E_{\nu,l})}
$$

(D.24)

By using the explicit form of $V$ given in Eq.(2.14) and in Eq.(2.15), and by using that the energies $E_{gg,n} = -\hbar \delta_c n$, $E_{\pm,n} = -\hbar \Delta - \hbar \delta_c n$ and $E_{ee,n} = -2\hbar \Delta - \hbar \delta_c n$, we can write the result of the transitions as

$$
\langle gg,n | H_{\text{eff}} | gg,n \rangle = \left( \frac{g_+^2 (x_1, x_2) + g_-^2 (x_1, x_2)}{\Delta} \right) n 
+ \left( \frac{[g_+^2 (x_1, x_2) - g_-^2 (x_1, x_2)]^2}{\Delta^3} \right) (n + 2) (n + 1)
$$

(D.25)

$$
\langle gg,n + 1 | H_{\text{eff}} | gg,n \rangle = \left( \frac{\sqrt{2} \Omega}{\Delta} g_+ (x_1, x_2) \right) \sqrt{n} + 1
$$

(D.26)

$$
\langle gg,n + 2 | H_{\text{eff}} | gg,n \rangle = \left( \frac{2 \Omega^2}{\Delta^3} [g_+^2 (x_1, x_2) - g_-^2 (x_1, x_2)] \right) \sqrt{n} + 2 \sqrt{n} + 1
$$

(D.27)
Finally the total effective Hamiltonian reads

\[
H_{\text{eff}} = H_{\text{cav}} + \left( \frac{g^2_+ (x_1, x_2) + g^2_- (x_1, x_2)}{\Delta} \right) n |n\rangle \langle n| \\
+ \left( \sqrt{\frac{2\Omega}{\Delta}} g_+ (x_1, x_2) \right) \sqrt{n+1} |n\rangle \langle n+1| + \text{h.c.} \\
+ \left( \frac{\left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right]^2}{\Delta^3} \right) (n+2) (n+1) |n+2\rangle \langle n+2| \\
+ \left( \frac{2\Omega^2}{\Delta^3} \left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right] \right) \sqrt{n+2} \sqrt{n+1} |n\rangle \langle n+2| + \text{h.c.} \\
= (\bar{\theta} - \delta_c) a^\dagger a + \bar{\beta} \left( a^\dagger + a \right) + \bar{\chi} a^\dagger a^\dagger a a + \bar{\alpha} \left( a^2 + a^\dagger a \right), \quad (D.28)
\]

where

\[
\bar{\theta} = \frac{g^2_2 (x_1, x_2) + g^2_- (x_1, x_2)}{\Delta} \quad (D.29) \\
\bar{\beta} = \frac{\sqrt{2\Omega}}{\Delta} g_+ (x_1, x_2) \quad (D.30) \\
\bar{\chi} = \frac{1}{\Delta^3} \left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right]^2 \quad (D.31) \\
\bar{\alpha} = \frac{2\Omega^2}{\Delta^3} \left[ g^2_+ (x_1, x_2) - g^2_- (x_1, x_2) \right] \quad (D.32)
\]
Equations for field operators

The equations for the field operators (Eq. 3.5) can be written in matrix form,

\[ \dot{A} = \mathcal{M}A + \mathcal{N} \]  \hspace{1cm} (E.1)

where

\[ A = \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \]  \hspace{1cm} (E.2)

\[ \mathcal{M} = \begin{pmatrix} -\kappa' & -i\alpha \\ i\alpha & -\kappa' \end{pmatrix} \]  \hspace{1cm} (E.3)

\[ \mathcal{N} = \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \]  \hspace{1cm} (E.4)

A formal solution is given by

\[ A(t) = e^{\mathcal{M}t}A(0) + e^{\mathcal{M}t}\int_0^t e^{-\mathcal{M}\tau}\mathcal{N}(\tau)\,d\tau \]  \hspace{1cm} (E.5)

The eigenvalues and eigenfunctions of \( \mathcal{M} \) (Eq. (E.3)) reads

\[ \lambda_1 = -\kappa' - \alpha \]  \hspace{1cm} (E.6)

\[ \lambda_2 = -\kappa' + \alpha \]  \hspace{1cm} (E.7)

\[ v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \]  \hspace{1cm} (E.8)
\[ v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix} \]  

(E.9)

The terms of Eq.(E.5) reads now

\[ e^{-\lambda v_1} = e^{-\lambda_1 v_1} \frac{1}{\sqrt{2}} \left( -i\eta + \eta^\dagger \right) + e^{-\lambda_2 v_2} \frac{1}{\sqrt{2}} \left( i\eta + \eta^\dagger \right) \]

\[ = e^{(\kappa' + \alpha) v_1} \frac{1}{\sqrt{2}} \left( -i\eta + \eta^\dagger \right) + e^{(\kappa' - \alpha) v_2} \frac{1}{\sqrt{2}} \left( i\eta + \eta^\dagger \right) \]

(E.10)

and

\[ e^{\lambda t} A(0) = e^{\lambda_1 t} v_1 \frac{1}{\sqrt{2}} \left( -ia(0) + a^\dagger(0) \right) + e^{\lambda_2 t} v_2 \frac{1}{\sqrt{2}} \left( i a(0) + a^\dagger(0) \right) \]

\[ = e^{(-\alpha - \kappa') t} v_1 \frac{1}{\sqrt{2}} \left( -ia(0) + a^\dagger(0) \right) + e^{(\alpha - \kappa') t} v_2 \frac{1}{\sqrt{2}} \left( i a(0) + a^\dagger(0) \right) \]

(E.11)

By inserting Eqs.(E.6, E.7, E.10) and Eq.(E.11) into Eq.(E.5) we can write

\[ A(t) = e^{(\kappa' - \alpha) t} v_1 \frac{1}{\sqrt{2}} \left( -ia(0) + a^\dagger(0) \right) + e^{(\alpha - \kappa') t} v_2 \frac{1}{\sqrt{2}} \left( i a(0) + a^\dagger(0) \right) \]

\[ + \int_0^t \left[ e^{(\kappa' + \alpha)(\tau - t)} v_1 \frac{1}{\sqrt{2}} \left( -i\eta + \eta^\dagger \right) + e^{(\kappa' - \alpha)(\tau - t)} v_2 \frac{1}{\sqrt{2}} \left( -i\eta + \eta^\dagger \right) \right] d\tau \]

(E.12)

The separated equations reads now

\[ a(t) = \frac{1}{2} e^{(\kappa' - \alpha)t} \left( a(0) + ia^\dagger(0) \right) + e^{(\alpha - \kappa') t} \left( a(0) - ia^\dagger(0) \right) \]

\[ + \frac{1}{2} \int_0^t \left[ e^{(\kappa' + \alpha)(\tau - t)} \left( \eta + i\eta^\dagger \right) + e^{(\kappa' - \alpha)(\tau - t)} \left( \eta - i\eta^\dagger \right) \right] d\tau \]

(E.13)
E. Equations for field operators

\[ a(t) = e^{-\kappa' t} \left( a(0) \cosh(\alpha t) - i a^\dagger(0) \sinh(\alpha t) \right) + \frac{1}{2} \int_0^t \left[ e^{(\kappa' + \alpha)(\tau - t)} (\eta + i\eta^\dagger) + e^{(\kappa' - \alpha)(\tau - t)} (\eta - i\eta^\dagger) \right] d\tau \]
(E.14)

By the same procedure, the conjugate operator is described by

\[ a^\dagger(t) = e^{-\kappa' t} \left( i a(0) \sinh(\alpha t) + a^\dagger(0) \cosh(\alpha t) \right) + \frac{1}{2} \int_0^t \left[ e^{(\kappa' + \alpha)(\tau' - t)} (-i\eta + \eta^\dagger) + e^{(\kappa' - \alpha)(\tau' - t)} (i\eta + \eta^\dagger) \right] d\tau' \]
(E.15)

By multiplying Eq. (E.14) and Eq. (E.15) and evaluating its expectation value, we can write

\[ \langle a^\dagger a \rangle = e^{-2\kappa' t} \left\{ i \left( \langle a^2(0) \rangle - \langle a^\dagger a \rangle \right) \right\} \cosh(\alpha t) \sinh(\alpha t) + \langle a(0) a^\dagger(0) \rangle \sinh^2(\alpha t) + \langle a^\dagger(0) a(0) \rangle \cosh^2(\alpha t) \}
+ \frac{1}{2} \alpha^2 + e^{-2\kappa' t} \left( \kappa'^2 - \alpha^2 - \kappa' (\kappa' \cosh(2\alpha t) + \alpha \sinh(2\alpha t)) \right) \frac{\kappa'^2 - \alpha^2}{\kappa'^2 - \alpha^2} \]
(E.16)
Two-time correlation functions

Let us assume $c(t)$ being a system operator that fulfills

$$\left[ c(t), \sqrt{2\kappa a_{\text{in}}(t)} \right] = \kappa \{ c(t), a(t) \} \quad (F.1)$$

with,

$$\left[ c(t), \sqrt{2\kappa a_{\text{in}}(t')} \right] = 0, \quad t' > t \quad (F.2)$$
$$\left[ c(t), \sqrt{2\kappa a_{\text{out}}(t')} \right] = 0, \quad t' < t \quad (F.3)$$

with the input-output (Eq.(1.103)) relation we can write

$$\left[ c(t), -\sqrt{2\kappa a_{\text{in}}(t')} + 2\kappa a(t) \right] = 0, \quad t' < t \quad (F.4)$$

that implies

$$\left[ c(t), \sqrt{2\kappa a_{\text{in}}(t')} \right] = \left[ c(t), 2\kappa a(t) \right], \quad t' < t \quad (F.5)$$

As a result from the previous equation and Eq(F.1)

$$\left[ c(t), \sqrt{2\kappa a_{\text{in}}(t')} \right] = 2\kappa \theta(t - t') \left[ c(t), a(t') \right] \quad (F.6)$$

being $\theta = 1$ for $t > 0, 1/2$ for $t = 0$ and 0 for $t < 0$ the step function.

In this way, the commutator for the output field is

$$\left[ a_{\text{out}}(t), a_{\text{out}}^\dagger(t') \right] = \left[ a_{\text{in}}(t), a_{\text{in}}^\dagger(t') \right] \quad (F.7)$$
If the input state can be considered as a coherent vacuum, we can rewrite the variances of the output in terms of the internal system. The terms with $a_{in}(t')$ will factorize and the two-time correlation functions of the output field can now be related to the internal cavity field as

$$\langle a_{\text{out}}^\dagger(t), a_{\text{out}}(t') \rangle = 2\kappa \langle a^\dagger(t), a(t) \rangle$$

The phase dependent two time correlation function read

$$\langle a_{\text{out}}(t), a_{\text{out}}^\dagger(t') \rangle = \delta(t-t') + \langle a_{\text{out}}^\dagger(t'), a_{\text{out}}(t) \rangle$$

$$\langle a_{\text{out}}^\dagger(t), a_{\text{out}}^\dagger(t') \rangle = \delta(t-t') + 2\kappa \langle a^\dagger(t'), a(t) \rangle$$

and the corresponding correlation function for the hermitian conjugate operators read

$$\langle a_{\text{out}}(t), a_{\text{out}}^\dagger(t') \rangle^* = \langle a_{\text{out}}(t'), a_{\text{out}}(t) \rangle$$

$$\langle a_{\text{out}}^\dagger(t), a_{\text{out}}^\dagger(t') \rangle = 2\kappa \langle a^\dagger(t'), a^\dagger(t) \rangle.$$

with $\tau = \max[t, t']$ and $\tau' = \min[t, t']$. The two time correlation function of the output is related with the temporal order of the two time correlation function of the cavity field. The spectrum of the output field, given by the Fourier transform of $\langle a_{\text{out}}(t), a_{\text{out}}(t') \rangle$ will be equal to the spectrum of the cavity field.
Derivation of the secular equations for fast vibrating atoms

After inserting Eq. (3.39) into the Eqs. (3.37)-(3.38), we obtain

$$\dot{A}(t) = MA(t) + N(t) + \sum_{j=1,2} k^2 q_j^2 \cos^2(\nu t + \phi_j) \left[ VA(t) + (-1)^j B \right]$$

where

$$A(t) = \begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix}, \quad (G.2)$$

$$M = \begin{pmatrix} -\kappa' - i(\theta - \delta_c) & -i\alpha \\ i\alpha & -\kappa' + i(\theta - \delta_c) \end{pmatrix}, \quad (G.3)$$

$$N(t) = \begin{pmatrix} \eta(t) \\ \eta^\dagger(t) \end{pmatrix}, \quad (G.4)$$

$$V = \begin{pmatrix} i\theta/2 & i\alpha/2 \\ -i\alpha/2 & -i\theta/2 \end{pmatrix}, \quad (G.5)$$
G. Derivation of the secular equations for fast vibrating atoms

and

\[ B = \begin{pmatrix} -\beta & \beta \\ \beta & \beta \end{pmatrix}. \]  

We indicate with

\[ \tilde{f}(t) = \frac{1}{T} \int_t^{t+T} d\tau f(\tau) \]  

the time average of a variable \( f(t) \) over a period of oscillation \( T = 2\pi/\nu \) of the atomic motion. Since

\[ \frac{\partial}{\partial t} \tilde{f}(t) = \frac{1}{T} [f(t + T) - f(t)] = \tilde{f}', \]

we find

\[ \frac{\partial}{\partial t} \tilde{A}(t) = M\tilde{A}(t) + \tilde{N}(t) + k^2 \bar{q}^2 V \tilde{A}(t) \]

\[ + k^2 \bar{q}^2 V \sum_{j=1,2} \frac{1}{T} \int_t^{t+T} d\tau \cos(2\nu \tau + 2\phi_j) A(\tau) \]  

where we have used the relation \( \cos^2(y) = \frac{1}{2} [1 + \cos(2y)] \) and we have assumed that the two atoms have the same energy, such that \( \bar{q}_1^2 = \bar{q}_2^2 = \bar{q}^2 \). We now identify the conditions under which we can neglect the second line of Eq. (G.8). Integrating by part the second line of Eq. (G.8) an using Eqs. (G.1) and (G.8) we obtain

\[ \frac{\partial}{\partial t} \tilde{A}(t) = M\tilde{A}(t) + \tilde{N}(t) + k^2 \bar{q}^2 V \tilde{A}(t) \]

\[ + k^2 \bar{q}^2 C(t) + k^4 \bar{q}^4 D(t) + k^4 \bar{q}^4 E \]  

(G.9)
where

\[ C(t) = \frac{V}{4\nu} \sum_j \{ \sin(2\nu t + 2\phi_j) [M\tilde{A}(t) + \tilde{N}(t)] \}
\]
\[
- \frac{1}{T} \int_t^{t+T} \, d\tau \sin(2\nu\tau + 2\phi_j) [MA(\tau) + N(\tau)] \},
\]

\[ D(t) = \frac{V^2}{8\nu T} \sum_{jj'} \int_t^{t+T} \, d\tau
\times \left[ \sin(2\nu t + 2\phi_j) \cos(2\nu\tau + 2\phi_{j'}) - 2 \sin(2\nu t + 2\phi_j) \cos^2(\nu\tau + \phi_{j'}) \right] A(\tau),
\]

\[ E = \frac{VB}{8\nu} \sin[2(\phi_2 - \phi_1)]. \quad (G.10)
\]

The terms \( k^2 \bar{q}^2 C(t) + k^4 \bar{q}^4 D(t) \) are negligible with respect to \( k^2 \bar{q}^2 V \) when
\[ \langle \theta \rangle \kappa'/8\nu \ll \langle \alpha \rangle /2 \text{ and } \langle \theta(\theta - \delta_c) \rangle /8\nu \ll \langle \alpha \rangle /2 \]
which reduce to

\[ \nu \gg \frac{g^2}{\langle \Delta \rangle}, \quad (G.11)
\]
\[ \nu \gg \frac{k^2 \bar{q}^2}{8} \left\langle \frac{g^2 \Delta}{\Omega^2} \right\rangle \quad (G.12)
\]

when \(|\alpha|\) and \(\kappa'\) are of the same order of magnitude and \(\delta_c = \theta(1 - k^2 \bar{q}^2 /2)\), see Eq. (3.43). The term \( k^4 \bar{q}^4 E \) in Eq. (G.9) can be neglected when
\[ k^4 \bar{q}^4 \langle \theta\beta \rangle /16\nu \ll k^2 \bar{q}^2 \langle \alpha \rangle /2, \]
that is

\[ \nu \gg \frac{k^2 \bar{q}^2}{16} \left\langle \frac{g\Delta}{\Omega} \right\rangle. \quad (G.13)
\]

When conditions (G.11)-(G.13) are satisfied we approximate Eq. (G.8) with

\[ \frac{\partial}{\partial t} \tilde{A}(t) = M\tilde{A}(t) + \tilde{N}(t) + k^2 \bar{q}^2 V \tilde{A}(t). \quad (G.14)
\]

which then leads to Eqs. (3.41) and (3.42). Finally we show that the averaged noise operators, \( \tilde{\eta}(t) \) and \( \tilde{\eta}^\dagger(t) \), which appear in the term \( \tilde{N}(t) \), are delta
G. Derivation of the secular equations for fast vibrating atoms

Correlated. The only non-vanishing correlation function is

\[ \langle \tilde{\eta}(t)\tilde{\eta}^\dagger(t') \rangle = \frac{2\kappa'}{T^2} \int_t^{t+T} d\tau \int_{t'}^{t'+T} d\tau' \delta(\tau - \tau') \]

which is not zero only if the two integration intervals \([t, t+T]\) and \([t', t'+T]\) have finite overlap. Therefore if \(f(t)\) varies slowly over the time \(T\), so that \(\tilde{f}(t) \simeq f(t)\), then one has

\[ \int_{-\infty}^{\infty} dt f(t) \langle \tilde{\eta}(t)\tilde{\eta}^\dagger(t') \rangle \simeq 2\kappa' f(t'), \quad (G.16) \]

that is \(\langle \tilde{\eta}(t)\tilde{\eta}^\dagger(t') \rangle \simeq 2\kappa' \delta(t-t').\)
Hamiltonian in second quantization

The second-quantized form of Hamiltonian in Eq. (4.8) is obtained after introducing the field operators $\Psi(x)$ and $\Psi^\dagger(x)$, which are defined by the commutation rules Eq. (4.10). The field operators are defined in the Hilbert space of the states of the quantized field. In this appendix we show that this Hilbert space contains the Hilbert space of a given $N$-particle system. More details are provided for instance in [101].

The evolution of the quantized field is determined by Hamiltonian $H = \Gamma + \Lambda$, with

\begin{align*}
\Gamma & = \int d^3x \Psi^\dagger(x) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_0 \cos(kx)\right) \Psi(x) \tag{H.1} \\
\Lambda & = \frac{1}{2} \int d^3x_i d^3x_j \Psi^\dagger(x_i) \Psi^\dagger(x_j) V(x_i, x_j) \Psi(x_i) \Psi(x_j), \tag{H.2}
\end{align*}

We first observe that $[H, N] = 0$, with $N$ the number operator defined in Eq. (4.11). Hence, they can be simultaneously diagonalized. In particular, a simultaneous eigenstate of operators $H$ and $N$ is an energy eigenstate of a system with a definite number of particles. In order to show it, we denote by $\{|\Psi_{EN}\rangle\}$ the vectors of the orthonormal basis, which are simultaneously
eigenstates of $H$ and $N$. In detail, they fulfill the following properties

$$
\langle \psi_{EN} | \psi_{EN} \rangle = 1 \\
H |\psi_{EN} \rangle = E |\psi_{EN} \rangle \\
N |\psi_{EN} \rangle = N |\psi_{EN} \rangle 
$$

The vacuum state $|0\rangle$, in particular, is one of these eigenstates at zero energy and zero atom number. It is here assumed to be unique. From the commutation properties of the field operators it is easily verified that

$$
[\Psi (x), N] = \Psi (x) \longrightarrow N\Psi (x) |\psi_{EN} \rangle = (N-1) \Psi (x) |\psi_{EN} \rangle \\
[\Psi^\dagger (x), N] = -\Psi^\dagger (x) \longrightarrow N\Psi^\dagger (x) |\psi_{EN} \rangle = (N+1) \Psi (x) |\psi_{EN} \rangle 
$$

from which follows that $\Psi (x)$ and $\Psi^\dagger (x)$ annihilates and creates, respectively, a particle. From the property, that the norm is semi-positive definite, one finds that the eigenvalues of the spectrum of operator $N$ have to be semi-positive definite,

$$
< \Psi_{EN} | \Psi^\dagger (x) \Psi (x) | \Psi_{EN} > = N - 1 \geq 0 \quad (H.3)
$$

which implies that the eigenvalues are positive integers, $N = 0, 1, 2, \ldots$. Since operator $\Psi (x)$ decreases $N$ by 1, and the state at $N = 0$ is assumed to be unique, then the identity holds

$$
|\Phi_n \rangle |\Psi (x_1) |\Psi (x_2) \ldots |\Psi (x_N) |\psi_{EN} \rangle = 0 \text{ unless } |\Phi_n \rangle \equiv |0\rangle 
$$

We will define a function of $N$ position coordinates $x_1, \ldots, x_N$ as

$$
\psi_{EN} (x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \langle 0 | \Psi (x_1) \ldots \Psi (x_N) |\psi_{EN} \rangle \quad (H.4)
$$

This function is symmetric with respect to the exchange of any two coordinates for bosons, and the norm is unity

$$
\int d^3N x \psi_{EN}^* (x_1, \ldots x_N) \psi_{EN} (x_1, \ldots, x_N) = 1 \quad (H.5)
$$

Our aim is to establish the connection between the quantized field and a $N$-body system by proving the following theorem.
\begin{equation}
\left( -\frac{\hbar^2}{2m} \sum_{j=1}^{N} (\nabla_j^2 + V_j) + \sum_{i<j} v_{ij} \right) \psi_{EN} (x_1, \ldots, x_N) = E\psi_{EN} (x_1, \ldots, x_N)
\end{equation}

(H.6)

We start with

\begin{equation}
\frac{1}{\sqrt{N!}} \langle 0 | [\Psi (x_1), \ldots, \Psi (x_N)] H |\psi_{EN} \rangle = E\psi_{EN} (x_1, \ldots, x_N)
\end{equation}

(H.7)

Since $H \langle 0 \rangle = 0$ and $H$ is hermitian ($\langle 0 | H = 0$) by using the identity $[AB, C] = [A, C] B + A [B, C]$ one can find

\begin{equation}
J = \frac{1}{\sqrt{N!}} \langle 0 | [\Psi (x_1), \ldots, \Psi (x_N), H] |\psi_{EN} \rangle = \frac{1}{\sqrt{N!}} \langle 0 | \Psi (x_1), \ldots, [\Psi (x_j), H] \ldots \Psi (x_N) \rangle |\psi_{EN} \rangle
\end{equation}

(H.8)

We should now find $[\Psi (x_j), H] = [\Psi (x_j), K] + [\Psi (x_j), \Lambda]$

\begin{equation}
[\Psi (x_j), K] = -\frac{\hbar^2}{2m} \int d^3x \left[ \Psi (x_j), \Psi (x) \right] (\nabla^2 + V_i (x)) \Psi (x)
\end{equation}

\begin{equation}
= -\frac{\hbar^2}{2m} \int d^3x \left[ \Psi (x_j), \Psi (x) \right] \Psi (x)
\end{equation}

\begin{equation}
= -\frac{\hbar^2}{2m} (\nabla_j^2 + V_{lj}) \Psi (x_j)
\end{equation}

(H.9)

\begin{equation}
[\Psi (x_j), \Lambda] = \frac{1}{2} \int d^3x_1 d^3x_2 \left[ \Psi (x_j), \Psi (x_1) \Psi (x_2) \right] v_{12} \Psi (x_1) \Psi (x_2)
\end{equation}

\begin{equation}
= \frac{1}{2} \int d^3x_1 d^3x_2 \left[ \Psi (x_j), \Psi (x_1) \Psi (x_2) \right] \Psi (x_1) \Psi (x_2)
\end{equation}

\begin{equation}
= \int d^3x \Psi (x_j) v (x, x_j) \Psi (x) \Psi (x_j)
\end{equation}
We have then

$$[\Psi(x_j), H] = \left[ -\frac{\hbar^2}{2m} \nabla_j^2 + V_{ij} + X(x_j) \right] \Psi(x_j) \quad (H.11)$$

where

$$X(x_j) = \int d^3x \Psi^\dagger(x) v(x, x_j) \Psi(x) \quad (H.12)$$

It can be shown that

$$[\Psi(x_j), X(x_j)] = v_{ij} \Psi(x_i)$$

$$X(x_j)|0\rangle = 0 \quad \text{and} \quad \langle 0| X(x_j) = 0 \quad (H.13)$$

The left part of equation (H.6) becomes

$$J = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \left( \nabla_j^2 + V_{ij} \right) \psi_{EN}(x_1 \ldots x_N)$$

$$+ \frac{1}{\sqrt{N!}} \sum_{j=1}^{N} (0| \Psi(x_1) \ldots \Psi(x_j - x_1) X(x_j) \Psi(x_j) \ldots \Psi(x_N)|\psi_{EN}) \quad (H.14)$$

By commuting X(j) all the way to the left

$$[\Psi(x_1) \ldots \Psi(x_j - x_1) X(x_j) \Psi(x_j) \ldots \Psi(x_N)]$$

$$= [\Psi(x_1) \ldots \Psi(x_j - x_2) X(x_j) \Psi(x_j - x_1) \ldots \Psi(x_N)] + v_{j-1,1} [\Psi(x_1) \ldots \Psi(x_N)]$$

$$= [\Psi(x_1) \ldots \Psi(x_j - x_3) X(x_j) \Psi(x_j - x_2) \ldots \Psi(x_N)] + (v_{j-2,1} + v_{j-1,j}) [\Psi(x_1) \ldots \Psi(x_N)]$$

$$= \left[ X(x_j) \sum_{i=1}^{j-1} v_{ij} \right] [\Psi(x_1) \ldots \Psi(x_N)] \quad (H.15)$$

we obtain

$$J = \left[ -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \left( \nabla_j^2 + V_{ij} \right) + \sum_{i<j} v_{ij} \right] \psi_{EN}(x_1 \ldots x_N) \quad (H.16)$$
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Publications

This thesis is based on the following publications:

Part I

• *Nonlinear optics with two trapped atoms*
  S. Fernandez-Vidal, S. Zippilli and G. Morigi

Part II

• *Quantum stability of Mott-insulator states of ultracold atoms in optical resonators*
  J. Larson, S. Fernandez-Vidal, G. Morigi, M. Lewenstein

• *The quantum ground state of self-organized atomic crystals in optical resonators*
  S. Fernandez-Vidal, G. De Chiara, J. Larson, G. Morigi
  Accepted in Phys. Rev. A.

The following articles were published during my PhD studies although they are not discussed along this thesis:

• *Coherent Manipulation of Holes in Dipole Trap Arrays*
  A. Benseny, S. Fernandez-Vidal, J. Baguda, R. Corbalan, A. Picon, L.
• Universal decoherence induced by an environmental quantum phase transition

F. M. Cucchietti, S. Fernandez-Vidal, J. P. Paz

Bibliography


