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## Strong correlation effects with atoms in optical lattices

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I've become frogproof

## Abstract

Our work concerns the effects of strong correlations of ultracold atoms in optical lattices in three different scenarios. First, we analyze the influence of dissipative processes on the superfluid–Mott insulator transition in the Bose–Hubbard model, observing a shift of the well-known phase transition. In a second setup, atoms are trapped in state-dependent lattices; we show that any asymmetry in the contact interaction produces a form of correlated hopping, which results in a pair superfluid phase with interesting correlation properties that differentiate it from an ordinary atomic Bose–Einstein condensate. Finally, we investigate a two-species Bose–Hubbard model including a conversion term, which can be implemented experimentally through a Feshbach resonance. We are particularly interested in the exotic incompressible, yet superfluid "super-Mott" phase.

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## A short overview

Light controlling particles — to some, it could seem to be a magic trick in which the thin strings cannot be seen. This interplay is certainly awe-inspiring but not magic. Physics, and its ever-blooming and never-ending path of achievements and developments, pulls the strings behind the veil. Today, our understanding of nature is used as a tool to trap, then cool, store and manipulate neutral atoms in intensity patterns created via laser arrangements [78].

As some particles are cooled to unimaginably low temperatures<sup>\*</sup>, their characteristic thermal de Broglie wavelength<sup>†</sup> exceeds their mean interparticle separation, thus favoring the particles to occupy a single ground state and form a Bose–Einstein condensate (BEC) [15, 35]. A BEC is a "social" phenomenon in which the population of this ground state becomes macroscopic, based on the quantum statistics of bosons (particles with zero or integer spin). Since its prediction in the mid-twenties, other phenomena such as superfluidity in liquid helium [71, 106], high-temperature superconductivity in some materials [69] and condensation of pions in neutron stars [52], have been considered as manifestations of bosonic condensation. The capability of trapping and cooling atoms with light forms the basis for the experimental observation of BEC, achieved for the first time in dilute alkali atomic gases in 1995 [6, 25, 17]. Since then, the opportunity to produce these degenerate bosonic (and fermionic) quantum gases, combined with the ability to trap them, has promoted exciting developments in fields ranging from atom and condensed matter physics [58, 14] to quantum information processing [22]. As of yet, we can use simple dipole traps [95], microtraps [32], surface microtraps [21] and optical lattices [94, 5, 12], that is plenty of choice of configurations to fulfill our wishes.

Ultracold neutral atoms trapped in optical lattices are a wonderful tool to study manybody physics and strong correlation effects. One of the great advantages of these systems is that generally, the physical behavior of the atoms is perfectly described by a simple underlying lattice Hamiltonian, a description ultimately known as the Hubbard model [58, 49]. The Hubbard model allows us to use these artificial crystals as analogues to real systems in condensed matter physics. For instance, quantum magnetism can be studied through the implementation of spin Hamiltonians [31, 44, 61], and the origin of high-temperature superconductivity is believed to be explained by the physics within the Hubbard Hamiltonian [69, 55] (an idea that has been experimentally pursued by the cooling of fermionic atoms to study Cooper pairing and the BCS<sup>‡</sup> to BEC transition

<sup>\*</sup>Temperatures going down to the nK regime ( $\sim -273^{\circ}C!$ ).

<sup>&</sup>lt;sup>†</sup>Wave-like property of matter appearing in the wave-particle duality.

<sup>&</sup>lt;sup>‡</sup>Fermions forming loose pairs like Cooper pairs in BCS theory, the microscopic theory of supercon-

[89, 125, 16]). Furthermore, these quantum simulators have enabled the prediction of novel and exotic many-body quantum phases, as well as new physical phenomena (*e.g.* quantum Hall effect with bosons [84], lattice gauge theories [60, 82]).

The present study uses these artificial crystals of light to create and investigate fundamental quantum phases of bosonic many-body systems. The focus is threefold: atoms undergoing dissipation as an open quantum system, atoms with correlated hopping, and atoms and molecules coupled through a Feshbach resonance.

**Atoms in a noisy environment** Cold atoms in an optical lattice are coupled to a large reservoir (also described by the Bose–Hubbard model) to investigate how the occurrence of dissipation modifies the system's phase diagram. Our interest lies on the new features arising in the quantum state of an otherwise conservative system when it undergoes a superfluid–Mott insulator phase transition in the presence of dissipation. Related studies have been carried out later by Diehl et al. [30], Kraus et al. [66] and Verstraete et al. [110], where quantum reservoirs and system-reservoir couplings are specially designed with two aims: to generate quantum phases and entangled states in the steady-state regime of the system and to implement universal quantum computation [28]. An advantage of this new method is that it makes possible to prepare states that correspond to excited many-body states, allowing the study of increasingly complex systems. It is remarkable that there is a master equation yielding any one multipartite pure state of the system as unique stationary state — the relaxation occurs within a time scale that does not depend on the number of subsystems [66]. Dissipative state engineering can be used to prepare ground states of frustration-free Hamiltonians [110, 66]. Engineering a reservoir is akin to choosing for jump operators  $c_l$  in the master equation [47] those that have the desired state  $|\psi\rangle$  as a dark state  $c_l |\psi\rangle = 0$ , while the dissipation is kept quasi-local [30]. Our study focuses on two kinds of decoherence processes: number dissipation and phase dissipation. Number dissipation corresponds to an exchange of particles between the system and the reservoir, while phase dissipation refers to collisions between both sets of particles inducing the dephasing of the system. Controlling the level of noise, we can access different regimes and learn more about dissipative phenomena. We observe that dissipation shifts the phase transition in a direction related to the state of the reservoir, agreeing with later findings [30].

Atoms with correlated hopping The second topic takes us to a different setup, where atoms are trapped in state-dependent lattices [73] and a novel mechanism for pairing based on transport-inducing collisions is introduced. As illustrated in figure 1, when two atoms collide they can mutate their internal state  $(|+\rangle, |-\rangle)$ . If these atoms are placed in one of two state-dependent optical lattices, a collision will force hopping of atoms to a site associated to their new state. For deep enough lattices, as in the Mott insulator experiments [49], this coordinated jump of pairs will be the dominant hopping process and the atoms will become a superfluid of pairs. In the most general case, deriving the effective lattice Hamiltonian for the atoms we show that any asymmetry in the contact interaction  $(g_{\uparrow\uparrow} \neq g_{\downarrow\downarrow}, g_{\uparrow\downarrow} \neq g_{\downarrow\uparrow})$  [75, 121] translates into a form of correlated

ductivity proposed by Bardeen, Cooper, and Schrieffer in 1957.



Figure 1: (left) Two atoms in state  $|+\rangle$  collide and change of state in free space. (right) When these atoms are confined in overlapping state-dependent optical lattices, shifted out-of-phase from one another in space, their change of state will be accompanied by a tunneling event to a neighboring site (solid). This leads to correlated hopping of atom pairs along the x direction, as other tunneling processes (dashed) are forbidden.

hopping: either environment-biased hopping  $n_i a_j^{\dagger} a_k$  [34] or pair hopping  $a_j^{2^{\dagger}} a_k^2$  [33]. Our most relevant finding is evidence of a pair superfluid, which exists for a wide range of interaction asymmetries and has interesting correlation properties that differentiate it from an ordinary atomic Bose–Einstein condensate. Other phases that this model presents are ordinary Mott insulators, a double feature of a superfluid with a pair superfluid, and charge-density waves.

Atoms in a Feshbach resonance The last investigated topic concerns a two-species Bose–Hubbard model including a conversion term, by which two particles of a species can be converted into one particle of a second species, and vice versa. This model can be related to ultracold atom experiments where a Feshbach resonance [105, 29] is used to tune the scattering length of the atoms in order to produce molecules (figure 2). The motivation to investigate the phase diagram of this system lies in recent results using quantum Monte Carlo simulations [91, 92], where the existence of an exotic, so-called "super-Mott" phase has been proposed. They report an unusual combination of properties: the system has a vanishing compressibility, simultaneously with the flow of individual species in opposite directions. In their first work [91], they use the world line algorithm [11, 10]. The compressibility of the system is determined through the slope of the particle density  $\rho$ as a function of the chemical potential. The superfluidity of the mixture is evaluated using the Pollock and Ceperley formula [87], which relates the superfluid density to the fluctuations of the winding number  $W^{\S}$ . Given that atoms may turn into molecules and vice versa, pseudowinding numbers are defined for each species. The authors have found that certain regions are incompressible and have, at the same time, individual species flowing — but without a net mass current. In a following study [92], they use the stochastic Green function algorithm [90]. This method is useful to easily estimate the superfluid fraction of atoms and of molecules, used to probe the quasi-condensation of individual species. Using also the winding numbers, they draw the phase diagram for a system with a fixed occupation number and find the "super-Mott" phase for strong interactions. This "super-Mott" phase has not been observed in previous mean-field studies [98], due to the incapability of the method to describe dynamical correlations. To deepen our

<sup>&</sup>lt;sup>§</sup>A quantity defined for a given configuration in the algorithm as the difference between the number of times that a world line crosses the boundaries of the system in one direction and in the other.



Figure 2: Representation of a Feshbachresonant atomic collision: two atoms collide and form a molecule in another part of the Hilbert space, here indicated by the spin arrangement.

knowledge about this intriguing phase and the details behind its mechanism, we use a different approach based on quasi-exact diagonalizations. This method enables the study of the spatial structure of correlations, which is completely missing within a meanfield approach and gives additional information to the superfluid density. Moreover, we consider parameter values comparable to those in experiments, thus constraining possible scenarios in which this mixed phase may be observed in experiments.

#### Outline of this study

To this dissertation concerns the study of strong correlation effects with ultracold atoms in optical lattices in three different scenarios: noise, correlated hopping and Feshbach resonances. This leads naturally to structure this dissertation in 3 + 1 parts, as described in the following.

In the introductory part *Background: Atoms in an optical lattice*, we want to acquaint the reader with the concepts and techniques that are common to all subsequent studies. In the first chapter we start explaining how optical lattices are created and the principles behind their action on neutral atoms (section 1.1). Here we find the ideal occasion to present the Bloch and Wannier states (section 1.2), which are going to be used in the derivation of the Bose–Hubbard model (section 1.3). This last section finishes with a discussion about the physics arising from this model and its phases.

In the second chapter we present the analytical and numerical techniques used to study ultracold atoms in optical lattices and to predict the properties of the emerging phases. Analytical methods like the quantum rotor model (section 2.1) and the strong coupling expansion (section 2.2) are usually used to study regions of the parameter space which cannot be solved exactly and require some approximations. On the other hand, numerical methods like the Gutzwiller ansatz (section 2.3) and the Matrix Product State algorithms (section 2.4) come into play in those regions that lie outside the possible analytical approximations: typically near to transition points, where the complexity of the system increases; or when the size of the system cannot be otherwise handled. In the study of *Atoms in a noisy environment*, we analyze the effects of dissipative processes on the superfluid–Mott insulator transition in the Bose–Hubbard model, where a shift of the phase transition is observed. The dynamics of a system coupled to an environment can be described in two ways: following an exact treatment to solve the composed system and tracing out the environment from the solution; or using an approximate model for the system where the environment is treated as noise. In the third chapter we introduce the basics of the theory needed to elaborate this approximate model: the master equation formalism (section 3.1). We continue presenting the system and the environment in detail, their Hamiltonians, and the dissipative mechanisms that are going to be considered (section 3.2).

In the fourth chapter we proceed with the application of the analytical and numerical methods. We apply the quantum rotor model (section 4.1) for both, the complete and the approximate model. These results show how dissipative processes may be used to change the state of a system and drive it into a different phase. The strong coupling expansion (section 4.2) and the Gutzwiller ansatz (section 4.3) agree on the observation of a shift of the phase transition, which is equivalent to a renormalization of the parameters of the Bose-Hubbard model.

In the study of *Atoms with correlated hopping* we move to a different setup, where atoms are trapped in state-dependent lattices and transport-inducing collisions appear naturally from the engineering of the system. In the fifth chapter we introduce a model for correlated hopping (equation 5.1), qualitatively discussing its origin and the quantum phases that are expected to appear in the different parameter regimes (section 5.2). We present a possible way to implement this model, which is based on optical superlattices and atoms with asymmetric interactions.

The sixth chapter presents the theoretical results obtained using analytical and numerical methods, starting with exact diagonalizations for a small number of atoms and sites (section 6.1). These calculations reveal the existence of insulating and coherent regimes, as well as pairing; they will be the basis for later analysis. Further work is done on the understanding of the pair-superfluid phase introducing a toy model inspired in the ordinary superfluid (section 6.2). Having gained some insight into the basics of our system, we continue studying the many-body physics of larger lattices with correlated hopping using a variety of techniques: insulating regime (section 6.3), perturbation theory (section (6.4) and quantum rotor model (section (6.5)). These methods suggest a number of possible phases, including a Mott insulator, a pair superfluid, a normal superfluid and a chargedensity wave state; and give estimations of the parameters for which these phases appear. We also develop two numerical methods to study our system: a Gutzwiller ansatz (section 6.6) and an infinite Matrix Product State method (section 6.7). With these simulations we confirm the predicted phases and locate the quantum phase transitions, which are found to be of second order. Finally, in section 6.8 we suggest some currently available experimental methods to detect and characterize these phases.

Finally comes the study of *Atoms in a Feshbach resonance*, where we investigate a Bose–Hubbard model that includes a mixture of atoms and molecules, and a conversion term between these species. This model is interesting because it can be related to ultra-

cold atom experiments where a Feshbach resonance produces molecules. In the seventh chapter, we start introducing the theory of Feshbach resonances (section 7.1) and follow presenting the Hamiltonian of our system (section 7.2).

In the eighth chapter we discuss the results. We apply an adiabatic elimination of the molecular state (section 8.1), where the effect of this level is seen as a renormalization of the Bose–Hubbard model. A strong coupling expansion (section 8.2) and the mean-field theory (section 8.3) are used to give further insight into this model, observing already with the latter the appearance of a hybrid phase. We close this chapter formulating a Density Matrix Renormalization Group algorithm using Matrix Product States (section 8.4) to study the long-range correlations of the system, with special interest to verify the existence of the exotic "super-Mott" phase, which has been recently reported.

This dissertation also includes four appendices, where some derivations used in this study are explained in detail. In appendix A we explain how a Density Matrix Renormalization Group algorithm using Matrix Product States can be numerically implemented, as used in sections 6.7 and 8.4. In appendix B we derive the master equations for a dissipative system that undergoes either exchange of particles or collisions with a reservoir, as considered in section 4.1. In appendix C we include the detailed derivation of the model presented in section 5.2. At last, in appendix D we derive from microscopical considerations the physical parameters used in section 7.2 and following sections.

# Background: Atoms in an optical lattice

## Chapter 1

## Cold atoms in optical lattices

#### **1.1 Optical Lattices**

An optical lattice is a light structure used to capture, cool and manipulate neutral atoms, which have been typically already precooled in a magneto-optical trap<sup>\*</sup> (MOT) and later further cooled down to the  $\mu K$  regime using other laser techniques.

The idea to confine atoms in wavelength-size regions of a standing wave by means of the dipole force appears for the first time in 1968 [70]. But it was only 20 years later when its earliest realization came to light, with the experimental observation of the channeling of atoms from an atomic beam into paths between the peaks of a one-dimensional (1D) standing wave [94]. Since then, optical lattices have played a very important role in the development of cooling techniques [24, 88] and in the study of atoms confined to a wavelength scale, with applications ranging from the simulation of condensed matter systems [58, 13] to the processing of quantum information [18, 72], where in the latter localized atoms can be seen as a natural quantum register. These realizations rely on the fact that optical lattices allow to produce an artificial crystal for quantum matter which is free of defects, has an exactly known structure and whose potential depth can be varied through the laser parameters without changing the lattice vectors, while these latter may be changed independently redirecting the laser beams. More sophisticated arrangements than the 1D introduced here, may allow to move the confined particles around and attain a large number of diverse configurations.

The simplest optical lattice that we can consider is the periodic intensity pattern of light formed when a  $1D^{\dagger}$  arrangement of two counterpropagating laser beams of the same polarization interfere. The incoming laser passes through the atomic cloud in the MOT and it is collimated and retro-reflected on a mirror (see figure 1.1 (up)). Then, these two beams form a stationary distribution of light with a periodicity of half the laser wavelength, a standing wave with its first node at the surface of the mirror. If the intensity of these beams is large and their frequency is relatively close to the internal transition of the atoms, we will have that when the MOT is turned off the AC Stark shift creates a

<sup>\*</sup>A MOT is a hybrid trap, it uses inhomogeneous magnetic fields and circularly polarized laser light, able to cool down neutral atoms to temperatures below 1mK.

<sup>&</sup>lt;sup>†</sup>For simplicity, we omit the description of the confinement in the other two dimensions.



**Figure 1.1:** (up) Stationary wave formed by a red detuned laser, where the atoms are trapped in the intensity maxima. (down) Schematic representation of the underlying potential, the optical lattice.

periodic potential

$$V(x) = V_0 \sin^2(kx) \tag{1.1}$$

that can be used to trap the atoms. Here,  $k = 2\pi/\lambda$  with  $\lambda$  being the wavelength of the laser and  $V_0$  denotes the potential depth of the lattice, which is proportional to the intensity of the laser beams and is easily controllable in the experiments. This kind of setup will confine the atoms in pancake-like discs, as shown in figure 1.1 (up).

To keep the atoms from distributing over a long distance, this lattice is superimposed with a trap  $V_{trap}(x)$  generated by a red detuned laser beam focused at the position of the atom cloud. This beam creates a Gaussian intensity profile, which is harmonic around the trap center. This additional trap, resulting from the spatial variation of the laser intensity, concentrates the atoms along a line which is typically of the order of  $100\mu m$ , the beam waist of the laser.

Most experiments in laser cooling and trapping are performed with alkali atoms, like <sup>7</sup>Li, <sup>23</sup>Na, <sup>39,41</sup>K and <sup>87</sup>Rb, because of their closed optical transitions lying in a convenient spectral range. As an example, the experiments by Bloch [1] and Rempe [2] concentrate on <sup>87</sup>Rb atoms, using blue detuned lasers with  $\lambda = 830 - 850nm$  ( $\Delta \simeq 80 - 60nm$ ) which results in a lattice spacing of 415 - 425nm. The lattice depth can vary from a few recoil energies<sup>‡</sup> up to  $30E_r$ , having for this species  $E_r/\hbar \sim 20kHz$ . These potentials yield wavepacket sizes that range from  $\sim 90nm$  for the shallow lattices to  $\sim 60nm$  for the deeper ones. These values are small compared to the lattice spacing  $\lambda/2$ , allowing to consider localized states. To obtain 1D confinement, lattices with  $V_{0\perp} \sim 30E_r$  in the orthogonal directions are used. After the BEC has been created in a magnetic trap, the lattice potential is ramped up, splitting the BEC in up to  $\sim 10^5$  lattice sites. The potential is ramped up slowly, in about 80ms, ensuring the permanence of the atoms in the ground state of the system.

<sup>&</sup>lt;sup>‡</sup>The recoil energy is a natural measure of energy scales in optical lattice potentials, it is the recoil energy of an atom after the absorption of a photon from the lattice.

#### Theory of AC-Stark shift trapping

As already mentioned, this varying light intensity creates a periodic potential for the atoms. This occurs because the oscillating electric field of the beams interacts with the atoms, inducing an oscillating atomic dipole moment. This dipole moment oscillates at the same frequency  $\omega$  of the field, with an amplitude  $d = \alpha(\omega)E$ . Here,  $\alpha(\omega)$  is the polarizability of the atoms, depending on the laser frequency, and E is the amplitude of the electric field.

The potential arising from this interaction is the time average over  $\vec{d} \cdot \vec{E}$ . Within a two-level model for the atom and using standard approximations [51], one obtains the dipole potential

$$V_{dip}(\vec{r}) = -\frac{1}{2} \langle dE(\vec{r}) \rangle \sim \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} I(\vec{r})$$
(1.2)

where  $\Delta = \omega - \omega_0$  denotes the detuning of the laser with respect to the atomic transition frequency  $\omega_0$ . The second equality comes from relating the dipole moment of the atom to its decay rate  $\Gamma$  and considering a far detuned laser.

In equation 1.2, we see that the potential is proportional to the intensity of the field. For an optical lattice, the intensity is space dependent  $I(\vec{r}) = I_0 \sin^2(x)$ . Thereof, for a blue detuned laser ( $\omega > \omega_0$ ) the atoms will tend to the minima of intensity, and for a red detuned laser ( $\omega > \omega_0$ ) to the maxima. As in the lattice both maxima and minima of intensity are arranged periodically in space, the dipole interaction creates the egg-crate potential we expect and that is usually represented as in figure 1.1 (down).

#### **1.2** Single-particle states

The dynamics of atoms in these periodic potentials can be described in terms of Bloch wavefunctions and energy bands, as it is done in solid state physics for electrons in a crystal.

An atom moving in a 1D optical lattice is described by the single-atom Hamiltonian

$$H_1 = -\frac{\hbar^2 \nabla^2}{2m} + V(x) + V_{trap}(x).$$
(1.3)

Here, V(x) is the periodic potential (1.1) and the slowly varying potential  $V_{trap}(x)$  prevents the atoms from escaping through the ends of the optical lattice. For simplicity, we neglect this latter term throughout this work.

Following from equation 1.1, our potential V(x) has a periodicity of  $a = \lambda/2$ . According to Bloch's theorem [9], the eigenstates of the single-atom Hamiltonian (1.3) have the Bloch form  $\psi_{nk}(x) = e^{ikx}u_{nk}(x)$ , where  $u_{nk}(x)$  are the solutions of the eigenvalue problem

$$\left[\frac{(-i\hbar\nabla + \hbar k)^2}{2m} + V(x) - E_{nk}\right] u_{nk}(x) = 0, \ k \in [-\pi/a, \pi/a]$$
(1.4)

with the boundary condition  $u_{nk}(x) = u_{nk}(x+a)$ . These Bloch functions have two labels: the quasimomentum k and the band index n. The quantum number n identifies the different independent eigenstates that exist for a given value of k. In this way, solutions labeled by the same n form energy bands with energies  $E_{nk}$ , as it is pictured in figure 1.2 for different lattice depths. Observing figure 1.2 (center), we can see that for a potential barrier  $V_0$  of already a few  $E_r$  the bands located below  $V_0$  are rather flat and well separated from other bands by a large energy gap. For deeper potentials (figure 1.2 (right)), these features are reinforced and as we will see, the eigenstates of the particles become more localized in each lattice site. This latter occurs because the atoms lack enough energy to jump from one site to the other.

Localized states are usually described through the complete and orthogonal set of Wannier functions [117]

$$w_n(x-x_i) \sim \sum_{k \in [-\pi/a, \pi/a]} e^{-ikx_i} u_{nk}(x)$$
 (1.5)

where the *i*-th Wannier function describes a state localized in the *i*-th lattice site and in some given band n. An advantage of using this base is that it allows to assign a mean position to the particles, hence to account for interactions when the wavefunctions of two or more particles overlap.

In the harmonic limit  $(V_0 >> E_r)$  each lattice minimum can be considered as a harmonic oscillator

$$V(x) = V_0 \sin^2(kx) \simeq V_0 k^2 x^2 \simeq \frac{1}{2} m \omega_{ho} x^2 = V_{ho}(x), \qquad (1.6)$$

with a frequency  $\omega_{ho} = \sqrt{4V_0 E_r/\hbar^2}$  that defines the separation to the first excited Bloch band. In this limit, the Wannier states can be approximated by Gaussian functions and the size of the Gaussian ground state wave-packet in each of these pows is given by  $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ .

We can assume that only the lowest band is going to be occupied as long as neither thermal excitations nor the considered interactions are able to populate the excited bands. Following from the harmonic approximation, this implies that  $\hbar\omega_{ho} >> k_B T, U\bar{n}(\bar{n} - 1)/2$ . In the case of <sup>87</sup>Rb, we have that for shallow lattices the separation to the first band is  $\omega_{ho} \sim 90kHz$ , and 220kHz for deeper ones. Therefore, we need to go down to temperatures in the nK regime and to have occupations of few atoms per lattice site

**Figure 1.2:** Energy bands for potential depths  $V_0 = E_r$  (left),  $V_0 = 5E_r$  (center) and  $V_0 = 20E_r$  (right). We use the recoil energy of the atoms  $E_r$  as unit of energy, which is typically of the order of a few  $\mu K$ .



 $(\bar{n} \leq 4)$ , which coincides with current experiments [1, 2], to assume safely that only the ground state is populated.

#### 1.3 Many-body Hamiltonian: the Bose–Hubbard model

One of the great advantages of cold atoms in optical lattices is that the physical behavior of the atoms is usually perfectly well described by a simple underlying Hamiltonian, allowing us to use these systems as models for modern condensed matter theories. More precisely, a system of interacting bosonic particles in an optical lattice is very well described by the Bose–Hubbard Hamiltonian in second quantization [58]. In this section we sketch the derivation of this model<sup>§</sup> and although we specify it for bosons, the reasoning for a fermionic system follows in the same way.

The Hamiltonian of a bosonic gas in an optical lattice with contact interactions is

$$H = \int dx\psi(x)^{\dagger} \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) + V_{trap}(x) \right) \psi(x) + \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \psi(x)^{\dagger} \psi(x)^{\dagger} \psi(x) \psi(x)$$
(1.7)

where  $\psi(x)$  ( $\psi(x)^{\dagger}$ ) is the bosonic field operator that annihilates (creates) a particle at position x,  $a_s$  the s-wave scattering length and  $4\pi a_s \hbar^2/m$  the interaction strength between two atomic particles. Assuming, as discussed in the previous section, that neither the thermal excitations nor the interaction energy are able to take the atoms out of the lowest Bloch band of the optical lattice (figure 1.2), we can expand the field operators in terms of the Wannier functions (1.5) for the lowest energy band (n = 0)

$$\psi(x) \sim \sum_{i=1}^{L} a_i w_0(x - x_i).$$
(1.8)

Here,  $a_i$  is the operator annihilating a particle in site *i*, and *L* the total number of sites in the lattice. Then, expanding equation 1.7 in terms of equation 1.8, we can exploit the localized nature of the Wannier states  $w_0(x)$ . This means that we can neglect the interaction of particles at different sites and the tunneling to sites other than nearest neighbors, which are indeed from one to several orders of magnitude smaller than the on-site interaction and the nearest-neighbor tunneling amplitude [57]. The resulting Hamiltonian is the Bose–Hubbard model

$$H = \frac{U}{2} \sum_{i} n_i (n_i - 1) - j \sum_{\langle i,j \rangle} a_i^{\dagger} a_j.$$
(1.9)

In this notation we have that  $\langle i, j \rangle$  denotes the sum over nearest neighbors, including double counting, and  $n_i = a_i^{\dagger} a_i$  the number operator corresponding to site *i*. For simplicity, we have neglected the trapping potential  $V_{trap}(x)$ . Nevertheless, when working in the grand canonical ensemble, the chemical potential  $\mu$  plays a similar roll than this trapping potential. Having this additional trap is equivalent to use a chemical potential that starts

<sup>&</sup>lt;sup>§</sup>For similar detailed examples see section 5.2 and appendix D.2.

Figure 1.3: Representation of the parameters in the Bose–Hubbard model. The local interaction U is the energy required to add a particle to a site that is already occupied. The hopping amplitude j is the energy compensation for a particle tunneling to a neighboring site.



with some given value in the middle of the trap and decreases until it has dropped to zero towards the edges.

In the Hamiltonian (1.9), the first term corresponds to the potential energy of the system. This term is characterized by the on-site interaction energy

$$U = \frac{4\pi a_s \hbar^2}{m} \int dx |w_0(x)|^4$$
(1.10)

a parameter that tells us how much energy does it cost to put a second atom into a lattice site which is already occupied by another atom (see figure 1.3).

The second term in the Hamiltonian refers to the kinetic energy. This term is specified by the tunneling matrix element between adjacent sites

$$j = -\int dx w_0(x - x_i) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) w_0(x - x_{i+1}).$$
(1.11)

which is basically determined by the overlap between adjacent localized wavefunctions, giving the probability of tunneling while decreasing exponentially with the lattice depth.

To gain some qualitative insight into these parameters and their relation to experimental specifications, let us consider the limit where  $V_0 >> E_r$ . There, we can apply the harmonic approximation around the potential minima and replace the Wannier wavefunctions with Gaussians [124], obtaining

$$U = \sqrt{\frac{8}{\pi}} a_s k V_0^{1/4} V_{0\perp}^{1/2} E_r^{1/4}, \qquad (1.12a)$$

$$j = \frac{4}{\sqrt{\pi}} V_0^{3/4} E_r^{1/4} e^{-2\sqrt{V_0/E_r}}.$$
(1.12b)

Going back to the case of <sup>87</sup>Rb mentioned earlier, the interaction energy U may vary from 10kHz for shallow lattices to 16kHz for deeper ones. At the same time, the hopping amplitude j may nearly reach values of 2kHz for shallow lattices, decreasing dramatically to 10Hz for deeper ones.

Consequently, the properties of ultracold atoms in optical lattices depend only on the ratio between these two competing energies U/j (equivalently j/U may also be considered). This parameter U/j characterizes the strength of the interactions in relation to the tunnel coupling between neighboring sites, a quantity that is proportional to the potential



Figure 1.4: Schematic zerotemperature phase diagram of the Bose– Hubbard model in the grand canonical ensemble. Dashed lines in the SF region correspond to constant-integer density. For  $\langle n \rangle = 1, 2, 3$  these lines touch the corresponding MI phases at the tips of the lobes for some critical value of j/U. This critical ratio decreases with increasing the density  $\bar{n}$ . For  $\langle n \rangle = 1 + \epsilon$ the line of constant density stays outside the MI region because a fraction  $\epsilon$  of the particles remains superfluid down to the lowest values of j/U.

depth  $V_0$ . This makes the system controllable just through one parameter, the intensity of the laser used to create the lattice. The phenomenology is characterized by two limits. For a shallow lattice, U/j is small (~ 6 for <sup>87</sup>Rb) and equation 1.9 will be dominated by the kinetic energy term, yielding a *superfluid* ground state. Whereas for a deep lattice, U/j becomes large (~ 1600 for <sup>87</sup>Rb) and the Hamiltonian will be dominated by the interaction energy term, resulting in a *Mott insulating* ground state. These phases are explained in more detail as follows.

#### Phases of the Bose–Hubbard model

The Bose-Hubbard model was first introduced in [39], showing that it exhibits a quantum phase transition [93] from a superfluid (SF) to a Mott insulating (MI) phase at a critical value of the ratio j/U. In this passage we introduce these two phases, which are well described in the limiting cases of U = 0 and j = 0 at each side of the transition. We will also consider variations depending on the density of the system.

**Superfluid phase** In the case of an ideal gas  $j/U \to \infty$ , the interactions become unimportant and the atoms behave like independent particles. Each atom is completely delocalized over the entire lattice and, for periodic boundary conditions, the ground state of the system can be written as

$$|\psi_{SF}\rangle = \frac{1}{\sqrt{N!}} \left(\sum_{i=1}^{L} \frac{1}{\sqrt{L}} a_i^{\dagger}\right)^N |0\rangle \tag{1.13}$$

where N is the total number of particles in the lattice. Equation 1.13 is a coherent state  $\langle a_i \rangle \neq 0$  with a well defined phase for each lattice site. Its spectrum of excitations in the density is gapless, which means that it is compressible:  $\partial \bar{n}/\partial \mu \neq 0$ . This state is a superposition of different number states with a binomial atom number distribution per lattice site and thereof, nonzero number fluctuations  $\Delta n \neq 0$  are found.

A superfluid in 1D is also characterized by algebraically decaying long-range offdiagonal correlations  $\langle a_i^{\dagger}a_{i+\Delta}\rangle$  with the distance  $\Delta$ . This does not happen for equation 1.13, as these two-body correlations turn out to be constant in  $\Delta$ . This occurs because the ansatz (1.13) is only well suited to model a superfluid in 3D or in 2D, though the latter may only be a superfluid when the temperature is strictly zero. A true condensate at finite temperature can only occur in 3D, as it can be rigorously proofed¶ that Bose–Einstein condensation at T > 0 does not exist in 1D and 2D system, because thermal fluctuations destroy the long-range order that characterizes this state. Nevertheless, given that the decay of the correlations is power law, rather than exponential as in normal fluids, they are usually termed quasi-condensates. Whenever we use the term "condensate", whether we refer to a real condensate or to a quasi-condensate can be said from the context, *i.e.* the dimensionality of the system.

**Mott phase** In the opposite case  $j/U \rightarrow 0$ , the interactions dominate the physics of the system and the particles try to repel each other the best they can to minimize repulsion (we need U > 0 to avoid the collapse of the system), becoming completely localized to lattice sites. For commensurate filling the ground state of the system can be conveniently written as

$$|\psi_{MI}(\bar{n})\rangle = \prod_{i=1}^{L} \frac{1}{\sqrt{\bar{n}!}} \left(a_i^{\dagger}\right)^{\bar{n}} |0\rangle$$
(1.14)

where  $\bar{n} = N/L$  is an integer number and represents the particle occupation per site. This strongly correlated phase can be described by a Fock state with a well defined number of atoms per site and thereby, it has a vanishing number fluctuation  $\Delta n = 0$ . If the filling is not commensurate, the number of particles will vary from site to site, leading to a series of degenerate ground states for equivalent distributions (position of defects over a homogeneous background). In a Mott insulator there is no coherence  $\langle a_i \rangle = 0$ , as with a minimized number-uncertainty the phase-uncertainty is maximized. Moreover, as the system is now incompressible  $\partial \bar{n}/\partial \mu = 0$ , an energy gap of order U appears in the excitation spectrum. This means that in this case an energy has to be paid to introduce another particle into the system.

**Charge-density wave** When next-neighbor interactions are added to the Hamiltonian (1.9), *i.e.* a term like  $V \sum_{i} n_{i}n_{i+1}$ , a charge-density wave may appear in the system in the limit of large interactions U, |V| >> j. This phase has similar properties to a Mott insulator, only differing in the particle distribution. Depending on the value of the interaction strength V, and for integer or half-integer filling, we would obtain either one of two configurations: for V > 0 there could be alternating filled and unfilled lattice sites, while for V < 0 we could have alternating filled sites with one particle difference  $(n_{2i} = n^*$  and  $n_{2i+1} = n^* + 1$ , when  $\bar{n} = (2n^* + 1)/2$ ). Other non-integer fillings would give rise to similar states introducing defects, as mentioned before for the Mott insulator.

<sup>&</sup>lt;sup>¶</sup>The Mermin-Wagner-Hohenberg theorem [77, 56] shows that the mean number of excited quasiparticles of momentum  $\vec{k}$  in the gas at equilibrium at temperature T diverges in the infrared limit for any dimensionality  $D \leq 2$  unless the condensate fraction vanishes.



Figure 1.5: Visualization of a superfluid (up), where particles are delocalized over the whole lattice; a Mott insulator (center), where for commensurate filling the atoms are pinned to sites; and a charge-density wave (down), an insulator with an alternating filling factor. These phases are predicted by the Bose-Hubbard model in the limits  $j/U \rightarrow \infty$ ,  $j/U \rightarrow 0$  and, when considering nearest-neighbor interactions  $V, j/U, j/|V| \rightarrow 0$  respectively.

In our analysis we indistinguishably refer to two pictures: a system where the total number of particles is externally imposed; and the free energy or grand canonical picture, where the total number of particles is not fixed and the chemical potential is used as a lagrangian multiplier to fix it. Nevertheless, one should be aware that in the grand canonical ensemble it is not always possible to reproduce some states with incommensurate filling, precisely those which are insulating states (the Mott insulator and the chargedensity wave) presenting defects; but it does not mean that they would not appear in the real physical system.

## Chapter 2

## Description of theoretical methods

In this chapter we describe the methods used throughout this work to analyze the behavior of cold atoms in optical lattices in different parameter regimes. In general, these methods offer the possibility to calculate correlators and other expectation values, thereby permitting the characterization of the states.

We start with the analytical methods which are specifically shown for the Bose-Hubbard model (1.9), but their application to other cases will be presented eventually in other parts of this work when judged to be required. In general, solving an eigenvalue problem exactly is not possible: only for very few Hamiltonians we can find solutions in an analytical form. However, there are some approximation methods that in certain cases allow to obtain analytically approximate solutions of the eigenvalue equation. We introduce some of the analytical methods used to study cold atoms in optical lattices in regions of the parameter space where an exact solution cannot be found. Given the complexity of the system when it undergoes a phase transition, the analytical methods presented here are only reliable away from this point<sup>\*</sup>. For a better treatment of critical points, numerical methods will be required. Here, we first present the quantum rotor or phase model [76, 45], which becomes relevant in the case of systems with a high average occupation per site, either in the limit of strong or weak interactions. Then, the Mottphase diagram is obtained from a strong coupling expansion [42, 43]. This approximation to the phase boundaries is only valid in the limit of strong interactions U >> j, as it is a perturbation theory expansion around the incompressible regions when j = 0.

Then later, we continue with the numerical methods which are presented in a general framework and may be applied as well to other quantum lattice problems. We introduce some variational methods which can be implemented numerically, to find a mathematical description and a physical characterization of lattice systems in cases where an analytical treatment is no longer possible. This may happen due to the complexity of the problem, either in the presence of a phase transition or in the limit of a reasonably sized system. We start with the simplest of the methods treated here, the Gutzwiller ansatz [67]. This is a product state which gives a mean-field description of the system, being able to reveal some characteristics of its physical phases. In the case of a homogeneous system, it may be able to treat the limit of  $L \to \infty$ . Later on, we introduce an implementation of the more

<sup>\*</sup>There are other methods, as the renormalization group and the conformal field theory.

elaborated Density Matrix Renormalization Group method (DMRG) [112, 109] which is able to give us detailed information about phase transitions and correlations decay. Finally, we introduce the infinite Time-Evolving Block Decimation algorithm (iTEBD) [113] to study systems in the thermodynamic limit. Both DMRG and iTEBD are based on a Matrix Product State ansatz [111], which is also shortly introduced in this section.

#### 2.1 Quantum Rotor model: the phase approximation

In this section we move from the number occupation or Fock basis  $|\vec{n}\rangle$  to the basis of phase states  $|\vec{\phi}\rangle$ 

$$\left|\vec{n}\right\rangle \to \left|\vec{\phi}\right\rangle$$
$$\vec{n}\left|\vec{\phi}\right\rangle = \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{L/2}} \quad \text{with} \quad \vec{\phi} \in [-\pi,\pi]^{\otimes L}.$$
(2.1)

Here, the notation as vectors is used to collect the values of a variable at each site under one symbol, as to each site of the lattice corresponds an element of the vector (*e.g.*  $|\vec{\phi}\rangle = |\phi_1 \phi_2 \dots \phi_L\rangle$ ). It is interesting to work in the phase basis when the relevant physical states are concentrated around large occupation numbers,  $\langle n_i \rangle = \bar{n} >> 1$ , otherwise some non-physical states, as Fock states with negative particle number, would be also included. This is due to the symmetry of the phase interval in equation 4.1 with respect to zero. Throughout this section we have ignored the constant terms in the Hamiltonians.

We start with the Bose–Hubbard Hamiltonian in equation 1.9. Expanding the configuration of the lattice in Fock states  $\psi = \sum_{\vec{n}} c_{\vec{n}} |\vec{n}\rangle$  and considering as said, a large average number of particles per site, we may approximate the hopping term as

$$a_i^{\dagger} a_j |\psi\rangle = \sqrt{\bar{n}(\bar{n}+1)} \mathcal{P} A_i^+ A_j^- |\psi\rangle + |\Delta_{ij}\rangle$$
(2.2)

where  $A^{\pm}$  are ladder operators,  $A^{\pm} |n\rangle = |n \pm 1\rangle$ , and  $\mathcal{P}$  is the projector onto the states with non-negative occupation numbers, *i.e.* physical states. To the lowest order in the Taylor expansion the error  $|\Delta_{ij}\rangle$  is

$$|\Delta_{ij}\rangle = \sum_{\vec{n}} c_{\vec{n}} \frac{(\bar{n}+1)(n_i - \bar{n}) + \bar{n}(n_j - \bar{n})}{2\sqrt{\bar{n}(\bar{n}+1)}} |\vec{n}\rangle$$

and its norm is bounded by

$$||\Delta_{ij}|| \le \sqrt{\frac{\bar{n}^2 + (\bar{n}+1)^2}{2\bar{n}(\bar{n}+1)}}\sigma_j$$

where  $\sigma_i^2 = \langle (n_i - \bar{n})^2 \rangle$  is the dispersion in the number of particles in the *i*-th site. We observe that the validity of this approximation is restricted to the cases of lattices with a high mean number of particles per site  $\bar{n}$  and a small uncertainty compared to this average value,  $\sigma_i \ll \bar{n}$ . Besides, when applied to equation 1.9, the interaction energy must exceed the neglected terms in (2.2),  $U\bar{n}(\bar{n}-1) \gg j\sigma$ .

#### 2.1. Quantum Rotor model: the phase approximation

Following this procedure, we can rewrite our Hamiltonian (1.9) as

$$H = \mathcal{P}\sum_{i=1}^{L} \left[ -\varrho j (A_{i+1}^{+} A_{i}^{-} + A_{i}^{+} A_{i+1}^{-}) + \frac{U}{2} (A_{i}^{z})^{2} \right]$$
(2.3)

with  $\rho = \sqrt{\bar{n}(\bar{n}+1)}$  being approximately the density per site and  $A_i^z = a_i^{\dagger}a_i - \bar{n}$  the fluctuations of the number operator around the mean  $\bar{n}$ , having  $\sum_i A_i^z |\psi\rangle = 0$  for states with a fixed and commensurate filling.

Given that the physically interesting states are around large occupations, any contribution from negatively occupied states to the wavefunction of the system will be negligible. This allows us to safely drop the projector  $\mathcal{P}$  and move to the phase basis (4.1). To do this, we have to translate the operators from the Fock to the phase basis using the relation between these two

$$\left|\vec{\phi}\right\rangle = \sum_{\vec{n}} \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{M/2}} \left|\vec{n}\right\rangle \tag{2.4}$$

which derives from equation 4.1. The operators we need to rewrite the Hamiltonian (2.3) are the ladder operators

$$\begin{aligned} A_{j}^{\pm} |\vec{\phi}\rangle &= \sum_{\vec{n}} \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{M/2}} A_{j}^{\pm} |\vec{n}\rangle = \sum_{\vec{n}} \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{M/2}} |\vec{n}\pm 1_{j}\rangle \\ &= \sum_{\vec{n}} \frac{e^{i\vec{n}\mp 1_{j}\cdot\vec{\phi}}}{(2\pi)^{M/2}} |\vec{n}\rangle = e^{\mp i\phi_{j}} |\vec{\phi}\rangle, \end{aligned}$$
(2.5a)

and the deviation of the mean from the number operator

$$A_{j}^{z}|\vec{\phi}\rangle = \sum_{\vec{n}} \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{M/2}} A_{j}^{z} |\vec{n}\rangle = \sum_{\vec{n}} \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{M/2}} (n_{j} - \bar{n}) |\vec{n}\rangle$$
$$= \left(-i\frac{\partial}{\partial\phi_{j}} - \bar{n}\right) |\vec{\phi}\rangle.$$
(2.5b)

These equations lead us to the equivalent of Hamiltonian (2.3) in the phase basis

$$H = \sum_{i=1}^{L} \left[ -2\varrho j \cos(\phi_i - \phi_{i+1}) - \frac{U}{2} \frac{\partial^2}{\partial \phi_i^2} \right].$$
(2.6)

To minimize the energy in the limit of  $j \gg U$ , the wavefunction will concentrate around the equilibrium configuration where the phase at each site has the same value  $\phi_i \simeq \phi_j$ . In this range of parameters we are in the superfluid regime, where the phase fluctuations are small. Therefore it becomes reasonable to apply the harmonic approximation, expanding the cosine in equation 2.7 to first order in  $\phi_i - \phi_{i+1}$ 

$$H = \sum_{i=1}^{L} \left[ \varrho j (\phi_i - \phi_{i+1})^2 - \frac{U}{2} \frac{\partial^2}{\partial \phi_i^2} \right].$$
 (2.7)

In general, a state in this basis can be written as

$$|\psi\rangle = \frac{1}{(2\pi)^{L/2}} \int e^{i\vec{n}\cdot\vec{\phi}} \Psi(\vec{\phi}) |\phi\rangle \,\mathrm{d}\vec{\phi}$$
(2.8)

where  $\vec{n} \cdot \vec{\phi} = \bar{n} \sum_{j} \phi_{j}$  and  $d\vec{\phi} = d\phi_{1} d\phi_{2} \dots d\phi_{L}$ . The wavefunction  $\Psi(\vec{\phi})$  that is solution of equation 2.7 can only depend on the phase difference between neighboring sites  $\xi_{i} = \phi_{i} - \phi_{i+1}$ . In the limit of large lattices, we can assume that these differences are independent from each other and write the wavefunction as

$$\Psi(\vec{\phi}) = \prod_{i=1}^{L} f(\phi_i - \phi_{i+1}).$$
(2.9)

In the Mott insulating regime, when  $j/U \to 0$  and the phases are independent from each other, the appropriate solution is  $f_{MI}(\xi) = 1$  whereas in the superfluid limit, when  $j/U \to \infty$  and the phases tend to the same value, it is  $f_{SF}(\xi) = \sum_n \delta(\xi - 2\pi n)$ , where *n* are integer numbers. This can be checked by substitution in equation 2.8.

For other parameter values or variations from the simple Bose–Hubbard model, the solution (2.8) is not exact and a variational method should be use to identify the best fitting wavefunction. In the following chapters we will proceed differently. We will look for the normal modes of equation 2.7, with the help of a real discrete Fourier transform to decouple the variables, and use a Gaussian ansatz to find the optimal ground state of the system.

#### 2.2 Strong coupling expansion

In the limit of weak hopping  $j \ll U$  the boundaries to the superfluid phase can be calculated using perturbation theory around the insulating phases [42, 43]. Degenerate perturbation theory is a very standard approximation method in Quantum Mechanics, which is extensively explained in several textbooks, *e.g.* [23]. Its ubiquity in the field relies on the philosophy behind it: first solve the main part of the problem giving the dominating features and then the corrections given by weaker terms, for which perturbation theory is typically used.

Applied to our case, the boundary between the incompressible phase (MI) and the compressible phase (SF) is then determined when the energy difference between the Mott insulator and the defect state vanishes. With this, it is assumed that the compressibility  $\partial_{\mu}n$  approaches zero continuously at the phase boundary. The defect state may be either an additional hole or an additional particle in the system, giving the lower and upper branches of the Mott lobe respectively. Here, we apply this approximation method up to second order in the hopping amplitude j, computing the boundaries for the Mott insulator of one and two particles per site.

Following from equation 1.9 and still considering the case of homogeneous trapping, we separate H into two terms

$$H = H_0 + W \tag{2.10}$$



Figure 2.1: Three of the subspaces considered for the strong coupling expansion, those with a total of L - 1, L and L + 1 particles in the system, where L is the number of sites in the lattice. They correspond to the ground state configurations when j = 0, and it is around them that the perturbation is applied.

where  $H_0$  corresponds to a part that we know how to solve exactly, and W is a perturbation which together with  $H_0$  cannot be treated exactly. For the Bose–Hubbard Hamiltonian (1.9) we consider

$$H_0 = \sum_{i} \frac{U}{2} n_i (n_i - 1) - \mu \sum_{i} n_i$$
(2.11)

$$W = -\sum_{i} j \ (c_{i}^{\dagger} c_{i+1} + c_{i} c_{i+1}^{\dagger})$$
(2.12)

with the condition  $j \ll U$ . We want to study the modifications introduced by W in the well-known discrete set of energies and stationary states of  $H_0$  — note that  $H_0$  is already diagonal in the Fock basis. Furthermore, to emphasize the perturbation character of W, we will write it in general as  $W = \sum_x f_x(j) \hat{W}_x$  where  $f_x(j)$  are dimensionless parameters much smaller than 1.

As the eigenvectors  $|\psi_M^i\rangle$  of  $H_0$  belong to the Fock basis, they have a fixed and welldefined number of particles per site. Therefore, their corresponding eigenvalues  $E_M^i$  are grouped into well differentiated manifolds  $\mathcal{E}_M^0$ ,  $\mathcal{E}_{M+1}^0$ ..., where each of these manifolds corresponds to M, M + 1... particles in the lattice and the index *i* denotes a possible degeneracy according to the configurations of the particles

$$H_0 \left| \psi_M^i \right\rangle = E_M^i \left| \psi_M^i \right\rangle. \tag{2.13}$$

We define  $P_M$  as the projector over the manifold  $\mathcal{E}_M^0$ 

$$P_M = \sum_i \left| \psi_M^i \right\rangle \left\langle \psi_M^i \right|. \tag{2.14}$$

Adding W to our initial Hamiltonian  $H_0$  will not mix these manifolds, they will remain separate from each other because W does not contain terms connecting states with a different total number of particles. Therefore, the energy levels of H will be clustered as in  $H_0$ . This is also reflected in the fact that for both Hamiltonians H and  $H_0$ , the total number of particles N is a good quantum number. The consequence of this coupling will be an internal mixing of the states within the manifolds and a change in their energies.

Considering periodic boundary conditions, our problem acquires translational invariance and we have that states within the same subspace are degenerate. Therefore, in contrast to equation 2.13, for the unperturbed problem we have

$$H_0 \left| \psi_M^i \right\rangle = E_M \left| \psi_M^i \right\rangle \tag{2.15}$$

and we are looking for the solutions of the full problem

$$H\left|\psi_{M}^{i}(j)\right\rangle = E_{M}(j)\left|\psi_{M}^{i}(j)\right\rangle.$$
(2.16)

To be able to draw the phase diagram of our system as j grows, given by vanishing energy difference between the Mott insulators and the defect states, we will need to study the perturbation of the levels  $E_M$  for consecutive values of M.

We start assuming that the solutions for the energy of equation 2.16 can be expanded in powers of the parameter j

$$E_M(j) = E_M^{(0)} + jE_M^{(1)} + j^2 E_M^{(2)} + \dots$$
(2.17)

At zero order  $E_M(j)$  should approach  $E_M$  when j goes to zero, therefore we have that  $E_M^{(0)} = E_M$ . The first energy correction comes from solving the eigenvalue equation

$$\hat{W}_{x}^{(M)} |0\rangle = E_{M}^{1,x} |0\rangle \tag{2.18}$$

for each term in  $W = \sum_{x} f_x(j) \hat{W}_x$ , and summing up all contributions  $E_M^{1,x}$ . Here,  $\hat{W}^{(M)}$  is the restriction of the operator  $\hat{W}$  to the eigensubspace  $\mathcal{E}_M^0$  (corresponding to the eigenvalue  $E_M^{(0)}$ ) and the vector  $|0\rangle$  belongs to the space spanned by the unperturbed states  $|\psi_M^i\rangle$ . It is important here to remember that all the degenerate states  $|\psi_M^i\rangle$  are equivalent due to the translational invariance of system. The second energy correction has a more complicated expression

$$E_{M}^{2,x} = \sum_{p,i'} \frac{\langle \psi_{M}^{i} | \hat{W} | \psi_{M,p}^{i'} \rangle \langle \psi_{M,p}^{i'} | \hat{W} | \psi_{M}^{i} \rangle}{E_{M} - E_{M}^{p}}$$
(2.19)

where the summation over p corresponds to all those states that incorporate one excitation created by  $\hat{W}$ , and the possible indices i' are the degeneracies of those.

Application to Bose–Hubbard model For the sake of illustration, and also to compare with later results in this work, we will now sketch the strong coupling expansion for the Bose–Hubbard model. Let us consider the subspaces L - 1, L and L + 1, where the lowest energy states of  $H_0$  are those pictured in figure 2.1. Here, L is the total number of sites and as said, we are considering periodic boundary conditions. These unperturbed states are labeled as  $\{|\psi_{L-1}^i\rangle\}_{i=1,...L}, |\psi_L\rangle$  and  $\{|\psi_{L+1}^i\rangle\}_{i=1,...L}$ , with respective energies

$$E_{L-1} = 0, \ E_L = 0, \ E_{L+1} = U.$$
 (2.20)

The subspace  $\mathcal{E}_{L+1}^0$  ( $\mathcal{E}_{L-1}^0$ ) consists of the defect states: one particle per site except from one that is doubly occupied (empty), as shown in figure 2.1, so it is *L*-degenerate.

We are going to treat explicitly the subspace  $\mathcal{E}_{L+1}^{0}$ , while the others can be treated analogously. For the first energy correction, we have processes like the depicted in figure 4.2 (i), where the defect moves to a neighboring site and the resulting state is still in the same subspace  $\mathcal{E}_{L+1}^{0}$ . Therefore  $E_{L+1}^{1,x} = -2j$ , for all x. On the other hand, the second energy correction refers to processes of the type shown in figure 4.2 (ii). We proceed to calculate the actual value of that precise process using equation 2.19. The energy of



Figure 2.2: Possible processes in the perturbation of the subspace with L + 1 particles in the system. Note that for systems with L - 1 and L particles, only virtual processes like the pictured in (ii) are possible.

each configuration is calculated according to the Hamiltonian in the strong coupling limit (2.11)

$$E_{L+1} = U, \ E_{L+1}^1 = 2U \tag{2.21}$$

where the superscript <sup>1</sup> denotes p = 1 in equation 2.19, one of the excited states upon action of the hopping (2.12). The transition probability from the ground state to the excited level is calculated using equation 2.12

$$\left\langle \psi_{L+1,p}^{i'} \middle| W \middle| \psi_{L+1}^{i} \right\rangle = -\sqrt{2}j.$$
(2.22)

Putting equations 2.21 and 2.22 together according to equation 2.19, we have that the correction to this order is

$$\sum_{x} E_{L+1}^{2,x} = \sum_{p,i'} \frac{\left\langle \psi_{L+1}^{i} \middle| W \middle| \psi_{L+1,p}^{i'} \right\rangle \left\langle \psi_{L+1,p}^{i'} \middle| W \middle| \psi_{L+1}^{i} \right\rangle}{E_{L+1}^{0} - E_{L+1}^{p}} = -\frac{4j^{2}}{U}(L-1) - \frac{3j^{2}}{U} \qquad (2.23)$$

where the second term refers to the virtual process of a particle jumping to the doublyoccupied site and back, as in figure 4.2 (ii).

In a similar way, all other energies can be calculated for L - 1, L and L + 1 particles in the lattice

$$E_{L-1} = -2j - \frac{4j^2}{U}(L-1),$$
 (2.24a)

$$E_L = -\frac{4j^2}{U}L, \qquad (2.24b)$$

$$E_{L+1} = U - 4j - \frac{4j^2}{U}(L-1) - \frac{3j^2}{U}, \qquad (2.24c)$$

and as well for 2L - 1, 2L and 2L + 1 particles in the system

$$E_{2L-1} = U(L-1) - 4j - \frac{12j^2}{U}(L-1) - \frac{3j^2}{U}, \qquad (2.25a)$$

$$E_{2L} = UL - \frac{12j^2}{U}L,$$
 (2.25b)

$$E_{2L+1} = U(L+2) - 6j - \frac{12j^2}{U}(L-1) - \frac{8j^2}{U}.$$
 (2.25c)



**Figure 2.3:** Phase diagram of the Bose–Hubbard model using the strong coupling expansion. The first two Mott regions are drawn from an expansion to second order in the perturbation. The corresponding mathematical expressions are are shown on the right side. In the inset is the phase diagram by Freericks and Monien [43] using a third order strong-coupling calculation (solid). They compare their results with a fit to a Kosterlitz-Thouless form [43] (dotted) and the result of the quantum Monte Carlo calculation of Scalettar *et al.* [10] (circles). The inset of this figure is published with the kind permission of H. Monien.

We would like to remark that processes like the depicted in figure 4.2 (i) do not exist in  $\mathcal{E}_L^0$ , as it does not return to the unperturbed initial configuration  $|\psi_L^i\rangle$  after an application of any term of the perturbation  $\hat{W}_x$ .

With equations 2.24 and 2.25 we can calculate the boundary of the insulating regions to second order in the hopping strength j. For the insulator with M/L particles per site, the system becomes compressible at the point where the energy of the Mott state is degenerate with a defect state. Those points are the chemical potential at which a hole or a particle can be introduced,  $\mu_h(M) = E_M - E_{M-1}$  and  $\mu_p(M) = E_{M+1} - E_M$  respectively. The results for our case are shown in figure 2.3 and they are in agreement with the presented by Freericks and Monien in [42, 43]. We observe that for high values of the interaction strength, the system is a conductor wherever the compressibility becomes finite, as in the defect state there is an additional particle/hole that moves coherently through the lattice. As the hopping strength increases, the range of the chemical potential  $\mu$  about which the system is still incompressible decreases. Hence, for each value of  $\mu$ , the Mott insulator phase will completely disappear at some critical value of j and beyond this, the system is a superfluid.

#### 2.3 Mean-field approach: the Gutzwiller ansatz

The Gutzwiller ansatz [67] assumes that the state of a lattice system  $|\psi\rangle$  can be written as a product of possibly different functions  $|\psi_i\rangle$  describing the state of each corresponding site *i*
Given its product nature, at T = 0 mean-field theory is operationally equivalent to a Gutzwiller wavefunction calculation as the self-consistent condition is automatically fulfilled at each step of the minimization [99]. This type of ansatz can be easily generalized to higher dimensional systems and to inhomogeneous trapping potentials. Although its simplicity, and despite this approach cannot capture the correct behavior of the spatial quantum correlations, it provides a qualitatively satisfactory picture of the phases of strongly correlated systems, and thereof it has been used in many different studies [58, 59, 50, 37, 19].

Here we consider each of these  $|\psi_i\rangle$  written in the Fock basis

$$|\psi_i\rangle = \sum_{n=1}^N f_n^{(i)} |n\rangle \tag{2.27}$$

where N is the cutoff of the local Hilbert space, typically taken to be the same in all lattice sites, but not necessarily. Given a Hamiltonian H, the value of the ground state energy may be calculated as

$$E(\{f_n^{(i)}\}) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}, \qquad (2.28)$$

using  $|\psi\rangle$  from equation 2.26, and minimized as a function of the coefficients  $\{f_n^{(i)}\}$ , using the normalization constrain  $\sum_n |f_n^{(i)}|^2 = 1$  for all *i*. Normally, this optimization process is done numerically.

As already mentioned, a drawback of this method is that, approximating the state of the system by a product state cannot give us neither the decay of the correlations with distance nor precise information about the location of phase transition. Nevertheless, we are still able to calculate some correlation functions and this ansatz does give us a qualitative idea of the overall behavior of the system.

## 2.4 DMRG and the Matrix Product State algorithms

In this section we start introducing what the Matrix Product State ansatz is and its derivation through the Schmidt decomposition [111]. These states are the underlying structure of the Density Matrix Renormalization Group method [83, 109] and the infinite Time-Evolving Block Decimation algorithm [113], which will be also described in the following. The first is a numerical technique used to classically simulate some quantum many-body systems with unprecedented precision [86], based on the controlled truncation of the Hilbert space. The latter is specially well suited to deal with systems in the thermodynamic limit.

#### Matrix Product State ansatz

A general position-dependent Matrix Product State for a one-dimensional system of size L is defined as

$$|\psi\rangle = \sum_{s_1,\dots,s_L=1}^d Tr\left(A[1]^{s_1}A[2]^{s_2}\dots A[L]^{s_L}\right)|s_1,\dots,s_L\rangle$$
(2.29)

 $A[i]^{s_i}: \begin{array}{l} \text{Matrix associated to site } i \\ \text{and its state } s_i, \text{ whose} \\ \text{dimension is bounded by} \\ \text{some fixed number } D_i \times D_{i+1}. \\ \text{They parametrize the state.} \end{array}$ 

 $d: \begin{array}{c} \text{Dimension of the Hilbert} \\ \text{space corresponding to} \\ \text{the physical system.} \end{array}$ 

They conform a class of states that yields local descriptions of multipartite quantum states, giving a very good approximation with only a polynomial number of parameters in some 1D problems [107]. In the special case of open boundary conditions we have  $D_1 = D_{L+1} = 1$ .

An ansatz for slightly entangled states The approach we introduce here to derive MPS was proposed by Vidal in 2003 [111], and it was developed independently to other contemporary works [36, 109]. We will introduce it here because it is a generalization of [109] and it is the starting point for the infinite-size simulations [113] treated at the end of this section.

This is a particular decomposition<sup>†</sup> for the coefficients  $c_{s_1 \cdots s_L}$  of an arbitrary state written in the product basis  $|s_1\rangle \otimes \cdots \otimes |s_L\rangle$ 

$$|\psi\rangle = \sum_{s_1,\dots,s_L=1}^{d} c_{s_1\dots,s_L} |s_1\rangle \otimes \dots \otimes |s_L\rangle$$
$$c_{s_1s_2\dots,s_L} = \sum_{\alpha_1,\dots,\alpha_L} \Gamma[1]_{\alpha_1}^{s_1} \lambda[1]_{\alpha_1} \Gamma[2]_{\alpha_1\alpha_2}^{s_2} \lambda[2]_{\alpha_2} \Gamma[3]_{\alpha_2\alpha_3}^{s_3} \cdots \Gamma[L]_{\alpha_{L-1}}^{s_L}$$
(2.30)

which employs L tensors  $\{\Gamma[1], \ldots \Gamma[L]\}$  and L - 1 vectors  $\{\lambda[1], \ldots \lambda[L - 1]\}$ , whose indices  $s_i$  and  $\alpha_i$  take values in  $\{1, \ldots d\}$  and  $\{1, \ldots D_i\}$ , respectively. Contracting  $\Gamma \leftrightarrow \lambda$ or  $\lambda \leftrightarrow \Gamma$  together, the structure obtained can be readily identified with a Matrix Product State as in equation (2.29).

The optimal size of the tensors  $D_i$  is related to the von Neumann entropy  $S_i$  [80] of the partition  $1 \dots i : i + 1 \dots L$ , as  $S_i \leq 2 \log_d D_i$ . If this quantity is well-behaved, we would be able to represent our state efficiently with a number of parameters that grows linearly with the size of the system instead of exponentially, as when the full Hilbert space is used. This is the idea behind [111], where they show that any quantum computation with pure states can be efficiently simulated with a classical computer, provided that the amount of entanglement involved ( $\sim D_i$ ) is sufficiently restricted. Here we restrict to sketch the decomposition of the state.

In general, this decomposition can be found for all possible states. It consists of a concatenation of L - 1 Schmidt decompositions, and depends on the particular way the sites have been ordered from 1 to L. Here, we consider the systematic truncation of the Hilbert space, taking the first  $D_i$  Schmidt vectors in each partition<sup>‡</sup> to achieve an efficient description of the system in compromise with the computational resources. The procedure can be described as follows:

<sup>&</sup>lt;sup>†</sup>For simplicity, we describe it for open boundary conditions.

<sup>&</sup>lt;sup>‡</sup>An exact decomposition would keep all Schmidt vectors.

#### 2.4. DMRG and the Matrix Product State algorithms

1. do the first Schmidt decomposition of  $|\psi\rangle$  at the partition 1: 2...L, keeping the  $D_1$  first Schmidt vectors with highest Schmidt value

$$\begin{aligned} |\psi\rangle &= \sum_{\alpha_1=1}^{D_1} \lambda[1]_{\alpha_1} |\phi[1]_{\alpha_1}\rangle |\phi[2\dots L]_{\alpha_1}\rangle \\ &= \sum_{\underline{s_1},\alpha_1} \underline{\Gamma[1]_{\alpha_1}^{s_1}} \lambda[1]_{\alpha_1} |\underline{s_1}\rangle |\phi[2\dots L]_{\alpha_1}\rangle \end{aligned}$$

where we have  $\underline{expanded}$  each Schmidt vector for site 1 in terms of a local-space basis.

2. expand each Schmidt vector  $|\phi[2...L]_{\alpha_1}\rangle$  in a local-space basis for site 2

$$|\phi[2\dots L]_{\alpha_1}\rangle = \sum_{s_2} |s_2\rangle |\tau[3\dots L]_{\alpha_1 s_2}\rangle$$

3. write  $|\tau[3...L]_{\alpha_1 s_2}\rangle$  in terms of at most  $D_2$  Schmidt vectors corresponding to the partition  $1 \ 2 : 3 \dots L$  for the second half<sup>§</sup>

$$|\tau[3\dots L]_{\alpha_1 s_2}\rangle = \sum_{\alpha_2=1}^{D_2} \Gamma[2]_{\alpha_1 \alpha_2}^{s_2} \lambda[2]_{\alpha_2} |\phi[3\dots L]_{\alpha_2}\rangle$$

4. substitute this in the previous decomposition of  $|\psi\rangle$  to obtain

$$|\psi\rangle = \sum_{\substack{s_1, s_2 \\ \alpha_1, \alpha_2}} \Gamma[1]_{\alpha_1}^{s_1} \lambda[1]_{\alpha_1} \Gamma[2]_{\alpha_1 \alpha_2}^{s_2} \lambda[2]_{\alpha_2} |s_1 s_2\rangle |\phi[3 \dots L]_{\alpha_2}\rangle.$$

Iterating these steps for the Schmidt vectors  $|\phi[3...L]_{\alpha_2}\rangle$ ,  $|\phi[4...L]_{\alpha_3}\rangle$ , ...  $|\phi[L]_{\alpha_{L-1}}\rangle$  one can finally express  $|\psi\rangle$  as

$$|\psi\rangle = \sum_{\substack{s_1\cdots,s_L\\\alpha_1\cdots,\alpha_{n-1}}} \Gamma[1]^{s_1}_{\alpha_1}\lambda[1]_{\alpha_1}\Gamma[2]^{s_2}_{\alpha_1\alpha_2}\lambda[2]_{\alpha_2}\Gamma[3]^{s_3}_{\alpha_2\alpha_3}\cdots\Gamma[L]^{s_L}_{\alpha_{L-1}}|s_1\cdots s_L\rangle$$

which corresponds exactly to the decomposition given in equation 2.30.

When such a decomposition uses  $D \sim D_i$  Schmidt vectors at each step such that  $dLD^2 << d^L$ , this description results in a great improvement for classical simulations. In that case, only poly(L) parameters are required to represent the state  $|\psi\rangle$ , instead of the  $d^L$  coefficients  $c_{s_1\cdots s_L}$  needed for the full expansion in the computational basis.

<sup>&</sup>lt;sup>§</sup>We can do this because  $\{|\tau[3...L]_{\alpha_1 s_2}\rangle\} \in span\{|\phi[3...L]_{\alpha_2}\rangle\}.$ 

### Density Matrix Renormalization Group algorithm: optimization of Matrix Product States

Density Matrix Renormalization Group [118, 119] (DMRG) is a numerical technique for finding accurate approximations of the ground state and the low-lying excited states of strongly interacting quantum lattice systems. It traces its roots to Wilson's numerical renormalization group (RG) treatment of the impurity problem [122] and it is weakly related to real space renormalization groups [108]. The accuracy of this method, just employing a modest amount of computational effort, is remarkable for 1D systems and it is limited by the dimensionality or range of the interaction. This fact was already noticed by Östlund et al. [83] who for White's infinite algorithm [118, 119], established DMRG's mathematical foundations in terms of the MPS. The standard DMRG method was originally introduced in a partially *ad hoc* manner, without fully understanding the reasons of its success, but with MPS there exists now a coherent theoretical picture of it which underlies Quantum Information Theory concepts [109].

DMRG is closely related to exact diagonalization methods and to Wilson's numerical Renormalization Group. They may be seen to form a chain of improvements on top of each other, as described in the following:

- **Exact Diagonalization** gives an exact solution, but the maximum system size that can be treated is severely limited by the exponential growth of the Hilbert space with the number of particles in the system. To circumvent this drawback, one would require the formulation of a variational diagonalization scheme that also truncates the Hilbert space used to represent the Hamiltonian in a controlled way.
- Wilson's Numerical Renormalization Group implements this idea progressively integrating out unimportant degrees of freedom, using a succession of renormalization group (RG) transformations, where only the low-energy eigenstates obtained for a system of size L will be important in making up the low-energy states of a system of size L + 1. The process could be described as:
  - a) we start with a block of length L and its m (some prefixed number) lowest energy eigenstates, determined in some previous steps, as an approximate basis

 $L \qquad \{|\psi_j\rangle\}_{j=1\dots,m}$ 

In the initial step, L is small enough to exactly diagonalize the Hamiltonian.

b) we add a new site to the block



Our basis is then  $\{ |\psi_j\rangle |i\rangle \}$ .

c) we project our enlarged basis onto a subspace of dimension m, keeping the lowenergy states of the system and recovering again a small basis

$$L+1 \qquad \{|\tilde{\psi}_j\rangle\}_{j=1\dots,m}$$

The truncation scheme is iterated.

How to treat the boundaries of the isolated block after its enlargement is crucial in formulating an accurate RG procedure, and it has been the main problem for Wilson's method. In the case of interacting systems, this could be solved at best by embedding the block of interest in a larger superblock. At this point a dilemma arises, as one state of the superblock can, in general, project onto many states of the system block.

**Density Matrix Renormalization Group** chooses an optimal way to do this projection. After the enlargement of the block (step b in Wilson's method), it proceeds introducing an environment block, which is the mirror image of the enlarged block, as it is assumed to have reflection symmetry,



The result is what is called the superblock. The reduced density matrix of the enlarged system (not the whole superblock) is built and its most probable eigenstates are kept as the new basis. This last step is the so-called density matrix projection. The whole procedure is iterated until the quantities of interest, computed at every step, have converged to the desired accuracy.

DMRG can be formulated as a variational method within the class of MPS [83, 109]. The calculation of the energy  $\langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$  for a Hamiltonian H with nearest-neighbor interactions leads to a multiquadratic function of the matrices A[i] defining the MPS, which can be solved using the standard technique of alternating least squares to do the minimization. More in detail, this is done by first fixing all the matrices but the one for site j and writing the effective Hamiltonian for that site H[j], which includes the rest of the matrices A[i] with  $i \neq j$  (see equation A.9)

$$E(A[j]) = \frac{\vec{A}[j]^{\dagger} H[j] \vec{A}[j]}{\vec{A}[j]^{\dagger} \vec{A}[j]}.$$
(2.31)

Then, the minimization is done at each of these sites, sweeping back and forth over all lattice sites i until the desired convergence is achieved. At the end one obtains the set of matrices A[i] defining the ground state of the system.

In practice, the convergence of this method is excellent [68, 107]. A detailed description of the algorithm in terms of MPS can be found in appendix A.

#### Infinite Time-Evolving Block Decimation algorithm

The infinite Time-Evolving Block Decimation algorithm (iTEBD) [113] simulates 1D quantum lattice systems in the thermodynamic limit. The attainment of this limit is important to study bulk properties of matter, avoiding finite-size corrections and boundary effects. To introduce iTEBD we will first describe the Time-Evolving Block Decimation algorithm (TEBD) [112], as it gives the basis for the infinite-size extension.

**Time-Evolving Block Decimation algorithm** allows the simulation of quantum manybody dynamics [112] using a MPS like equation 2.30.



Figure 2.4: Schematic representation of two steps of the iTEDB algorithm in a constrained region of the lattice. After each application of the time evolution operator  $U^{AB}$  ( $U^{BA}$ ) the matrices  $\Gamma^A$ ,  $\Gamma^B$  and  $\lambda^A$ ( $\Gamma^A$ ,  $\Gamma^B$  and  $\lambda^B$ ) have to be updated, which is indicated here with a tilde.

For example, consider that we want to calculate the state  $|\psi_t\rangle$ , obtained as the time evolved state of  $|\psi_0\rangle$  according to the Hamiltonian H

$$\psi_t \rangle = e^{-iHt} \left| \psi_0 \right\rangle \tag{2.32}$$

where H contains only local and nearest-neighbor interactions. The main idea of TEBD is to separate the Hamiltonian describing the dynamics of the 1D system  $H = \sum_{i} h^{[i,i+1]}$  into its even and odd terms H = F + G, where by even we mean  $F = \sum_{i} h^{[2i,2i+1]}$  and by odd  $G = \sum_{i} h^{[2i-1,2i]}$ . Note that the terms within one partition act on different sites and thus commute with each other  $[h^{[i,i+1]}, h^{[i',i'+1]}] = [h^{[2i-1,2i]}, h^{[2i'-1,2i']}] = 0$ .

We approximate the time evolution operator in equation 2.32 using a Suzuki-Trotter expansion of order p for small  $\delta > 0$  [102]

$$e^{-iHt} = [e^{-i(F+G)\delta}]^{t/\delta} \simeq [f_p(e^{-iF\delta}, e^{-iG\delta})]^{t/\delta}$$

This approximates the time evolution operator by a product of  $\mathcal{O}(t/\delta)$  N-body transformations, which can be expressed as a product of the two-sites operators  $e^{-ih^{[2i,2i+1]}\delta}$  and  $e^{-ih^{[2i-1,2i]}\delta}$ .

The time evolution in equation 2.32 is then accomplished by iteratively applying the operators  $e^{-iF\delta}$  and  $e^{-iG\delta}$  a number of  $\mathcal{O}(t/\delta)$  times to the initial state  $|\psi_0\rangle$ , which has been previously decomposed in the form of equation 2.30. After the application of each operator at sites i and i + 1 the decomposition (2.30) has to be updated, involving at each step only the transformation of the tensors  $\Gamma[i], \lambda[i]$  and  $\Gamma[i + 1]$  [111].

In the case of an infinite chain which is translational invariant, the state can be written in the form of equation 2.30 with  $\Gamma[i]$  and  $\lambda[i]$  independent of *i*. Thus, given that the time evolution is generated by two-sites operators

$$U^{AB} = \bigotimes_{i} e^{-iF[2i,2i+1]\delta}, \ U^{BA} = \bigotimes_{i} e^{-iG[2i-1,2i]\delta}$$
(2.33)

the representation is chosen to be of the form

$$\Gamma[2i] = \Gamma^A, \ \lambda[2i] = \lambda^A \tag{2.34}$$

$$\Gamma[2i+1] = \Gamma^B, \ \lambda[2i+1] = \lambda^B \tag{2.35}$$

taking only explicit invariance under shifts by two sites. For  $L \to \infty$ , the action of  $U^{AB}$  and  $U^{BA}$  preserves the invariance of the evolved state under these shifts. As a consequence, only tensors  $\Gamma^A, \Gamma^B, \lambda^A$  and  $\lambda^B$  need to be updated, having a reduction in the cost of the simulation by a factor of L in comparison to the simulation of finite systems.

The computation of the ground state is achieved by simulating an evolution in imaginary time, where the two-sites unitary gates  $U_{AB}$  and  $U_{BA}$  are replaced by the non-unitary gates

$$U^{AB} = \bigotimes_{i} e^{-F[2i,2i+1]\delta}, \ U^{BA} = \bigotimes_{i} e^{-G[2i-1,2i]\delta}$$
(2.36)

using  $\delta t \ll 1$  to minimize the errors introduced by a non-unitary evolution. The state should also be normalized adequately.

Atoms in a noisy environment

# Chapter 3

# The physical system for dissipation

## **3.1** A mathematical toolbox for dissipative systems

#### Master equation formalism

The master equation describes the time evolution of a system that is coupled to an environment, while this coupling induces in the system a dynamic that is in general not coherent [116, 47, 20]. The description is given in terms of the reduced density matrix of the system and the master equation governs the time evolution of probabilities (diagonal elements of the density matrix) and of variables containing information about quantum coherence between the states of the system (non-diagonal elements of the density matrix).

**Derivation of the master equation** To derive this equation, we consider that the system S we want to study is coupled to a reservoir R through a weak interaction V. System and environment are modeled by the Hamiltonians  $H_S$  and  $H_R$ , respectively. The full Hamiltonian describing the dynamics has the following form

$$H = H_S + H_R + V. \tag{3.1}$$

If  $\omega(t)$  is the density operator of the total system S + R, its evolution in the interaction picture<sup>\*</sup> with respect to the free Hamiltonian  $H_S + H_R$  is dictated by

$$\frac{d\omega(t)}{dt} = -\frac{i}{\hbar} [V(t), \omega(t)]$$
(3.2)

and we are interested in the evolution of the reduced density operator of the system

$$\rho(t) = Tr_R[\omega(t)]. \tag{3.3}$$

We consider that initially between the system and the reservoir there are no correlations, as they had not been in contact before

$$\omega(0) = \rho(0) \otimes \rho_R(0). \tag{3.4}$$

<sup>\*</sup>We want to see the effect of the small perturbation on the state of the system.

With this ingredients, we are going to derive the Markovian<sup>†</sup> non-unitary evolution of the system.

Integrating the evolution equation for the total system (3.2), we obtain a formal solution for the density matrix

$$\omega(t) = \omega(0) - \frac{i}{\hbar} \int_0^t dt_1[V(t_1), \omega(t_1)].$$
(3.5)

This recurrent integral equation for  $\omega(t)$  can be indefinitely iterated, inserting it as the solution for the  $\omega(t_1)$ ,  $\omega(t_2)$ , ... appearing in the commutator of the integral. The solution may now be written as

$$\omega(t) = \omega(0) + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \\ \int_0^{t_{n-1}} dt_n [V(t_1), [V(t_2), \dots [V(t_n), \omega(0)] \dots ]].$$
(3.6)

Then, to obtain the state of the system S, we trace out the modes of the bath as in (3.3)

$$\rho(t) = \rho(0) + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \\
\int_0^{t_{n-1}} dt_n Tr_R[V(t_1), [V(t_2), \dots [V(t_n), \rho(0) \otimes \rho_R(0)] \dots]] \\
= [1 + U_1(t) + U_2(t) + \dots] \rho(0) = U(t)\rho(0)$$
(3.7)

where in the last equality we have defined the operators giving the weak coupling expansion of the master equation

$$U_i(t)[\cdot] = \left(-\frac{i}{\hbar}\right)^i \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{i-1}} dt_i Tr_R[V(t_1), [V(t_2), \dots [V(t_i), (\cdot) \otimes \rho_R(0)] \dots]].$$

Using these operators, we can write the exact evolution of the density operator  $\rho(t)$  as

$$\frac{d\rho(t)}{dt} = [\dot{U}_1(t) + \dot{U}_2(t) + \dots] U(t)^{-1}[\rho(t)] = \mathcal{L}(t)[\rho(t)]$$
(3.8)

where  $\mathcal{L}(t)$  is the generator of the temporal evolution, the so-called Liouvillian.

To be able to evaluate the trace of  $\omega(t)$  (3.7) over the reservoir degrees of freedom, we need to know how the reservoir evolves under the influence of the coupling. We are going to assume that the *bath relaxes much faster* than the system. This is reasonable when the reservoir is very big, much bigger than the system, having an immense number of degrees of freedom. As a result, the correlation time of the reservoir  $t_{res}$  is very small compared with  $t_{damp}$ , the characteristic time scale of the system evolving under dissipation; meaning that the system looses all memory of its past. This is known as the "first Markovian

<sup>&</sup>lt;sup>†</sup>Local in time.

approximation". Considering that the reservoir is much bigger than the system, we can assume that the changes in the reservoir are negligible ( $\rho_R(t) \simeq \rho_R(0)$ ) and that it is always in thermal equilibrium. This is the so-called "Born approximation"

$$\omega(t) = \rho(t) \otimes \rho_R(0) + \rho_{correl} \tag{3.9}$$

where, following from the Markov approximation,  $\rho_{correl}$  is negligible. Given that the bath is at finite temperature, it does not have quantum fluctuations. As a result, it cannot excite quantum fluctuations in the system. There are only thermal fluctuations, but these are negligible at first order. Thereof, we assume that the coupling between the system and the reservoir is such that

$$Tr_R[V(t), \rho_R(0)] = 0.$$
 (3.10)

This condition ensures that  $U_1(t)$  vanishes. Moreover, if the *perturbation to the system is weak*, we can neglect the terms of order greater than two in equation 3.8 and approximate the Liouvillian as

$$\mathcal{L}(t)[\cdot] = \dot{U}_2(t)[\cdot] = -\frac{1}{\hbar^2} \int_0^t dt_1 T r_R[V(t), [V(t_1), (\cdot) \otimes \rho_R(0)]]$$
(3.11)

where the next correction is at least of fourth order in the coupling.

Hence, the evolution of our system under the effect of dissipation through a reservoir can be described as

$$\frac{d\rho(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt_1 Tr_R[V(t), [V(t_1), \rho(t) \otimes \rho_R(0)]] = \mathcal{L}[\rho], \qquad (3.12)$$

that is the master equation for the system S. The assumptions taken to obtain this expression are the standard ones taken in quantum optics [116, 47, 20].

#### Heisenberg equations of motion

The general equation of motion for a system operator; or in other words, the time evolution of the mean value of some system observable A

$$\langle A \rangle(t) = Tr_S[A\rho(t)], \qquad (3.13)$$

can be easily calculated applying the chain rule for derivation to  $\langle A \rangle(t)$  and using conveniently the master equation of the system.

Applying the derivative, we have

$$\frac{d}{dt}\langle A\rangle(t) = Tr_S \left[ A \frac{d\rho(t)}{dt} \right] + Tr_S \left[ \frac{dA}{dt} \rho(t) \right]$$
(3.14)

where the second term denotes the possibility of an implicit time dependency of the operator. In the first term of equation 3.14, we can substitute  $d\rho(t)/dt$  by the master equation

$$\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H_S, \rho(t)] + \mathcal{L}[\rho(t)].$$
(3.15)

In equation 3.15 we have separated explicitly the coherent part of the evolution for a closed system, the term with the commutator; and the incoherent evolution, typical of an open system and described by the Liouvillian. Combing equations 3.14 and 3.15, we obtain

$$\frac{d}{dt} \langle A \rangle(t) = Tr_{S} \left[ A \frac{d\rho(t)}{dt} \right] + Tr_{S} \left[ \frac{dA}{dt} \rho(t) \right]$$

$$= \frac{1}{i\hbar} Tr_{S} \left[ Tr_{S} [H_{S}, \rho(t)] A \right] + Tr_{S} \left[ \mathcal{L}[\rho(t)] A \right] + Tr_{S} \left[ \frac{dA}{dt} \rho(t) \right]$$

$$= \frac{1}{i\hbar} Tr_{S} \left[ [A, H_{S}] \rho(t) \right] + Tr_{S} \left[ \mathcal{L}[\rho(t)] A \right] + Tr_{S} \left[ \frac{dA}{dt} \rho(t) \right]. \quad (3.16)$$

The first and last terms refer solely to the free evolution of the system, they form the so-called "Ehrenfest's theorem" for closed systems. Equation 3.16 is the generalization of this theorem to open systems. This equation allow us to describe the dynamics of a system undergoing dissipation, through the calculation of relevant correlators<sup>‡</sup> to infer their behavior.

## **3.2** A Hamiltonian with dissipation

Consider a set of repulsively interacting bosonic cold atoms sitting in a 1D lattice, described by the Bose–Hubbard Hamiltonian (1.9)

$$H_{S} = \sum_{i=1}^{L} \left[ -j \left( a_{i+1}^{\dagger} a_{i} + a_{i}^{\dagger} a_{i+1} \right) + \frac{U}{2} n_{i} \left( n_{i} - 1 \right) \right].$$
(3.17)

This system S is embedded in a larger reservoir R, as depicted in figure 3.1, and these two interact in some way that will be specified later. We consider that the reservoir is a set of 1D optical lattices, orthogonal to system S, and trapping atoms in a different internal state, described as well by the Bose–Hubbard model

$$H_{R} = \sum_{i=1}^{L} H_{R}^{(i)} = \sum_{i=1}^{L} \sum_{k=1}^{L'} \left[ -j' \left( b_{ik+1}^{\dagger} b_{ik} + b_{ik}^{\dagger} b_{ik+1} \right) - j'' \left( b_{i+1k}^{\dagger} b_{ik} + b_{ik}^{\dagger} b_{i+1k} \right) + \frac{U'}{2} n_{ik}^{b} \left( n_{ik}^{b} - 1 \right) \right].$$
(3.18)

The operators used in equations 3.17 and 3.18 are the number operators for the system  $n_i = a_i^{\dagger} a_i$  and the reservoir  $n_{ik}^b = b_{ik}^{\dagger} b_{ik}$ , where  $a_i^{\dagger} (a_i)$  is the creation (annihilation) operator of atoms at the *i*-th site of the system, and  $b_{ik}^{\dagger} (b_{ik})$  the corresponding operators at the *k*-th site of the reservoir associated with *i*-th site of the system. Here, *j* and *U* represent the hopping and on-site interaction for the atoms in the system, j' and U' are the tunneling amplitude and interaction strength in the reservoir transverse tubes, while j'' is the hopping between these latter tubes. In our notation, *L* is the number of lattice

<sup>&</sup>lt;sup>‡</sup>In the context of cold atoms in optical lattices, they could be  $\langle n_i \rangle$ ,  $\langle a_i^{\dagger} a_{i+\Delta} \rangle$ , etc.



Figure 3.1: Schematic drawing for a system with dissipation in three different configurations: independent baths with number dissipation (left), independent baths with phase dissipation (center), and shared baths with number dissipation (right). The lattice sites of the system are shown in green and those of the reservoir in violet, where particles interact with a strength U and U', respectively. Black and gray lines indicate the possibility of tunneling between sites with an amplitude j (black), j' (dark gray), and j'' (light gray). At the crossing points, the colored lines indicate that the system and reservoir interact with a strength V, either through the exchange of particles (green) or collisions (orange).

sites in the system, and it is small compared to L', the number of sites in the reservoir in the orthogonal direction to the system axis. As usual, we consider periodic boundary conditions for both parties.

The atoms from the system and reservoir interact locally at the intersecting points of both chains according to an interaction Hamiltonian  $H_{SR}$ . As shown in figure 3.1, we will consider exchange of particles (left), collisions (center) and exchange of particles with shared baths (right), which are further described in section 3.2. All these kind of interactions are regarded to be the same for all lattice sites. In this way, the reservoir we consider may introduce irreversibilities in the system, through the exchange of particles or collisions. Nonetheless, whenever j'' = 0 and independent reservoirs are considered, coherences in the system cannot be established through the bath.

We want to focus our study on the properties of the main chain. Therefore, we will either study the complete evolution of the system and the environment, tracing afterwards the degrees of freedom of the latter, or describe directly our system using the master equation formalism.

#### Decoherence mechanisms

Now, we introduce the interaction mechanisms considered in this work, which have been already sketched in figure 3.1: collisions or phase dissipation, and the exchange of particles or number dissipation. This latter is developed for individual and shared baths between consecutive system sites. **Phase dissipation** Dissipation of the phase means that the particles of both parties, S and R, collide against one another, and this contact interaction should presumably lead to a loss of coherence

$$H_{SR} = V \sum_{i} n_i n_{i0}^b.$$
 (3.19)

This implies that the particles of the system  $(n_i)$  meet the ones of the reservoir  $(n_{i0}^b)$  at the points where these two systems overlap, interacting at a rate or strength V, as illustrated in figure 3.1 (center). We derived the Liouvillian for this process, as shown in appendix B, obtaining

$$\mathcal{L}_{\phi} = \frac{\gamma}{2} \sum_{i} \left\{ -n_i^2 \rho - \rho n_i^2 + 2n_i \rho n_i \right\}.$$
(3.20)

where  $\gamma$  is the damping rate (see equation B.17).

**Number dissipation** Dissipation in the number of particles means that there is an exchange of particles between the system and the reservoir, taking place at the points where they overlap at a rate or strength V. This is depicted in figure 3.1 (left) and it is described by the interaction Hamiltonian

$$H_{SR} = V \sum_{i} \left( a_{i}^{\dagger} b_{i0} + b_{i0}^{\dagger} a_{i} \right)$$
(3.21)

where the creation of a particle in the system  $(a_i^{\dagger})$  implies the destruction of another in the reservoir  $(b_{i0})$ , and vice versa. Deriving the Liouvillian for this interaction, as shown in appendix B, we obtain

$$\mathcal{L}_n = \frac{\gamma}{2} \sum_i \left\{ (N+1)(2a_i\rho a_i^{\dagger} - a_i^{\dagger}a_i\rho - \rho a_i^{\dagger}a_i) + N(2a_i^{\dagger}\rho a_i - a_ia_i^{\dagger}\rho - \rho a_ia_i^{\dagger}) \right\}$$
(3.22)

where  $\gamma$  is the damping rate (see equation B.17).

If we consider shared baths between neighboring sites, as shown in figure 3.1 (right), the operator  $a_i$  must be substituted by  $a_i + a_{i+1}$  in equation 3.21, as in this situation each of the baths interacts with the two nearest sites of the system. This results in an interaction Hamiltonian

$$H_{SR} = V \sum_{i} \left( (a_i + a_{i+1})^{\dagger} b_{i0} + b_{i0}^{\dagger} (a_i + a_{i+1}) \right).$$
(3.23)

Consequently, this substitution should be also done in equation 3.22, leading to the Liouvillian

$$\mathcal{L}_{n,shared} = \frac{\gamma}{2} \sum_{i,i'} \left\{ (N+1)(2(a_i+a_{i+1})\rho(a_{i'}+a_{i'+1})^{\dagger} - (a_i+a_{i+1})^{\dagger}(a_{i'}+a_{i'+1})\rho - \rho(a_i+a_{i+1})^{\dagger}(a_{i'}+a_{i'+1}) + N(2(a_i+a_{i+1})^{\dagger}\rho(a_{i'}+a_{i'+1}) - (a_i+a_{i+1})(a_{i'}+a_{i'+1})^{\dagger}\rho - \rho(a_i+a_{i+1})(a_{i'}+a_{i'+1})^{\dagger}) \right\}$$
(3.24)

where  $\gamma$  is the damping rate (see equation B.17).

# Chapter 4

# Description of theoretical results

We already know the behavior of ultracold atoms in optical lattices when there is no dissipation in the system ( $H_{SR} = 0$ ), as it corresponds to the Bose–Hubbard model presented in section 1.3. In this chapter we are now going to study the influence of dissipation on this model, or more precisely the effect of some dissipative processes on its phase diagram.

Let us recall that the Bose–Hubbard model presents mainly two phases, the superfluid in the limit j/U >> 1 and the Mott insulator when j/U << 1. The first methods of this chapter focus on distinct regimes. To study the superfluid region, in section 4.1 we introduce the phase and harmonic approximations, for contact (3.19) and exchange (3.21) interactions. After using these approximations, the problem can be solved applying a real Fourier transform to the variables and the state of the system is finally characterized through its reduced density matrix. To study the effect of the contact interaction (3.19) on the Mott-phase diagram, in section 4.2 we implement a strong coupling expansion to second order in the dissipation strength and the hopping amplitudes. For a general overview, in section 4.3 we consider a mean-field approach to study the complete phase diagram in the case of contact interaction (3.19), using a Gutzwiller ansatz.

# 4.1 Applying the Quantum Rotor model to a dissipative system

In this section we use the approximations introduced in section 2.1 for the Bose– Hubbard model, to describe our system in the limit of large hopping amplitudes j, j'and j''. Similarly as done there, we move from the Fock basis of the system  $|\vec{n}\rangle$  and the reservoir  $|\vec{n}^b\rangle$  to their basis of phase states  $|\vec{\phi}\rangle$  and  $|\vec{\xi}\rangle$ , respectively,

$$|\vec{n}\rangle \to \left|\vec{\phi}\right\rangle, \ |\vec{n}^b\rangle \to \left|\vec{\xi}\right\rangle$$
where  $\left\langle \vec{n}|\vec{\phi}\right\rangle = \frac{e^{i\vec{n}\cdot\vec{\phi}}}{(2\pi)^{L/2}}$ , with  $\vec{\phi} \in [-\pi,\pi]^{\otimes L}$  (4.1a)

and 
$$\left\langle \vec{n}^{b} | \vec{\xi} \right\rangle = \frac{e^{i\vec{n}^{b} \cdot \vec{\xi}}}{(2\pi)^{L'/2}}$$
, with  $\vec{\xi} \in [-\pi, \pi]^{\otimes L'}$ . (4.1b)

In this notation, as in section 2.1, to each site of the lattice corresponds an element of a given vector. For example,  $\phi_k$  is the phase corresponding to the k-th site of the main chain, and  $\xi_{kj}$  is the phase variable corresponding to the j-th site at the k-th chain of the bath.

Also as in section 2.1, throughout this section we ignore the constant terms in the Hamiltonians. We would also like to emphasize that it is interesting to work in the phase basis when the relevant physical states are concentrated around large occupation numbers  $(\bar{n}, \bar{n}^b >> 1)$ . Otherwise, some non-physical states, as Fock states with negative particle number, could be also included due to the symmetry of the phase intervals (equations 4.1) with respect to zero.

#### Hamiltonian for the full model

Our full Hamiltonian  $H = H_S + H_R + H_{SR}$  is composed by the free evolution of the system  $H_S$  (3.17), that of the reservoir  $H_R$  (3.18), and either the contact or the exchange interaction between them  $H_{SR}$  (3.19, 3.21). In the limit of large densities and weak interactions, as introduced in section 2.1, replacing the operators  $a_i$  ( $b_{ij}$ ) by the phases  $\sqrt{\bar{n}}e^{i\phi_i}$  ( $\sqrt{\bar{n}}be^{i\xi_{ij}}$ ), and the number operators  $a_i^{\dagger}a_i$  ( $b_{ij}^{\dagger}b_{ij}$ ) by the derivatives  $-i\partial/\partial\phi_i - \bar{n}$  ( $-i\partial/\partial\xi_{ij} - \bar{n}^b$ ), we obtain H expressed in the basis of phase states for the case of a contact interaction

$$H^{(\phi)} = -2j\varrho \sum_{i} \cos(\phi_{i} - \phi_{i+1}) - 2j'\varrho^{b} \sum_{i,j} \cos(\xi_{ij} - \xi_{ij+1}) - 2j''\varrho^{b} \sum_{i,j} \cos(\xi_{ij} - \xi_{i+1j})$$
$$-\frac{U}{2} \sum_{i} \frac{\partial^{2}}{\partial \phi_{i}^{2}} - \frac{U'}{2} \sum_{i,j} \frac{\partial^{2}}{\partial \xi_{ij}^{2}} - V \sum_{i} \frac{\partial^{2}}{\partial \phi_{i} \partial \xi_{i0}}$$
(4.2a)

and for an exchange interaction

$$H^{(n)} = -2j\varrho \sum_{i} \cos(\phi_{i} - \phi_{i+1}) - 2j'\varrho^{b} \sum_{i,j} \cos(\xi_{ij} - \xi_{ij+1}) - 2j''\varrho^{b} \sum_{i,j} \cos(\xi_{ij} - \xi_{i+1j}) - \frac{U}{2} \sum_{i} \frac{\partial^{2}}{\partial \phi_{i}^{2}} - \frac{U'}{2} \sum_{i,j} \frac{\partial^{2}}{\partial \xi_{ij}^{2}} + 2V\sqrt{\varrho\varrho^{b}} \sum_{i} \cos(\phi_{i} - \xi_{i0})$$
(4.2b)

where indices i and j run from 1 to L and from -(L'-1)/2 to (L'-1)/2, respectively. The constants  $\rho = \sqrt{\bar{n}(\bar{n}-1)}$  and  $\rho^b = \sqrt{\bar{n}^b(\bar{n}^b-1)}$  are approximately the density in the system and the chains of the reservoir. Given the high density in both systems, we have also approximated  $\sqrt{\bar{n}\bar{n}^b} \simeq \sqrt{\rho\rho^b}$ .

In the limit of strong tunneling, the full system has an equilibrium configuration where the phases of adjacent sites couple and tend to become equal,  $\phi_i \sim \phi_0$ ,  $\xi_{ij} \sim \xi_{00}$  and  $\phi_i \sim \xi_{i0}$ . In this limit we can apply the harmonic approximation, expanding the cosines in equations 4.2 around this equilibrium configuration and keeping up to the second order of the phase differences, to study the effect of the quantum fluctuations induced by the

#### 4.1. Applying the Quantum Rotor model to a dissipative system

interactions U, U' and V. The Hamiltonian (4.2a) is then approximated by

$$H^{(\phi)} = 2j\varrho \sum_{i} (\phi_{i}^{2} - \phi_{i}\phi_{i+1}) + 2j'\varrho^{b} \sum_{i,j} (\xi_{ij}^{2} - \xi_{ij}\xi_{ij+1}) + 2j''\varrho^{b} \sum_{i,j} (\xi_{ij}^{2} - \xi_{ij}\xi_{i+1j}) - \frac{U}{2} \sum_{i} \frac{\partial^{2}}{\partial\phi_{i}^{2}} - \frac{U'}{2} \sum_{i,j} \frac{\partial^{2}}{\partial\xi_{ij}^{2}} - V \sum_{i} \frac{\partial^{2}}{\partial\phi_{i}\partial\xi_{i0}}$$
(4.3a)

and equation 4.2b by

$$H^{(n)} = 2j\varrho \sum_{i} (\phi_{i}^{2} - \phi_{i}\phi_{i+1}) + 2j'\varrho^{b} \sum_{i,j} (\xi_{ij}^{2} - \xi_{ij}\xi_{ij+1}) + 2j''\varrho^{b} \sum_{i,j} (\xi_{ij}^{2} - \xi_{ij}\xi_{i+1j}) - \frac{U}{2} \sum_{i} \frac{\partial^{2}}{\partial\phi_{i}^{2}} - \frac{U'}{2} \sum_{i,j} \frac{\partial^{2}}{\partial\xi_{ij}^{2}} - V\sqrt{\varrho\varrho^{b}} \sum_{i} (\phi_{i}^{2} + \xi_{i0}^{2} - 2\phi_{i}\xi_{i0}).$$
(4.3b)

In equations 4.3 some of the variables are coupled by a circulant matrix, which is of the form  $Q(i, j) = -\delta_{ij-1} + 2\delta_{ij} - \delta_{ij+1}$ . Thus, both cases can be diagonalized by the same orthogonal transformation  $\omega_{pi}$ , a real discrete Fourier transformation dependent on the lattice size. Introducing the new variables

$$\tilde{\phi}_p = \sum_i \omega_{pi}(L)\phi_i \tag{4.4a}$$

$$\tilde{\xi}_{pq} = \sum_{ij} \omega_{pi}(L) \omega_{qj}(L') \xi_{ij}$$
(4.4b)

and using the orthogonality relations  $\sum_{i} \omega_{pi} \omega_{qi} = \delta_{pq}$  and  $\sum_{p} \omega_{pi} \omega_{pj} = \delta_{ij}$ , we arrive to a simpler model  $H^{(\cdot)} = \sum_{p} H_p^{(\cdot)}$ , where the Hamiltonian is made of different components for each momentum p

$$H_{p}^{(\phi)} = j\varrho\epsilon_{p}(L)\tilde{\phi}_{p}^{2} + \sum_{q} \varrho^{b}[j'\epsilon_{q}(L') + j''\epsilon_{p}(L)]\tilde{\xi}_{pq}^{2} - \frac{U}{2}\frac{\partial^{2}}{\partial\tilde{\phi}_{p}^{2}} - \sum_{q}\frac{U'}{2}\frac{\partial^{2}}{\partial\tilde{\xi}_{pq}^{2}}$$
$$-V\sum_{q}\frac{\partial^{2}}{\partial\phi_{p}\partial\tilde{\xi}_{pq}}\omega_{q0}(L')$$
(4.5a)

$$H_{p}^{(n)} = j\varrho\epsilon_{p}(L)\tilde{\phi}_{p}^{2} + \sum_{q} \varrho^{b}[j'\epsilon_{q}(L') + j''\epsilon_{p}(L)]\tilde{\xi}_{pq}^{2} - \frac{U}{2}\frac{\partial^{2}}{\partial\tilde{\phi}_{p}^{2}} - \sum_{q}\frac{U'}{2}\frac{\partial^{2}}{\partial\tilde{\xi}_{pq}^{2}}$$
$$-V\sqrt{\varrho\varrho^{b}}\left(\tilde{\phi}_{p}^{2} + \sum_{q,q'}\tilde{\xi}_{pq}\tilde{\xi}_{pq'}\omega_{q0}(L')\omega_{q'0}(L') - 2\sum_{q}\tilde{\phi}_{p}\tilde{\xi}_{pq}\omega_{q0}(L')\right) \quad (4.5b)$$

corresponding to equations 4.3a and 4.3b, respectively. Here,  $\epsilon_p(L)$  are the eigenvalues of the tridiagonal matrix that couples  $\phi_i$  with  $\phi_{i\pm 1}$  and  $\xi_{ij}$  with  $\xi_{i\pm 1j}$ , and  $\epsilon_q(L')$  those of the tridiagonal matrix coupling  $\xi_{ij}$  with  $\xi_{ij\pm 1}$ . For each value of p, equations 4.5 are Gaussian Hamiltonians. This allows us to write these  $H_p^{(\cdot)}$  in matrix form as

$$H_p^{(\cdot)} = \vec{\theta}_p^T D_p \vec{\theta}_p - \vec{\nabla}_{\theta_p}^T B_p \vec{\nabla}_{\theta_p}, \qquad (4.6)$$

where we have defined the vector of variables  $\vec{\theta}_p^T = (\tilde{\phi}_p, \tilde{\xi}_{p1}, \dots, \tilde{\xi}_{pL}) = (\tilde{\phi}_p, \{\tilde{\xi}_{pq}\})$  and the matrices

$$D_{p} = \begin{pmatrix} (j\varrho + j''\varrho^{b})\varepsilon_{p} & 0 & 0 & 0 & 0 \\ 0 & j'\varrho^{b}\varepsilon_{1} + j''\varrho^{b}\varepsilon_{p} & 0 & 0 & 0 \\ 0 & 0 & j'\varrho^{b}\varepsilon_{2} + j''\varrho^{b}\varepsilon_{p} & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & j'\varrho^{b}\varepsilon_{L'} + j''\varrho^{b}\varepsilon_{p} \end{pmatrix} + V_{n}$$
$$B_{p} = \begin{pmatrix} U/2 & 0 & 0 & \cdots & 0 \\ 0 & U'/2 & 0 & 0 & 0 \\ 0 & 0 & U'/2 & 0 & 0 \\ \vdots & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & U'/2 \end{pmatrix} + V_{\phi}$$

where the matrices  $V_n$  and  $V_{\phi}$  should be added depending on the type of dissipation present in the system, being either number dissipation or phase dissipation respectively. The expressions of these matrices are

$$V_{n} = \begin{pmatrix} -V\sqrt{\varrho\varrho^{b}} & V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & \cdots & V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} \\ V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' \\ V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' \\ \vdots & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' & \cdots & -V\sqrt{\varrho\varrho^{b}}/L' \\ V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' \\ V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' & -V\sqrt{\varrho\varrho^{b}}/L' \\ V\sqrt{\varrho\varrho^{b}}/\sqrt{L'} & 0 & 0 & 0 \\ V/\sqrt{L'} & 0 & 0 & 0 \\ \vdots & 0 & 0 & \cdots & 0 \\ V/\sqrt{L'} & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Given that H is a sum over L quadratic Hamiltonians  $H_p$ , it is possible to write its ground state as a product of the individual Gaussian solutions for each  $H_p$ 

$$\psi = \prod_{p} \psi_p(\vec{\theta_p}) \quad \text{with} \quad \psi_p(\vec{\theta_p}) = \left(\frac{\det A_p}{\pi^{L'+1}}\right)^{1/4} \exp\left[-\frac{\vec{\theta_p}^T A_p \vec{\theta_p}}{2}\right], \quad (4.7)$$

where the matrix  $A_p$  must satisfy the condition

$$D_p = A_p^T B_p A_p \tag{4.8}$$

for equation 4.7 to be a solution of  $H = \sum_{p} H_{p}$ . A possible solution to this problem is thus

$$A_p = B_p^{-1/2} \sqrt{B_p^{1/2} D_p B_p^{1/2}} B_p^{-1/2}$$
(4.9)

and it is the one we will consider in the following calculations.

#### Reduced density matrix of the system

To study the properties of the system S, we construct the S + R full density matrix using equation 4.7 and trace out the reservoir degrees of freedom to obtain the reduced density matrix of the system

$$\rho(\vec{\tilde{\phi}}, \vec{\tilde{\phi}}') = \int \prod_{ij} d\tilde{\xi}_{ij} \psi(\vec{\tilde{\phi}}, \{\tilde{\xi}_{ij}\}) \psi^{\star}(\vec{\tilde{\phi}}', \{\tilde{\xi}_{ij}\}).$$
(4.10)

Given that we have the state (4.7) decomposed into momentum states, it results more convenient to compute first the reduced density matrix for each of these and then consider their product

$$\rho(\vec{\tilde{\phi}}, \vec{\tilde{\phi}}') = \prod_{p} \int d\tilde{\xi}_{p1} \cdots d\tilde{\xi}_{pL} \psi_p(\tilde{\phi}_p, \tilde{\xi}_{p1}, \dots, \tilde{\xi}_{pL}) \psi_p^{\star}(\tilde{\phi}_p', \tilde{\xi}_{p1}, \dots, \tilde{\xi}_{pL}).$$
(4.11)

To proceed with this calculation, we start decomposing symbolically the matrix  $A_p$  into four blocks

$$A_p = \begin{pmatrix} A_{\phi\phi}^{(p)} & A_{\phi\bar{\xi}}^{(p)} \\ A_{\bar{\xi}\phi}^{(p)} & A_{\bar{\xi}\bar{\xi}}^{(p)} \end{pmatrix}$$
(4.12)

referring to the elements of the matrix in the Gaussian state (4.7) coupling the variables of the system and/or the reservoir. Considering that the matrix  $A_p$  is Hermitian and positive definite<sup>\*</sup>, the previous integral becomes

$$\rho(\vec{\phi}, \vec{\phi}') \sim \prod_{p} \int d\vec{\xi_p} \exp\left[-A^{(p)}_{\phi\phi}(\tilde{\phi}_p^2 + \tilde{\phi}_p'^2)/2 - \vec{\xi_p}^T A^{(p)}_{\vec{\xi}\vec{\xi}} \vec{\xi_p} - (\tilde{\phi}_p + \tilde{\phi}_p') A^{(p)}_{\phi\vec{\xi}} \vec{\xi_p}\right]$$
(4.13)

up to a normalization factor, and where we have defined the vector  $\vec{\xi}_p^T = (\tilde{\xi}_{p1}, \dots, \tilde{\xi}_{pL})$ . Applying the change of variables  $\chi_p = \tilde{\phi}_p + \tilde{\phi}'_p$ , we can express the integral in equation 4.13 as

$$\exp\left[-A^{(p)}_{\phi\phi}(\tilde{\phi}_p^2 + \tilde{\phi}_p'^2)/2\right] \int d\vec{\tilde{\xi}_p} \exp\left[-\vec{\tilde{\xi}_p}^T A^{(p)}_{\vec{\xi}\vec{\xi}} - \chi_p A^{(p)}_{\phi\vec{\xi}} \vec{\tilde{\xi}_p}\right]$$

which can also be written with a constant displacement in the variables of integration

$$\exp\left[-A_{\phi\phi}^{(p)}(\tilde{\phi}_{p}^{2}+\tilde{\phi}_{p}^{\prime 2})/2\right] \int d\vec{\xi_{p}} \exp\left[-(\vec{\xi_{p}}-\vec{v_{p}})^{T}A_{\vec{\xi}\vec{\xi}}^{(p)}(\vec{\xi_{p}}-\vec{v_{p}})+\vec{v}_{p}^{T}A_{\vec{\xi}\vec{\xi}}^{(p)}\vec{v}_{p}\right]$$

by defining a constant vector  $\vec{v}_p = -A_{\vec{\xi}\vec{\xi}}^{(p)-1}A_{\vec{\xi}\phi}^{(p)}\chi_p/2$ , that can be reabsorbed by the integration variables. This integral can now be written more clearly as

$$\exp\left[-A_{\phi\phi}^{(p)}(\tilde{\phi}_{p}^{2}+\tilde{\phi}_{p}^{\prime 2})/2+\vec{v}^{T}A_{\vec{\xi}\vec{\xi}}^{(p)}\vec{v}\right]\int d\vec{\xi}_{p}^{\vec{z}}\exp\left[-(\vec{\xi}_{p}^{\vec{z}}-\vec{v})^{T}A_{\vec{\xi}\vec{\xi}}^{(p)}(\vec{\xi}_{p}^{\vec{z}}-\vec{v})\right].$$

<sup>\*</sup>Actually, for periodic boundary conditions it is not the case, but we can neglect the degrees of freedom associated to zero eigenvalues since they are associated to the "center of mass" of the system and to the translational symmetry.

The integration over constants and degrees of freedom of the reservoir may be neglected, considering it part of the normalization of the state. Finally, the integral in equation 4.13 can be expressed as

$$\exp\left[-A_{\phi\phi}^{(p)}(\tilde{\phi}_{p}^{2}+\tilde{\phi}_{p}^{\prime 2})/2+A_{\phi\vec{\xi}}^{(p)}A_{\vec{\xi}\vec{\xi}}^{(p)-1}A_{\vec{\xi}\phi}^{(p)}(\tilde{\phi}_{p}+\tilde{\phi}_{p}^{\prime})^{2}/4\right]$$

upon normalization of the state. Therefore, the reduced density matrix of the system takes the form

$$\rho(\vec{\phi}, \vec{\phi}') = \frac{1}{\mathcal{N}} \prod_{p} \exp\left[-B^{(p)}(\tilde{\phi}_{p}^{2} + \tilde{\phi}_{p}'^{2})/2 + C^{(p)}\tilde{\phi}_{p}\tilde{\phi}_{p}'\right], \qquad (4.14)$$

where the diagonal and off-diagonal elements are given, respectively, by

$$B^{(p)} = A^{(p)}_{\phi\phi} - \frac{1}{2} A^{(p)}_{\phi\bar{\xi}} A^{(p)^{-1}}_{\bar{\xi}\bar{\xi}} A^{(p)}_{\bar{\xi}\phi}, \quad C^{(p)} = \frac{1}{2} A^{(p)}_{\phi\bar{\xi}} A^{(p)^{-1}}_{\bar{\xi}\bar{\xi}} A^{(p)}_{\bar{\xi}\phi}.$$
(4.15)

To give sense to the probability distribution that the density matrix describes, its trace should be one. This constrain defines the value of the normalization factor  $\mathcal{N}$ 

$$\mathcal{N} = \prod_{p} \int d\tilde{\phi}_{p} \exp\left[-\tilde{\phi}_{p}^{2}(B^{(p)} - C^{(p)})\right] = \prod_{p} \sqrt{\frac{\pi}{A^{(p)}_{\phi\phi} - A^{(p)}_{\phi\vec{\xi}}A^{(p)^{-1}}_{\vec{\xi}\vec{\xi}}A^{(p)}_{\vec{\xi}\phi}}}.$$
(4.16)

Furthermore, the state (4.14) can be more conveniently written as

$$\rho(\vec{\tilde{\phi}}, \vec{\tilde{\phi}}') = \frac{1}{\mathcal{N}} \exp\left[-\frac{\vec{\tilde{\phi}}^T B \vec{\tilde{\phi}}}{2} - \frac{\vec{\tilde{\phi}}'^T B \vec{\tilde{\phi}}'}{2} + \vec{\tilde{\phi}}^T C \vec{\tilde{\phi}}'\right],\tag{4.17}$$

where B and C are diagonal matrices with the ordered elements  $B^{(p)}$  and  $C^{(p)}$ , respectively. Using the discrete Fourier transform introduced in equation 4.4, we can return to the real space and obtain the reduced density matrix of the system

$$\rho(\vec{\phi}, \vec{\phi}') = \frac{1}{\mathcal{N}} \exp\left[-\frac{\vec{\phi}^T \bar{B} \vec{\phi}}{2} - \frac{\vec{\phi}'^T \bar{B} \vec{\phi}'}{2} + \vec{\phi}^T \bar{C} \vec{\phi}'\right],$$
(4.18)

where the matrices  $\bar{B}$  and  $\bar{C}$  are the corresponding Fourier transformed matrices B and C.

Having determined the state of our system (4.18), we can now continue calculating the expectation values that characterize its physical state and tell us more about its phases and properties.

#### Characterizing the state of the system: correlation functions

**Number fluctuation** The variance in the number of particles per site  $\Delta n_i^2$  tells us whether the particles in the system are pinned to the lattice sites  $\Delta n_i^2 = 0$  or are able to move the lattice  $\Delta n_i^2 \neq 0$ . In the phase model, this quantity may be calculated as

$$\Delta n_i^2 = \left\langle (a_i^{\dagger} a_i - \bar{n})^2 \right\rangle \simeq \left\langle -\frac{\partial^2}{\partial \phi_i^2} \right\rangle.$$
(4.19)

#### 4.1. Applying the Quantum Rotor model to a dissipative system

For the reduced density matrix (4.14), we compute this expected value as follows

$$\Delta n_i^2 = \int d\vec{\phi} d\vec{\phi}' \delta(\vec{\phi} - \vec{\phi}') \left( -\frac{\partial^2}{\partial \phi_i^2} \right) \rho(\vec{\phi}, \vec{\phi}').$$
(4.20)

We start taking explicitly the first and second derivatives with respect to the phase  $\phi_i$ 

$$\partial_{\phi_i}\rho(\vec{\phi},\vec{\phi}') = \left[-\sum_j \bar{B}_{ij}\phi_j + \sum_j \bar{C}_{ij}\phi'_j\right]\rho(\vec{\phi},\vec{\phi}'), \qquad (4.21a)$$

$$\partial_{\phi_i}^2 \rho(\vec{\phi}, \vec{\phi}') = \left\{ -\bar{B}_{ii} + \left[ -\sum_j \bar{B}_{ij} \phi_j + \sum_j \bar{C}_{ij} \phi'_j \right]^2 \right\} \rho(\vec{\phi}, \vec{\phi}')$$
(4.21b)

and then consider the trace of the second derivative of the state

$$\int d\vec{\phi}' \delta(\vec{\phi} - \vec{\phi}') \partial_{\phi_i}^2 \rho(\vec{\phi}, \vec{\phi}') = \left\{ -\bar{B}_{ii} + \left[ \sum_j (\bar{B}_{ij} - \bar{C}_{ij}) \phi_j \right]^2 \right\} \rho(\vec{\phi}, \vec{\phi}).$$
(4.22)

This allows us to write the problem as

$$\Delta n_i^2 = \frac{1}{\mathcal{N}} \int d\vec{\phi} \left\{ \bar{B}_{ii} - \left[ \sum_j (\bar{B}_{ij} - \bar{C}_{ij}) \phi_j \right]^2 \right\} \exp\left[ -\vec{\phi}^T (\bar{B} - \bar{C}) \vec{\phi} \right].$$
(4.23)

From this point, we proceed changing the variable of integration  $\vec{\phi}$  to  $\vec{\psi} = V^{-1}\vec{\phi}$ , where V is the unitary transformation that diagonalizes  $\bar{B} - \bar{C}^{\dagger}$ , while to simplify the notation we introduce  $X = \bar{B} - \bar{C}$ . This reduces the problem to

$$\Delta n_i^2 = \bar{B}_{ii} - \frac{1}{\mathcal{N}} \int d\vec{\psi} \left[ \sum_j (XV)_{ij} \psi_j \cdot \sum_k (XV)_{ik} \psi_k \right] \exp\left[ -\sum_l X^D{}_{ll} \psi_l^2 \right].$$
(4.24)

Finally, using the Gaussian integrals  $\int d\phi \exp(-\alpha \phi^2) = \sqrt{\frac{\pi}{\alpha}}$  and  $\int d\phi \exp(-\alpha \phi^2)\phi^2 = -\frac{d}{d\alpha}\sqrt{\frac{\pi}{\alpha}} = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$ , the fluctuations become

$$\Delta n_i^2 = \bar{B}_{ii} - \frac{1}{2}\bar{C}_{ii} \tag{4.25}$$

expressed as a function of the Gaussian solution (4.7) and its parameters.

Second-order correlation function We can also calculate the decay with the distance  $\Delta$  of the two-body correlations in our system. In the phase approximation it can be calculated as

$$\langle a_i^{\dagger} a_j \rangle = \langle e^{(ix^T \vec{\phi})} \rangle \tag{4.26}$$

where the only non-zero components of  $\vec{x}$  correspond to the *i*-th and *j*-th element  $(|i-j| = \Delta)$ , which are  $x_i = -1$ ,  $x_j = 1$ . For the reduced density matrix (4.14), this expected value can be computed as follows

$$\langle e^{(i\vec{x}\vec{T}\vec{\phi})} \rangle = \int d\vec{\phi} d\vec{\phi}' \delta(\vec{\phi} - \vec{\phi}') \exp(i\vec{x}\vec{T}\vec{\phi})\rho(\vec{\phi},\vec{\phi}').$$
(4.27)

<sup>†</sup>This means  $\bar{B} - \bar{C} = V(\bar{B} - \bar{C})^D V^{-1}$ , where  $(\bar{B} - \bar{C})^D$  is a diagonal matrix.

Considering first the trace of the product of the state and the exponential

$$\int d\vec{\phi}' \delta(\vec{\phi} - \vec{\phi}') \exp(i\vec{x}\vec{T}\vec{\phi})\rho(\vec{\phi},\vec{\phi}') = \exp(i\vec{x}\vec{T}\vec{\phi})\rho(\vec{\phi},\vec{\phi})$$
(4.28)

the problem becomes very simple

$$\langle e^{(i\vec{x}\vec{T}\vec{\phi})}\rangle = \frac{1}{\mathcal{N}} \int d\vec{\phi} \exp\left[i\vec{x}\vec{T}\vec{\phi} - \vec{\phi}\vec{T}(\bar{B} - \bar{C})\vec{\phi}\right]$$
(4.29)

and it can be solved defining the constant vector  $\vec{v} = i(\bar{B} - \bar{C})^{-1}\vec{x}/2$ , which can be reabsorbed in the variable of integration

$$\langle e^{(i\vec{x}\,\vec{T}\,\vec{\phi})} \rangle = \frac{1}{\mathcal{N}} \int d\vec{\phi} \exp\left[-(\vec{\phi} - \vec{v})^T (\bar{B} - \bar{C})(\vec{\phi} - \vec{v}) + \vec{v}\,\vec{T}(\bar{B} - \bar{C})\vec{v}\right]. \tag{4.30}$$

Finally, the correlator becomes

$$\langle e^{(i\vec{x}\vec{r}\vec{\phi})}\rangle = \exp\left[-\frac{1}{4}\vec{x}\vec{T}\left((\bar{B}-\bar{C})^{-1}\right)^T\vec{x}\right]$$
(4.31)

expressed as a function of the Gaussian solution (4.7), its parameters and the vector  $\vec{x}$  that determines between which sites the two-body correlator is taken.

In figure 4.1 we have the correlations in the system for two different sizes of the reservoir (in the upper plots L' = 101 and in the lower ones L' = 121), considering either number dissipation or phase dissipation through independent baths (left and right plots, respectively). All results coincide for V = 0, and we observe as expected that for a fixed value of the dissipation strength V, the hopping of the system j increases the number fluctuations and the second-order correlations in the system.

In the case of number dissipation (3.19), as the value of V increases, we observe that this kind of dissipation pushes the system to a state with characteristics more of a Mott kind, where the particles tend to be more localized, and loose the strong correlations. The size of the reservoir L' does not appear to affect the physics of the system.

In the presence of phase dissipation (3.21), for a small value of the dissipation strength V we observe that both correlators increase until the dissipation strength reaches a critical value ( $V \sim 0.06 - 0.07$  in figure 4.1 (right)), whereon the behavior is reverted. At this value there is a resonance where higher number fluctuations take place. The position of this resonance changes with the size of the environment L', happening at lower values of V for bigger reservoirs. A systematical study of this effect for longer values of L' is hindered by the computational resources.

A common feature of both dissipative mechanisms is that, for a strong dissipation strength V the second-order correlations decay, indicating a lost of coherence between neighbors. The systems is not a condensate anymore and tends to fragment, which can be understood as the emergence of a Mott-phase.

Interpreting these results for certain parameter values as a reinforcement of the phases, unveils a property of dissipation that is normally not seen in classical systems: it helps to create a desired quantum phase, with either strong or weak correlations. This idea has been later better developed by other authors [30, 66, 110].



Figure 4.1: All plots show the number fluctuations  $\Delta n$  (color gradient) and the second-order correlation function  $\langle a_i^{\dagger} a_{i+1} \rangle$  (solid). The systems we consider have lengths L = 50, L' = 101 (up) and L = 50, L' = 121 (down), undergoing either number dissipation (left) or phase dissipation (right). The reservoir is considered to be in a superfluid state, with  $\rho^b = \rho = 5$ , j'/U' = 1 and U' = U.

#### A generalized ansatz for the master equation

Instead of solving the Hamiltonian for the full system and tracing out the environment from its solution, another approach to deal with systems that present open quantum dynamics is to solve the master equation for their evolution, as it has been mentioned in section 3.1. To do this within the phase approximation, we will have to extend the description we have been using to density matrices.

A general mixed state in the phase model can be written as

$$\rho = \frac{1}{(2\pi)^L} \int d^L \phi d^L \phi' e^{i\vec{n} \cdot (\vec{\phi} - \vec{\phi'})} \rho(\vec{\phi}, \vec{\phi'}) \left| \vec{\phi} \right\rangle \left\langle \vec{\phi'} \right|.$$
(4.32)

Proceeding similarly as in the pure case, when equations 2.5 were derived, we find that the relevant operators acting over a density matrix in the phase basis (4.32) transform like

$$A_j^z \rho = i \partial_{\phi_j} \rho, \ \rho A_j^z = -i \partial_{\phi'_j} \rho \tag{4.33a}$$

$$A_j^{\pm}\rho = e^{\pm i\phi_j}\rho, \ \rho A_j^{\pm} = e^{\pm i\phi'_j}\rho \tag{4.33b}$$

depending on whether the operator acts from the left or from the right of the density matrix  $\rho$ .

Then, the master equation for phase dissipation (3.20) can be written as

$$\partial_{t}\rho = i\frac{U}{2}\sum_{j} \left[\partial_{\phi_{j}}^{2} - \partial_{\phi_{j}}^{2}\right]\rho + i\varrho j \sum_{j} \left[(\phi_{j} - \phi_{j+1})^{2} - (\phi_{j}' - \phi_{j+1}')^{2}\right]\rho + \gamma \sum_{j} \left[\partial_{\phi_{j}}^{2} + \partial_{\phi_{j}'}^{2} - 2\partial_{\phi_{j}}\partial_{\phi_{j}'}\right]\rho$$
(4.34)

and we shall consider the following ansatz

$$\rho(\vec{\phi},\vec{\phi}') = \mathcal{N} \exp\left[-\vec{\phi}^T A \vec{\phi} - \vec{\phi}'^T B \vec{\phi}' - \vec{\phi}^T C \vec{\phi}' + \vec{w}^T \vec{\phi} + \vec{v}^T \vec{\phi}'\right]$$
(4.35)

where  $\mathcal{N}$  is a suitable normalization constant, and the constants A, B, C,  $\vec{w}$  and  $\vec{v}$  can be found solving the system of equations obtained for the stationary solution of equation 4.34. Moreover, in the presence of phase dissipation we have an extra condition, namely the conservation of the number of particles in the system  $[\sum_{i} n_{i}, \rho] = 0$ , which translates into

$$\sum_{i} \left( \partial_{\phi_j} + \partial_{\phi'_j} \right) \rho(\phi, \phi') = 0 \tag{4.36}$$

where  $\rho(\phi, \phi')$  is the function defining the state in equation 4.32.

In the case of dissipation ( $\gamma \neq 0$ ), it is not possible to find a consistent solution for arbitrary values of the rest of the parameters.

**Heisenberg equations of motion** Another way of tackling this problem is to use equation 3.16 to derive the Heisenberg equations of motion for the correlation functions, which can be also used to characterize the state of the system.

For number dissipation in a system with shared baths between neighboring sites (3.24), using the expansion of  $a_i$  in terms of phase operators  $a_i = \sum_n (i\phi_i)^n / n!$ , we can calculate the equations for the second-order correlation functions in the phase-number representation

$$\begin{split} \dot{\langle n_{i}n_{j}\rangle} &= 2\gamma \left[ \langle n_{i}n_{j}\rangle - N \langle n_{i}\rangle - N \langle n_{j}\rangle + 2N \langle n_{i}\rangle \delta_{ij} \right] + \gamma \left[ \langle a_{i}^{\dagger}n_{j}a_{i}\rangle + \langle a_{j}^{\dagger}n_{i}a_{j}\rangle \right] + \\ \gamma N \left[ \langle a_{i+1}^{\dagger}a_{i}\rangle + \langle a_{i}^{\dagger}a_{i+1}\rangle \right] \delta_{ij+1} + \gamma N \left[ \langle a_{i+1}^{\dagger}a_{i}\rangle + \langle a_{i}^{\dagger}a_{i+1}\rangle \right] \delta_{ij-1} + \\ \frac{\gamma}{2} \left[ \langle n_{i}a_{j}^{\dagger}a_{j+1}\rangle + \langle n_{i}a_{j}^{\dagger}a_{j-1}\rangle + \langle a_{i+1}^{\dagger}a_{i}n_{j}\rangle + \langle a_{i-1}^{\dagger}a_{i}n_{j}\rangle \right] + \\ \frac{\gamma}{2} \left[ \langle a_{i}^{\dagger}n_{j}a_{i+1}\rangle + \langle a_{i}^{\dagger}n_{j}a_{i-1}\rangle + \langle a_{j+1}^{\dagger}n_{i}a_{j}\rangle + \langle a_{j-1}^{\dagger}n_{i}a_{j}\rangle \right] \right] \\ \dot{\langle \phi_{i}\phi_{j}\rangle} &= 0 \\ \dot{\langle \phi_{i}n_{j}\rangle} &= \frac{\gamma}{2} \left[ \langle a_{i}^{\dagger}a_{i-1}\phi_{j}\rangle + \langle a_{i-1}^{\dagger}a_{i}\phi_{j}\rangle + \langle a_{i}^{\dagger}a_{i+1}\phi_{j}\rangle + \langle a_{i+1}^{\dagger}a_{i}\phi_{j}\rangle \right] + \\ 2\gamma \left[ \langle n_{i}\phi_{j}\rangle - N \langle \phi_{j}\rangle \right] \end{aligned}$$

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#### 4.1. Applying the Quantum Rotor model to a dissipative system

where for simplicity we show only the dissipative part (*i.e.* as if U, j = 0), corresponding respectively to the number-number, the phase-phase and the phase-number correlations across the lattice, between sites *i* and *j*. The system of differential equations 4.37 is not closed, it mixes correlators of three different, consecutive orders. We encounter the same situation when considering shared baths with a phase in the interaction  $(a_i - a_{i+1})$  instead of  $a_i + a_{i+1}$  in equation 3.24).

For phase dissipation (3.20), using the commutation relation  $[\phi_i, n_j] = i\delta_{ij}$ , we can calculate the same second-order correlation functions

$$\langle n_{i}n_{j}\rangle = 2j\varrho \left[ \langle n_{i}\phi_{j-1}\rangle - 2\langle n_{i}\phi_{j}\rangle + \langle n_{i}\phi_{j+1}\rangle + \langle \phi_{i-1}n_{j}\rangle - 2\langle \phi_{i}n_{j}\rangle + \langle \phi_{i+1}n_{j}\rangle \right] \langle \dot{\phi_{i}\phi_{j}}\rangle = -U \left[ \langle n_{i}\phi_{j}\rangle + \langle \phi_{i}n_{j}\rangle \right] - \gamma\delta_{ij} \dot{\phi_{i}n_{j}}\rangle = 2j\varrho \left[ \langle \phi_{i}\phi_{j-1}\rangle - 2\langle \phi_{i}\phi_{j}\rangle + \langle \phi_{i}\phi_{j+1}\rangle \right] - U\langle n_{i}n_{j}\rangle.$$

$$(4.38)$$

If the system of equations 4.38 would be homogeneous, it could possibly have an interesting solution. On this basis, we introduce a toy model in which the phase dissipation (3.20) is modified, replacing  $n_i$  by  $n_i^2$  in the Liouvillian. This change ensures a system of homogeneous differential equations,

$$\langle n_{i}n_{j} \rangle = 2j\varrho \left[ \langle n_{i}\phi_{j-1} \rangle - 2\langle n_{i}\phi_{j} \rangle + \langle n_{i}\phi_{j+1} \rangle + \langle \phi_{i-1}n_{j} \rangle - 2\langle \phi_{i}n_{j} \rangle + \langle \phi_{i+1}n_{j} \rangle \right] \langle \dot{\phi_{i}\phi_{j}} \rangle = -U \left[ \langle n_{i}\phi_{j} \rangle + \langle \phi_{i}n_{j} \rangle \right] + 4\gamma \langle n_{i}n_{j} \rangle \delta_{ij} \dot{\langle \phi_{i}n_{j} \rangle} = 2j\varrho \left[ \langle \phi_{i}\phi_{j-1} \rangle - 2\langle \phi_{i}\phi_{j} \rangle + \langle \phi_{i}\phi_{j+1} \rangle \right] - U \langle n_{i}n_{j} \rangle.$$

$$(4.39)$$

The number of equations needed to solve this problem, can be reduced from  $4L^2$  to 4L considering periodic boundary conditions, such that  $\langle X_i Y_j \rangle = \langle X_1 Y_{|i-j|} \rangle$  for any local operators  $X_i$  and  $Y_i$ . Defining the relative distance  $\Delta = |i-j|$ , the 4L equations correspond to  $\langle n_1 n_\Delta \rangle$ ,  $\langle \phi_1 \phi_\Delta \rangle$ ,  $\langle \phi_1 n_\Delta \rangle$  and  $\langle n_1 \phi_\Delta \rangle$ . Using a vector to collect the operators at all relative distances  $\Delta$  under one symbol (*e.g.*  $\vec{X} = (X_1 X_2 \dots X_L)$ ), we can write the system of equations 4.39 as

$$\begin{pmatrix} \langle n_1 \vec{n} \rangle \\ \langle n_1 \vec{\phi} \rangle \\ \langle \phi_1 \vec{n} \rangle \\ \langle \phi_1 \vec{\phi} \rangle \end{pmatrix} = \begin{pmatrix} 0 & -2\varrho j B & -2\varrho j B & 0 \\ U & 0 & 0 & -2\varrho j B \\ U & 0 & 0 & -2\varrho j B \\ 4\gamma \delta_{0\Delta} & U & U & 0 \end{pmatrix} \begin{pmatrix} \langle n_1 \vec{n} \rangle \\ \langle n_1 \vec{\phi} \rangle \\ \langle \phi_1 \vec{n} \rangle \\ \langle \phi_1 \vec{\phi} \rangle \end{pmatrix}$$
(4.40)

where B is a circulant matrix, with  $B_{ii} = -2$  and  $B_{ii\pm 1} = 1$ . For j = 0, the equations 4.40 acquire simplified expression

yielding as solution a constant value of  $\langle n_1 n_\Delta \rangle$  in time, linearly growing correlators  $\langle \phi_1 n_\Delta \rangle$ and  $\langle n_1 \phi_\Delta \rangle$ , and a quadratically growing  $\langle \phi_1 \phi_\Delta \rangle$  that also grows with the dissipation. Implementing in the master equation  $\rho(\phi, \phi') = \rho_0 e^{-i(\vec{\phi} - \vec{\phi}') \cdot \vec{n}}$  as trial function, we find a constant  $\rho_0$  as stationary state of the system, corresponding to a Mott insulating state. We calculate the initial values of the second moments  $\langle n_1 n_\Delta \rangle$ ,  $\langle \phi_1 n_\Delta \rangle$ ,  $\langle n_1 \phi_\Delta \rangle$  and  $\langle \phi_1 \phi_\Delta \rangle$ using this state. Then, proceed with an adiabatic evolution of the system as j increases, but the resulting equations are not stationary. Considering  $j \neq 0$  and initially that  $\gamma = 0$ , the stationary state condition on (4.40) gives  $\langle n_1 n_\Delta \rangle = \frac{2j\varrho}{U} B \langle \phi_1 \phi_\Delta \rangle$  and  $\langle \phi_1 n_\Delta \rangle$ ,  $\langle n_1 \phi_\Delta \rangle =$ 0. Then, the correlation length

$$\xi^2 = \frac{\sum_{\Delta} \Delta^2 \langle \phi_1 \phi_{\Delta} \rangle}{\sum_{\Delta} \langle \phi_1 \phi_{\Delta} \rangle}$$

decreases as the interaction strength  $\gamma$  grows.

# 4.2 Strong coupling expansion around the interacting Mott

Proceeding as explained in section 2.2, we are going to calculate the Mott-phase diagram for an optical lattice undergoing phase dissipation (3.19) in a reservoir of independent baths (j'' = 0). We focus on the behavior of the first Mott lobe (one particle per site) drawn in figure 2.3, considering that the reservoir has also one particle per site.

The expansion to second order for weak coupling  $j, j'' \ll U, U', V$  yields for the lower boundary of the lobe (chemical potential required to add a hole to the system)

$$\mu_h(L) = V + 2j - \frac{4j^2}{U} + \frac{8j'^2}{U'} - \frac{8j'^2U'}{U'^2 - V^2}$$
  

$$\simeq V + 2j - \frac{4j^2}{U} - \frac{8j'^2V^2}{U'^3}$$
(4.41a)

and for the upper one (chemical potential required to add a particle to the system)

$$\mu_p(L) = U + V - 4j + \frac{j^2}{U} - \frac{8j'^2U'}{U'^2 - 4V^2} \left(\frac{3V^2}{U'^2 - V^2}\right)$$
  

$$\simeq U + V - 4j + \frac{j^2}{U} - \frac{24j'^2V^2}{U'^3}.$$
(4.41b)

Here, we see that the lobe shifts upwards proportionally to the strength of the on-site interaction V. The crossing point of these lines will give us an approximate behavior of the lobe tip under the influence of the dissipative process

$$\frac{5j^2}{U} - 6j + U - \frac{16V^2j'^2}{U'^3} = 0$$
(4.42)

which has as root the critical value of the hopping amplitude

$$\frac{j_c^{(2)}}{U} = \frac{6 \pm \sqrt{16 + 320 \frac{j'^2 V^2}{U U'^3}}}{10} \tag{4.43}$$

taking the solution with the negative sign (figure 4.2 (inset)), as we are in the perturbative regime. Therefore, we observe that the size of the lobe starts decreasing as the interaction is turned on, but also when the kinetic energy of the environment is increased.



Figure 4.2: Applying perturbation theory for V/U = 0 (solid), V/U = 0.1 (dashed) and V/U = 0.2 (dotdashed). In the inset the displacement of the lobe's tip to second order  $j_c^{(2)}$ with the hopping amplitude of the environment for a constant interaction strength V/U = 0.2.

## 4.3 A Gutzwiller ansatz for the system and reservoir

In this section we generalize the description introduced in section 2.3 to our manychains system. Namely, the state is modeled as a product of functions describing the state of each site

$$\left|\psi\right\rangle = \bigotimes_{i=1}^{L} \left|\psi_{i}^{(s)}\right\rangle \bigotimes_{i,j=1}^{L,L'} \left|\psi_{i,j}^{(r)}\right\rangle \tag{4.44}$$

where  $|\psi_i^{(s)}\rangle$  denotes the state of the *i*-th site of the system and  $|\psi_{i,j}^{(r)}\rangle$  the state of the *j*-th site of the *i*-th chain in the reservoir

$$\left|\psi_{i}^{(s)}\right\rangle = \sum_{n=1}^{N} f_{n} \left|n\right\rangle, \quad \left|\psi_{i,j}^{(r)}\right\rangle = \sum_{n=1}^{N} g_{n}^{(j)} \left|n\right\rangle \tag{4.45}$$

and  $f_n$  and  $g_n^{(j)}$  are the coefficients of these states when expanded in the Fock basis, considering translational invariance along the main chain as the index *i* is omitted. These coefficients are found by minimizing the free energy of whole system in the grand canonical ensemble, under the constrain of normalized states.

In figure 4.3 we have the phase diagrams calculated using a Gutzwiller ansatz. Each plot corresponds to a different value of the dissipation strength V in the case of phase dissipation (3.19). The lower plot will be our reference, displaying the results for the Bose–Hubbard model (*i.e.* V = 0). We identify the Mott insulating phases as those having vanishing number fluctuations ( $\Delta n = 0$ ) and vanishing coherence ( $\langle a \rangle = 0$ ). On the contrary, the superfluid regions show that these numbers acquire finite values ( $\Delta n, \langle a \rangle \neq 0$ ).

A Gutzwiller ansatz does not reveal any variations in the size of the Mott lobes when the dissipation strength V increases, as the strong coupling results had suggested (see inset figure 4.2). For  $V \neq 0$ , the lobes conserve the same size as in the Bose-Hubbard model (figure 4.3 (down)). This disagreement may come from the truncation of the strong coupling expansion to second order in V, neglecting changes that take place at higher values of V.



However, the results in figure 4.3 agree with the occurrence of a shift along the yaxis (chemical potential) that is linear in the dissipation strength V. In our mean-field simulations, the shift takes a magnitude of  $\sim 3.3V$ . This effect means that for the same value of the chemical potential, we have less particles per site as V increases. In other words, the phase dissipation induces a renormalization of the chemical potential, adding an effective repulsive potential at each site.

Less evident in the plots in figure 4.3 is an increase in the particle fluctuations and coherence in the superfluid area. The difference is significantly more pronounced around the Mott lobes (on top and near to the tips). For V = 0.05U we observe changes of up to  $\sim 20\%$  in the coherence  $\langle a \rangle$ , and  $\sim 12-15\%$  in the particle fluctuation  $\Delta n$ . For V = 0.1U both correlators grow as high as to a  $\sim 50\%$  more. This changes are not noticeable in the plots due to the small value that these quantities *per se* have in those locations.

Atoms with correlated hopping

# Chapter 5

# The physical system for correlated hopping

# 5.1 Correlated hopping model

Correlated hopping is not a new idea. It appears naturally in fermionic tight-binding models, where it has been used to describe systems as mixed valence solids [40] and, given that they are able to mimic the attractive interactions between electrons, high- $T_c$  superconductors [63, 64, 8, 7, 26, 114]. In most of these works, the correlated hopping appears also in the form  $n_i a_j^{\dagger} a_k$ , indicating that the environment can influence the hopping of a particle and may not seem to be related with the correlated motion of fermions. Nevertheless, even in this more elaborate form of correlated hopping, it has been shown to lead to the formation of bound electron pairs [7, 8] and it has been put forward as an explanation for high  $T_c$  superconductivity [54, 74].

It has been already shown in references [33, 34] that combining atomic collisions with optical superlattices can be used to induce correlated hopping. The basic idea is shown in figure 5.1 (right), where atoms are trapped in two orthogonal states called (+) and (-). The interaction terms change the state of the atoms, forcing them to hop to a different superlattice every time they collide. In this sense, interactions are responsible for transport. We would like to remark that the ideas presented here are not restricted to one dimension and could be implemented using other kinds of spin-dependent interactions. Also, we would like to point out that correlated hopping appears naturally in state-dependent lattices loaded with spinor atoms, because their interactions can change the hyperfine state of the atoms while preserving total angular momentum [120].

In this chapter we will introduce the most general model of correlated hopping that can be produced by means of state changing collisions. This model is presented in the following section, where we explain qualitatively the role of each Hamiltonian term. Later on, we will establish the connection between the parameters of this model and the underlying atomic model. This will be the foundation for the subsequent analytical and numerical studies.



**Figure 5.1:** (upper left) Atoms in two internal states  $\uparrow$  and  $\downarrow$  are trapped in an optical lattice and coupled by a Raman laser with Rabi frequency  $\Omega$ . (right) That setup is equivalent to two displaced superlattices for the dressed states  $|\pm\rangle \sim |\uparrow\rangle \pm |\downarrow\rangle$ . (lower left) When asymmetric contact interactions are considered and the hopping between superlattice cells neglected, the whole system behaves effectively as a 1D array of alternating  $|+\rangle$  and  $|-\rangle$  sites, with transitions of tunneling amplitude t between them.

## 5.2 A family of correlated hopping Hamiltonians

In this work we will study the ground state properties of a very general Hamiltonian that contains different kinds of correlated hopping. More precisely, the model will be

$$H = \sum_{i} \left\{ \frac{U}{4} : (n_{i} + n_{i+1})^{2} : + V \ n_{i}n_{i+1} - t \ (c_{i}^{\dagger 2}c_{i+1}^{2} + \text{H.c.}) - j \ [(n_{i} - 1)c_{i}^{\dagger}(c_{i-1} + c_{i+1}) + \text{H.c.}] \right\}.$$
(5.1)

Here,  $c_i^{\dagger}$  and  $c_i$  are bosonic operators for creation and annihilation of atoms according to the site numbering in figure 5.1 (lower left and right) and the colons :  $A_iB_j$ : denote normal ordering of operators  $A_i$  and  $B_j$ .

Let us qualitatively explain the roles of the different terms in equation 5.1. The first and second terms, with U and V, are related to on-site and next-neighbor interactions. When these terms are dominant, we expect the atoms in the lattice form an insulator. Such a phase is characterized by atoms being completely localized to lattice sites, having well-defined occupation numbers, the absence of macroscopic coherence and a gapped energy spectrum. Whether this insulating state is itself dominated by strong on-site interactions U or by nearest neighbor repulsion/attraction V will decide whether it presents a uniform density, a Mott insulator (MI), or a periodic density pattern with integer occupations, a charge density wave (CDW), respectively.

The third term is the key feature of our model. It describes the tunneling of pairs between neighboring lattice sites, with amplitude t. Given U, V, j = 0, we expect the atoms to travel along the lattice in pairs forming what we call a pair superfluid (PSF). The pairs in this phase will be completely delocalized, establishing long-range coherence along the lattice. The observable  $\langle a^2 \rangle$  would be the figure of merit describing this kind of delocalization, while a vanishing  $\langle a \rangle$  indicates the absence of the single-particle correlations appearing in a normal superfluid. Furthermore, this phase should have a critical velocity, similar to that of an atomic condensate, and the energy spectrum should be gapless.

When one considers the most general kind of atomic interaction, a second kind of correlated hopping will appear, described by the last term in equation 5.1 [34]. Here, individual atoms will hop only if there is already a particle in the site they go to  $(c_i^{\dagger}c_j(n_i-1))$  or leave at least a particle where they were  $((n_i - 1)c_jc_i^{\dagger})$ . One might be induced to think that this term is equivalent to an ordinary hopping term with a strength that depends on the average density, thus giving rise to a superfluid (SF) phase. However, this does not seem to be the case. We show that the correlated hopping j generates a mixed phase which contains features of both the ordinary BEC and the PSF created by t, a feature reflected by a non-zero value of  $\Delta a^2$ .

#### **Relation to atomic parameters**

We now establish the relation between the model in equation 5.1 and the dynamics of atoms in an optical superlattice. The actual setup, shown in figure 5.1 (upper left and right), is described in detail in appendix C.1. Roughly speaking, we have an optical superlattice that traps atoms in the dressed states  $|+\rangle$  and  $|-\rangle$ , while the atomic interaction is diagonal in the basis of the bare states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . The interaction will be described by a contact potential and, as we said, it is diagonal in the bare basis and parametrized by some real constants  $g_{\alpha\beta}$ 

$$H_{\text{int}} = \sum_{\alpha,\beta=\uparrow,\downarrow} \frac{g_{\alpha\beta}}{2} \int d^3x \psi^{\dagger}_{\alpha}(x) \psi^{\dagger}_{\beta}(x) \psi_{\beta}(x) \psi_{\alpha}(x)$$
$$= \sum_{\alpha,\beta=\uparrow,\downarrow} \frac{g_{\alpha\beta}}{2} \int d^3x : \rho_{\alpha}(x) \rho_{\beta}(x) :$$
(5.2)

These interaction constants are functions of the s-wave scattering lengths between different species  $g_{\alpha\beta} = 4\pi\hbar^2 a_{\alpha\beta}/m$ . In general, these scattering lengths are different for distinct atomic components, a situation that can be enhanced using optical or magnetic Feshbach resonances. Without loss of generality, we will use the parametrization

$$g_{\uparrow\uparrow} = g_0 + g_2, \quad g_{\downarrow\downarrow} = g_0 - g_2, \quad g_{\uparrow\downarrow} = g_0 + g_1 = g_{\downarrow\uparrow} \tag{5.3}$$

making these asymmetries more evident. Using this splitting we arrive to

$$H_{\text{int}} = \frac{g_0}{2} \int d^3 x : (\rho_{\uparrow}(x) + \rho_{\downarrow}(x))^2 :+ g_1 \int d^3 x : \rho_{\uparrow}(x) \rho_{\downarrow}(x) : \\ + \frac{g_2}{2} \int d^3 x : \rho_{\uparrow}(x)^2 - \rho_{\downarrow}(x)^2 :$$
(5.4)

The total Hamiltonian combines this interaction Hamiltonian with the kinetic energy and the trapping potential for one particle

$$H_1 = \sum_{s=\pm} \int dx \,\psi_s^{\dagger}(x) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_s(x) \right] \psi_s(x) \tag{5.5}$$

which is written in a different basis

$$\psi_{\uparrow}(x) = \frac{1}{\sqrt{2}}(\psi_{+} + \psi_{-}), \quad \psi_{\downarrow}(x) = \frac{1}{\sqrt{2}}(\psi_{+} - \psi_{-}).$$
(5.6)

Since the superlattice potential  $V_{\pm}(x)$  is the dominant term, we may approximate the bosonic fields as linear combinations of the Wannier modes in this superlattice and in the dressed state basis, a process detailed in appendix C. Note that out of all the terms in the interaction Hamiltonian (5.4), only the first one is insensitive to the state of the atoms. This is important because the asymmetries  $g_1$  and  $g_2$ , when expressed in the dressed basis, produce terms that change the state of the atoms during a collision. Once we introduce the effective interaction constants in the lattice

$$U_i = g_i \int d^3x \ |w(x)|^4 \quad \text{for } i = 0, 1, 2$$
(5.7)

where, w(x) is a Wannier wavefunction, we arrive to the effective Hamiltonian in equation 5.1 with the parameters U, V, t and j that relate to the microscopic model as follows

$$U = \frac{2U_0 + U_1}{4}, \quad V = -\frac{U_1}{8}, \quad t = \frac{U_1}{16} \text{ and } j = \frac{U_2}{8}.$$
 (5.8)
# Chapter 6 Description of theoretical results

In this chapter we start studying the eigenstates of Hamiltonian (5.1) for systems that we can diagonalize exactly. The goals are to characterize the effect of the different interaction and hopping terms, as well as to understand the structure of the ground state wavefunction. Although we are limited to a small number of particles, the following examples provide enough evidence of the roles of correlated hopping, nearest neighbor repulsion and the utility of different correlators to characterize the state. Later on we study the many-body physics of our model for a much larger number of particles using exact analytical methods. We begin with the regime in which the interaction terms Uand V dominate, obtaining the different insulator phases on the j = t = 0 plane. Then, using perturbation theory, we compute the phase boundaries of these insulating regions for growing j and t. Afterwards, we study the properties of the ground state and its excitations in the superfluid phase, with j = 0 and dominating t, proving indeed that this region describes a superfluid of pairs. Having drawn with these methods a rather complete picture of the possible ground states in our model, we close it with the application of some numerical methods. In the limit of strong interactions we find both uniform insulators and a breakdown of translational invariance forming a CDW, while for dominant hopping we expect both single-particle superfluidity and a new phase, a pair superfluid. We now confirm these predictions using two different many-body variational methods.

### 6.1 A two-sites example

Let us take the simplest interesting case, four particles in two sites. We write the Hamiltonian in the basis  $\{|40\rangle, |22\rangle, |04\rangle, |31\rangle, |13\rangle\}$ , where the notation  $|n_1n_2\rangle$  stands for  $n_1$  particles in the first site and  $n_2$  in the second restricting to  $n_1 + n_2 = 4$ ,

$$H_{4/2} = \begin{pmatrix} 0 & -4\sqrt{6}t & 0 & -12j & 0\\ -4\sqrt{6}t & 8V & -4\sqrt{6}t & -6\sqrt{6}j & -6\sqrt{6}j\\ 0 & -4\sqrt{6}t & 0 & 0 & -12j\\ -12j & -6\sqrt{6}j & 0 & 6V & -12t\\ 0 & -6\sqrt{6}j & -12j & -12t & 6V \end{pmatrix} + 6U.$$
(6.1)

Notice that in this particular case, U gives rise to a global energy shift and does not affect the different eigenstates. This is consistent with later studies where we will see that on-site interactions just add a global contribution to the energy that depends on the average density. To better understand the role of the remaining terms, we will consider separately three limiting cases, two of superfluid nature and an insulating one.

### Limit $j \neq 0, t = V = 0$ , single-particle delocalization

In this case we take for simplicity V = 0 and diagonalize equation 6.1, finding as normalized ground state

$$|\psi_{0,t=0}\rangle = \frac{1}{4} |40\rangle + \frac{1}{2} \sqrt{\frac{3}{2}} |22\rangle + \frac{1}{4} |04\rangle + \frac{1}{2} |31\rangle + \frac{1}{2} |13\rangle.$$
(6.2)

Note that this state coincides with the state describing a BEC of 4 particles spread over two sites

$$|\psi_{BEC}(4)\rangle = \frac{1}{\sqrt{4!}} \left(\frac{1}{\sqrt{2}} \sum_{i=1}^{2} c_{i}^{\dagger}\right)^{4} |00\rangle.$$
 (6.3)

This suggests that, at least in this small example, the correlated hopping proportional to j is equivalent to the single-particle hopping in the ordinary Bose–Hubbard model, giving rise to the delocalization of individual particles. However, as it will become evident later on, for larger systems and more particles this interpretation is wrong.

### Limit $j = 0, t \gg |V|$ , pair delocalization

In the presence of two particle hopping, the lowest energy state has the form

$$|\psi_{0,j=0}\rangle = c_{40}(t,V) |40\rangle + c_{22}(t,V) |22\rangle + c_{04}(t,V) |04\rangle$$
(6.4)

with coefficients

$$c_{22}(t,V) \propto -V + \sqrt{12t^2 + V^2}$$
  
$$c_{40}(t,V) = c_{04}(t,V) \propto \sqrt{6t}.$$

In particular, for dominant pair hopping  $t \gg |V|$  this is a state of delocalized pairs

$$|\psi\rangle = \frac{1}{2} |40\rangle + \frac{1}{\sqrt{2}} |22\rangle + \frac{1}{2} |04\rangle.$$
 (6.5)

Observe that this wavefunction is not equivalent to what one would naïvely understand as a "pair condensate" from analogy with the single-particle case

$$|\psi\rangle \neq \left(\sum_{i=1}^{2} c_{i}^{\dagger 2}\right)^{2} |\operatorname{vac}\rangle \sim \sqrt{\frac{3}{8}} |40\rangle + \frac{1}{2} |22\rangle + \sqrt{\frac{3}{8}} |04\rangle.$$

Instead, the previous wavefunction is isomorphic to the BEC of two bosons

$$|\psi_{BEC}(2)\rangle = \frac{1}{2}|20\rangle + \frac{1}{\sqrt{2}}|11\rangle + \frac{1}{2}|02\rangle$$
 (6.6)

under the replacement of each boson with two atoms. It is also interesting to remark that  $\psi_{BEC}(2)$  has larger pair-correlations than  $\psi$ .

#### Limit $|V| \to \infty$ , an insulator

Reusing the previous wavefunction (6.4) and taking the limit of dominant nearestneighbor interaction V, we obtain two possible states. For strong repulsion  $V \to +\infty$ , states  $|40\rangle$  and  $|04\rangle$  are favored, forming a charge density wave (CDW) with partial filling  $|\psi_{CDW}\rangle \propto |40\rangle + |04\rangle$ . On the other hand, for strong nearest-neighbor attractions  $V \to -\infty$ , the particles are evenly distributed forming a Mott insulator  $|22\rangle$ .

### 6.2 Toy model for pair-superfluidity

We have seen that a setup of four particles in a two-sites lattice with  $t \neq 0$ , V, U, j = 0 recreates the exact wavefunction of an ordinary BEC under the replacement of single bosons with pairs. We can test this idea for slightly bigger lattices with either 2 or 4 particles, diagonalizing numerically the Hamiltonian (5.1) containing only the pair hopping term. The resulting wavefunctions are compared side by side with the BEC-like ansatz we mentioned, that is a normal superfluid state for 1 or 2 particles considering each particle as a pair  $(1 \rightarrow 2 \text{ and } 2 \rightarrow 4)$ . In the case of two particles we get indeed the expected result

$$|\psi_2^{g.s.}\rangle = |\psi_2^{ideal}\rangle = \sum_{i=1}^L \frac{1}{\sqrt{2L}} a_i^{\dagger 2} |\text{vac}\rangle$$

whereas for 4 particles in 5 sites

$$\begin{aligned} |\psi_4^{g.s.}\rangle &= c_1 (|40000\rangle + |04000\rangle + |00400\rangle + |00040\rangle + |00004\rangle) + \\ &c_2 (|22000\rangle + |02200\rangle + |00220\rangle + |00022\rangle + |20002\rangle) + \\ &c_3 (|20200\rangle + |20020\rangle + |02020\rangle + |02002\rangle + |00202\rangle) \end{aligned}$$

we find a disagreement between the ideal case of a BEC-like state with coefficients  $c_1 = 1/5, c_2 = c_3 = \sqrt{2}/5$ , and the exact diagonalization with  $c_1 \sim 0.2735, c_2 \sim 0.3073$  and  $c_3 \sim 0.1754$ . We observe that when compared to the ideal BEC, our paired state breaks the translational symmetry, revealing an effective attraction between different pairs, that favors their clustering.

In figure 6.1 we plot the projection between these states, namely the solution of equation 5.1 with only  $t \neq 0$  and the *ideal* superfluid of pairs. In the nearby plot we also analyze two relevant correlators that will be used later on in the manuscript, namely, the single-particle coherence

$$C_{\Delta}^{1} = \frac{1}{L} \sum_{i} \left\langle a_{i+\Delta}^{\dagger} a_{i} \right\rangle \tag{6.7}$$

and the pair correlator

$$C_{\Delta}^{2} = \frac{1}{L} \sum_{i} \left\langle a_{i+\Delta}^{\dagger 2} a_{i}^{2} \right\rangle.$$
(6.8)

As it is evident from the wavefunction and from the plots, there is no single-particle coherence or delocalization because particles move in pairs. Hence,  $C_{\Delta}^1 \sim \delta_{\Delta 0}$ . The other



**Figure 6.1:** (left) Fidelity between the ground state of the Hamiltonian and the *ideal* PSF for the case of 2 particles (circle) and 4 (none). (right) Particle fluctuation (none), one-body correlator (dot-dashed) and two-body correlator (dashed) for the case of 2 particles (circle) and 4 (none) using the ground state of the Hamiltonian.

correlator,  $C^2_{\Delta}$ , which we identify with the delocalization of pairs, is rather large and it only decreases with increasing the lattice size because the total pair density becomes smaller.

### 6.3 No hopping limit: insulating phases

To analyze the phase diagram it is more convenient to work in the grand canonical picture, in which the occupation is determined by the chemical potential  $\mu$ . In this picture the ground state is determined by minimizing the free energy

$$F = H - \mu N, \tag{6.9}$$

where  $N = \sum_{n} n_k$  is the *total* number of particles, including both states  $|+\rangle$  and  $|-\rangle$ . The free energy has a very simple form in the absence of tunneling

$$F = \sum_{k} \left[ \frac{U}{4} : (n_{k} + n_{k+1})^{2} : +Vn_{k}n_{k+1} - \mu n_{k} \right]$$
  
$$= \sum_{k} \left[ \frac{U}{4} (n_{k} + n_{k+1})^{2} + Vn_{k}n_{k+1} - \left(\frac{2\mu + U}{4}\right) (n_{k} + n_{k+1}) \right]. \quad (6.10)$$

This function is defined over positive occupation numbers  $n_k \in \{0, 1, 2, ...\}$ . A discrete minimization will determine the different insulating phases and the regions where the system is stable against collapse.

For a translational invariant system with periodic boundary conditions, all solutions can be characterized as a function of two integers  $\vec{x}^t = (n, m)$ , representing the occupations of even  $n_{2k} = n$  and odd sites  $n_{2k+1} = m$ . The optimization begins by noticing that the



Figure 6.2: Phase diagram for U, V: different regions of stability and insulating phases for t, j = 0.

bond energy of two sites has a quadratic form

$$\varepsilon(\vec{x}) = \vec{x}^t \begin{pmatrix} U/4 & (U+2V)/4 \\ (U+2V)/4 & U/4 \end{pmatrix} \vec{x} - \vec{x}^t \begin{pmatrix} (U+2\mu)/4 \\ (U+2\mu)/4 \end{pmatrix} \\
= \vec{x}^t A \vec{x} - \vec{x}^t \vec{v}$$
(6.11)

where physical solutions are in the sector with  $n, m \ge 0$ . For these occupation numbers to remain bounded, the bond energy  $\varepsilon(\vec{x})$  has to increase as n, m or both grow. This gives us two conditions that need to be fulfilled to prevent collapse.

The first condition appears studying  $\varepsilon(\vec{x})$  along the boundaries of our domain  $(n \ge 0, m \ge 0)$ . Take for instance m = 0, this gives a total energy  $\varepsilon_B = (U/4)n^2 - [(U+2\mu)/4]n$ . For this function to have a local minimum at finite n, we must impose

$$U > 0. \tag{6.12}$$

The second condition comes from analyzing the interior of the domain. For this, we take the only eigenvector of A that lies in the region of positive occupation numbers, n = m = x/2. This line has an energy  $\varepsilon_+ = [(U + V)/4]x^2 - [(U + 2\mu)/4]x$  and, to have again a finite local minimum, we require

$$V > -U. \tag{6.13}$$

Given that equations 6.12 and 6.13 are satisfied, the system is stable and we have two possibilities to attain the minimum energy: either at the boundaries, n = 0 or m = 0, or right on the eigenvector of A. Inspecting  $\varepsilon_B$  and  $\varepsilon_+$  we conclude that a positive value of V will lead to the formation of charge density waves (CDW) of filled sites alternating with empty sites

$$V > 0 \Rightarrow n_{2k} = 0 \text{ or } n_{2k+1} = 0.$$
 (6.14)

If  $V \leq 0$  our energy functional will be convex and the minimum energy state will be a Mott insulator with n = m, when n + m is even, or a charge density wave with  $n = m \pm 1$ , when n + m is odd. The actual choice between these two insulating phases is obtained by computing the energy of both states

$$\epsilon(2n+1) = U(2n+1)^2/4 + Vn(n+1) - (U+2\mu)(2n+1)/4$$
(6.15)

$$\epsilon(2n) = U(2n)^2/4 + Vn^2 - (U+2\mu)2n/4.$$
(6.16)

Having  $\epsilon(2n+1) - \epsilon(2n) = 0$  defines the value of  $\mu$  at which the state with 2n particles every two sites, a Mott with n particles, stops being the ground state and becomes more favorable to acquire an extra particle to form a CDW. The boundaries of these insulating phases for t, j = 0 are given by

$$\mu(2n \to 2n+1) = (U+V)2n \tag{6.17}$$

$$\mu(2n - 1 \to 2n) = (U + V)2n - U. \tag{6.18}$$

Thus summing up, for  $\mu(2n-1 \rightarrow 2n) \leq \mu \leq \mu(2n \rightarrow 2n+1)$  the optimal occupation is n particles per site, forming a Mott, while for  $\mu(2n \rightarrow 2n+1) \leq \mu \leq \mu(2n+1 \rightarrow 2n+2)$  the occupation number is 2n + 1 particles spread over every two sites, and we have a CDW. The results of this section are summarized in figure 6.2.

#### 6.4 Perturbation theory around the Mott phase

The previous calculation can be improved using perturbation theory for  $t, j \ll U, V$ around the insulating phases, obtaining the phase boundaries around the insulators as tand j increase. This is done applying standard perturbation theory up to second order on both variables [42, 43], using as unperturbed Hamiltonian the operator (6.10) and as perturbation the kinetic energy term

$$W = \sum_{i} \left\{ -\left[ t \ c_{i}^{\dagger 2} c_{i+1}^{2} + j \ (n_{i} - 1) c_{i}^{\dagger} (c_{i-1} + c_{i+1}) \right] + \text{H.c.} \right\}.$$
 (6.19)

We start calculating analytically the ground state energies of the first four insulating phases according to (6.10), considering the perturbation W up to second order in j, t (see section 2.2). For the CDW with  $n_i = 1$  and  $n_{i+1} = 0$  this energy is obviously zero

$$E(L/2) = 0. (6.20)$$

For the MI with one particle per site we have virtual processes of the correlated hopping j, as environment-assisted hopping starts being allowed in a uniformly filled lattice

$$E(L) = (U+2V)L/2 - \frac{8j^2}{U-2V}L.$$
(6.21)

For the CDW with  $n_i = 2$  and  $n_{i+1} = 1$ , we find some doubly occupied sites and contributions from the pair hopping t appear

$$E(L+L/2) = (3U+4V)L/2 - \left(\frac{6t^2}{U} + \frac{24j^2}{U-6V} + \frac{32j^2}{U+2V}\right)L.$$
 (6.22)

#### 6.4. Perturbation theory around the Mott phase

Finally, for the MI with two particles per site the ground state energy is

$$E(2L) = (3U+4V)L - \frac{24t^2 + 216j^2}{U-2V}L.$$
(6.23)

Here L is the total number of sites and the results presented in this section are all for the case V < 0. The derivation of these formulas is very similar to the example treated in section 2.2.

At each value of j, t, the boundary of an insulating phase having an average density of  $\bar{n}$  particles per site is given by the degeneracy condition with a compressible state  $E(\bar{n}L) = E(\bar{n}L \pm 1)$ , which are the defect states with either an extra particle or an extra hole. Those points correspond to the chemical potential at which a hole can be introduced  $\mu_h(\bar{n}L) = E(\bar{n}L) - E(\bar{n}L - 1)$  and the one to introduce a particle  $\mu_p(\bar{n}L) =$  $E(\bar{n}L + 1) - E(\bar{n}L)$ . We show here the lower and upper limits of the first four insulating regions, corresponding to the CDW with  $n_i = 1, n_{i+1} = 0$ 

$$\mu_h(L/2) = 0$$
  

$$\mu_p(L/2) = U + 2V + j^2 \left(\frac{2}{V} - \frac{4}{U}\right)$$
(6.24)

the Mott-phase with one particle per site

$$\mu_h(L) = U + 2V + j^2 \left(\frac{4}{U} - \frac{2}{V} - \frac{16}{U - 2V}\right)$$
(6.25)

$$\mu_p(L) = E(L+1) - E(L)$$
  
=  $2U + 2V - 8j - \frac{4j^2}{U} + \frac{2j^2}{V} + \frac{8(j^2 - 6jt - 3t^2)}{U - 2V}$  (6.26)

the CDW with  $n_i = 2, n_{i+1} = 1$ 

$$\mu_h(L+L/2) = 2U + 2V + \frac{48t^2V}{U^2 - 2UV} + j^2 \left(\frac{4}{U} - \frac{2}{V} + \frac{96}{U - 6V} + \frac{24}{U - 2V} + \frac{128}{U + 2V}\right)$$
(6.27)  
$$\mu_p(L+L/2) = E(L+L/2+1) - E(L+L/2)$$

$$= 3U + 4V + j^{2} \left( -\frac{108}{U} + \frac{54}{V} + \frac{96}{U - 6V} + \frac{64}{U + 2V} \right) + 6t^{2} \left( \frac{4}{U} - \frac{8}{3U - 2V} - \frac{4}{U - 2V} - \frac{8}{U - 6V} \right)$$
(6.28)

and the MI with two particles per site

$$\mu_h(2L) = 3U + 4V + 8j + \frac{108j^2}{U} + 24t^2 \left(\frac{2}{U - 6V} + \frac{2}{3U - 2V}\right) - \frac{54j^2}{V} - \frac{24(35j^2 - 3\sqrt{2}jt + 3t^2)}{U - 2V}$$
(6.29)

$$\mu_p(2L) = 4U + 4V - 6\sqrt{6}j - \frac{108j^2}{U} - \frac{48t^2}{U - 6V} - \frac{48t^2}{3U - 2V} + \frac{54j^2}{V} + \frac{32(57j^2 - 12\sqrt{6}jt - 7t^2)}{3U - 6V}.$$
(6.30)



**Figure 6.3:** Phase diagrams for  $\mu$ ,  $j, t \ll |U|$  and V = -0.05. (left) Varying j for t = 0. (right) Varying t for j = 0. In both cases the lowest region is a CDW with alternating 0 and 1 particle occupation, followed upwards by a Mott of one particle per site, a CDW with 1 and 2 particles and the highest area a Mott of two particles.

The corresponding boundaries are plotted in figure 6.3. For small hopping amplitude, they match the values that are found later on with numerical methods. But even for larger values, this approximation anticipates that the insulating lobes are significantly larger for the correlated hopping j than for the pair hopping t.

# 6.5 Analysis of the pair-superfluid with the phase model

So far we have studied the many-body physics around the limit of strong interactions. However, the main goal of this work is to study the effect of correlated hopping and the creation of a pair superfluid. In absence of a mean field theory, but still in the limit of dominant two-body hopping  $U, V \ll t$ , we can use the number-phase representation, introduced in [45] for an ordinary BEC. Note, however, that the model in [45] cannot be directly applied here. Following that reference, one would assume a large number of particles per site,  $n_i > 1$ , and introduce the basis of phase states  $|\vec{\phi}\rangle$ 

$$\langle \vec{n} | \vec{\phi} \rangle = (2\pi)^{-L/2} e^{i\vec{n} \cdot \vec{\phi}}.$$
(6.31)

Using these states, one would then develop approximate representations for the operators  $a_i^2$ ,  $a_i^{\dagger 2}$  and  $n_i$ , and diagonalize the resulting Hamiltonian in the limit of weak interactions. However, after a few considerations one finds that the resulting phase model does not preserve an important symmetry of our system: if j = 0 particles can only hop around in pairs and therefore the parity of each site,  $(-1)^{n_i}$ , is a conserved quantity.

To describe correlated hopping we need to use a basis of states with fixed parity  $\nu$ 

$$\langle 2\vec{n} + \nu' | \vec{\phi} \rangle_{\nu} = (2\pi)^{-L/2} e^{i\vec{n} \cdot \vec{\phi}} \delta_{\nu\nu'}, \quad \nu \in \{0, 1\}$$
 (6.32)

which has to be  $\nu = 0$  for the ground state we are interested in. As mentioned before, we now have to find expressions for the different operators,  $a_i^2$ ,  $a_i^{\dagger 2}$  and  $n_i$ . We use the fact that our states will have a density close to the average value  $\bar{n}$  and approximate the action of the operators over an arbitrary state as

$$n_i \left| \vec{\phi} \right\rangle = \left( -i2\partial_{\psi_i} - \bar{n} \right) \left| \vec{\phi} \right\rangle$$
(6.33)

$$a_i^2 \left| \vec{\phi} \right\rangle = \sqrt{\bar{n}(\bar{n}-1)} e^{-i\phi_i} \left| \vec{\phi} \right\rangle$$
(6.34)

$$a_i^{\dagger 2} \left| \vec{\phi} \right\rangle = \sqrt{(\bar{n}+1)(\bar{n}+2)} e^{i\phi_i} \left| \vec{\phi} \right\rangle.$$
(6.35)

Introducing the constant  $\rho^2 = \bar{n}(\bar{n}-1)(\bar{n}+1)(\bar{n}+2)$  our Hamiltonian becomes similar to the quantum rotor model [45]

$$H = \sum_{i=1}^{L} \left[ 2U\partial_{\phi_i}^2 + (2U+4V)\partial_{\phi_i}\partial_{\phi_{i+1}} + 2\rho^2 t \cos(\phi_i - \phi_{i+1}) \right] - (U+V)L\bar{n}^2.$$
(6.36)

For small U and V, the ground state of this model is concentrated around  $\phi_i - \phi_{i+1} = 0$ . Expanding the Hamiltonian up to second order in the phase fluctuations around this equilibrium point, we obtain a model of coupled harmonic oscillators. This new problem can be diagonalized using normal modes that are characterized by a quasimomentum  $k = 2\pi n/L$ ,  $n \in [-(L-1)/2, (L-1)/2]$ . The result is

$$H = \sum \hbar \omega_k \left( b_k^{\dagger} b_k + \frac{1}{2} \right) + E_0 \tag{6.37}$$

with normal frequencies

$$\omega_k = 4\rho\sqrt{2Ut} \left|\sin(k/2)\right| \sqrt{1 + \left(1 + \frac{2V}{U}\right)\cos\left(k\right)}$$
(6.38)

and a global energy shift  $E_0 = 4(U+V)N^2 - 4L\bar{n}^2(U+V) - 2\rho^2 tL$ .

It is evident from equation 6.38 that our derivation is only self-consistent for negative values of V. Otherwise, when V > 0 some of the frequencies become imaginary signalling the existence of an unbounded spectrum of modes with  $|k| \ge \pi/4$  and that our ansatz becomes a bad approximation of the ground state. This strictly means that our choice  $\phi_i = \phi_{i+1}$  only applies in the case of attractive nearest neighbor interactions,  $-U \le V \le 0$ , as we know that this interaction can not destabilize a translational invariant solution such as the uniform Mott insulator. However, it does not mean by itself that the whole system becomes unstable for V > 0 — indeed, we will show numerically that it remains essentially in a similar phase for all values of V, but in the case of V > 0 the insulating phases are stable until values of the hopping slightly higher as in the V < 0 case.

If we focus on the regime of validity, we will find that the spectrum is very similar to that of a condensate. At small momenta we find the dispersion relation becomes linear,



Figure 6.4: Phase diagram with a Gutzwiller ansatz for U = 1, V = -0.5. We focus on (left) j = 0 and (right) t = 0, separately. Upper plots show average site occupation  $\langle n \rangle$  (color gradient), and number variance  $\Delta n$  (contour). Lower plots show single-particle coherence  $\langle a \rangle$  (color gradient) together with  $\Delta a^2$  (contour).

 $\omega_k \propto v_g k$ , with sound velocity  $v_g = 4\rho\sqrt{2Ut}/\hbar$ , while at larger energies the spectrum becomes quadratic, corresponding to "free" excitations with some mass. This is a consequence of the similarity between our approximate model for the pairs (6.36) and the phase model for a one-dimensional condensate. However, we can go a step further and conclude that the similarity extends also to the wavefunctions themselves, so that the state of a pair superfluid can be obtained from that of an ordinary BEC by the transformation  $n \to 2n$ . This is indeed consistent with what we obtained for the diagonalization of a two-particle state in the limit j, U, V = 0 (see equation 6.6), which was in contradiction with the results in section 6.2 but shows to recover validity when higher densities are considered.

### 6.6 Phase diagram using a Gutzwiller ansatz

The first numerical method that we use to study correlated hopping is a variational estimate of ground state properties based on a product state [67]

$$|\psi_{\rm GW}\rangle = \prod_{i} \sum_{n_i} f_n^{(i)} \frac{1}{\sqrt{n_i!}} c_i^{\dagger n_i} |0\rangle.$$
(6.39)

Minimizing the expectation value of the free energy  $F = H - \mu N$ , with respect to the variables  $f_n$ , under the constraint of fixed norm  $\sum_n |f_n|^2 = 1$ , we will obtain the phase diagram in the phase space of interactions and chemical potential,  $(U, V, j, t, \mu)$ .

In our study we have made several simplifications. First of all, we assumed period-two translational invariance in the wavefunction, using only two different sets of variational parameters,  $f_n^{(2i+1)} = f_n^1$  and  $f_n^{(2i)} = f_n^0$ . In our experience this is enough to reproduce effects such as the CDW. Next, since  $U \ge 0$  is required for the stability of the system, we have taken U = 1 as unit of energy. The limit U = 0 is approximated by the limits  $j, t \gg 1$  in our plots. Finally, in order to determine the roles of j and t, we have studied the cases j = 0 and t = 0 separately. The results are shown in figures 6.4 and 6.5 for V < 0 and V > 0, respectively.

The first interesting feature is that, as predicted by perturbation theory, we have large lobes both with integer (1, 2, ...) and with fractional (1/0, 2/1, ...) occupation numbers, forming uniform Mott insulators and CDW, respectively. The insulators are characterized by having a well defined number of particles per site, and thus no number fluctuations  $\Delta n^2 = \langle n^2 \rangle - \langle n \rangle^2 = 0$ . While the size of the lobes does not depend dramatically on the sign of V, these are significantly larger for the correlated hopping j than for the pair hopping t, as already seen with perturbation theory.

The boundary of the insulating areas marks a second order phase transition to a superfluid regime, where we find number fluctuations  $\Delta n \neq 0$ , and the transition to this gapless regime happens for smaller values of j than for t. In order to characterize these phases we have computed the order parameter of a single-particle condensate  $\langle a \rangle$ , and two quantities that we use to detect pairing. The first one is a two-particle correlation that generalizes the order parameter of a BEC to the case of a pair-BEC  $\langle a^2 \rangle$ . The second quantity  $\Delta a^2 = \sqrt{|\langle a^2 \rangle - \langle a \rangle^2|}$  is used to correct the previous value eliminating the contribution that may come from a single-particle coexisting with the pair-BEC.

When j = 0 we always find that  $\langle a \rangle = 0$ , even outside the insulating lobes. This marks the absence of a single-particle BEC, which is expected since we do not have single-particle hopping. On the other hand, we now find long range coherence of the pairs and thus  $\langle a^2 \rangle \neq 0$  all over the non-insulating area, which we identify with the pair-superfluid regime.

The situation is slightly different for t = 0. The single-particle order parameter  $\langle a \rangle$  no longer vanishes in the superfluid area, denoting the existence of single-particle coherence, but at the same time we find that the two-particle correlations exceed the contribution from the pure superfluid as  $\Delta a^2 \neq 0$ , which we attribute to a coexistence of both a single-particle and a pair-superfluid, or a state with both features.

This picture does not change substantially when V is positive or negative. The only differences are in the insulating region, where the CDW is either due to the incommensu-



Figure 6.5: Phase diagram with a GW ansatz for U = 1, V = 0.5. We focus on (left) j = 0 and (right) t = 0, separately. Upper plots show average site occupation  $\langle n \rangle$  (color gradient) and number variance  $\Delta n$  (contour). Lower plots show single-particle coherence  $\langle a \rangle$  (color gradient) together with  $\Delta a^2$  (contour).

rability of the particle number (V < 0) or really gives rise to the separation of particles alternating holes and filled sites (V > 0). However, in the superfluid regime we find no significant changes and in particular we see no breaking of the translational invariance or modulation of the coherent phase.

### 6.7 Quasi-exact diagonalizations and long-range pair correlations

The previous numerical simulations are very simple and cannot fully capture the single particle and two-particle correlators. To complete and verify the full picture we have searched the ground states of the full Hamiltonian using the so-called iTEBD algorithm introduced at the end of section 2.4, which uses an infinite Matrix Product State ansatz together with imaginary time evolution [113].

Roughly, this ansatz is based on an infinite contraction of tensors that approximates



Figure 6.6: Numerical simulations with the iTEBD algorithm. On the left we plot the results for j = 0, U = 1, V = -0.05 and on the right for V = 0.05, as a function of two-particle tunneling t. The upper row shows the density (dashed) and particle number fluctuations (solid), while the lower row shows  $(\Delta a)^2$  (solid) and two-particle coherence (dashed), which overlap indicating  $\langle a \rangle = 0$ . For each set of operators we show three lines, for  $\mu/U = 0.5$ , 1.5 and 2.5 corresponding to plain line, circle and star, respectively.

the wavefunction of a translational invariant system in the limit of infinite size. Adapting the ansatz to our problem we write it as

$$|\psi\rangle \sim \prod_{k\in\mathbb{Z}} \Gamma^{o}_{\alpha_{2k+1}\alpha_{2k+2}}(n_{2k+1})\lambda^{o}_{\alpha_{2k+2}}\Gamma^{e}(n_{2k+2})_{\alpha_{2k+2}\alpha_{2k+3}}\lambda^{e}_{\alpha_{2k+3}} \times \frac{1}{\sqrt{n_{2k+1}!n_{2k+2}!}}a^{\dagger n_{2k+1}}_{2k+1}a^{\dagger n_{2k+2}}_{2k+2} |\mathrm{vac}\rangle.$$
(6.40)

Here the  $\Gamma^{o}$  and  $\Gamma^{e}$  are matrices that depend on the state of the odd and even sites they represent, a dependence which is signaled by the  $n_{2k+1}$  and  $n_{2k+2}$  in the previous equation. These matrices are contracted with one-dimensional vectors of positive weights  $\lambda_{\alpha}^{e,o} \geq 0$ , which contract the tensors together and are related to the Schmidt coefficients of the equally named decomposition. This variational ansatz is known to work well for states

Figure 6.7: Correlator  $C_{\Delta}^2 = \langle a_{i+\Delta}^{\dagger 2} a_i^2 \rangle$ vs. site separation, for  $(t, \mu) = (0.1, 1.5)$ , (0.3, 0.5), (0.2, 1.5), (0.1, 2.5), from top to bottom. The line with  $t = 0.1, \mu =$ 1.5 (solid, circles) corresponds to a MI state and correlations decay to zero on the third site. The remaining lines have been rescaled and plotted in log-log scale in the inset, which shows that the twoparticle correlator decays approximately as  $\Delta^{-(1-\alpha)}$  with a power  $\alpha \sim 0.4 - 0.5$ .



with fast decaying correlations, but even in the critical phases it gives a good qualitative description of the states.

In order to optimize the iTEBD wavefunction we performed an approximate imaginary time evolution using a Trotter decomposition and local updates of the associated tensors, as described in [81]. Using the canonical forms for these tensors it is also straightforward to compute expectation values for different operators acting either on neighboring or separated sites.

In figure 6.6 we plot the most relevant results for three cuts across the phase diagram, namely for  $\mu = 0.5$ , 1.5 and 2.5, so that they cross both an insulating plateau and the superfluid region. We have used small tensor sizes from D = 16 up to 64, a value limited by the need of using large cutoffs for the site populations ( $n_{max} = 8$ ). As shown in these plots, when j = 0 the single-particle correlator is zero for distinct sites, and we are left only with two-particle correlations. In the MI case the pair correlations between neighboring sites decrease very quickly, while in the superfluid regime we see a critical behavior

$$C_{\Delta}^2 \sim \Delta^{-(1-\alpha)} \tag{6.41}$$

with an exponent that varies between  $\alpha = 0.4$  and 0.5, depending on the simulation parameters.

## 6.8 Some experimental considerations: detection of the phases

All the phases that this model presents are connected by second order quantum phase transitions and can be produced and identified using variations of current experiments [4, 97, 41]. The non-perturbative nature of the effect should help in that respect. The detection method required to discern the phases that our setup may present, depends directly on their characteristics and the particularities we want to observe.

The distinctive features of both the MI and the CDW is a well defined number of particles at each lattice site and the lack coherence. Therefore, their time-of-flight pictures will not reveal interference fringes [49] whereas the noise correlation will show peaks at certain momenta [3, 41]. To discern between this two phases either an adapted scanning electron microscopy [48], a fluorescence imaging [79, 65] of the system combined with pairwise light-assisted collisions [27], or a stimulated-emission-depletion fluorescence microscopy [53] would be adequate to recreate the density distribution along the lattice and determine whether the lattice is homogeneously filled or not. The energy gap in these insulators may be proved either by static [49] or spectroscopic means [100].

When the system enters a superfluid phase, it becomes a perfect "conductor" with a gapless excitation spectrum. The pair superfluid, lacking single-particle order  $C_{\Delta}^1 \sim 0$  a.e., will also lack interference fringes in the time-of-flight images [49]. In order to measure  $C_{\Delta}^2$  and confirm the pairing of the particles, we suggest to use Raman photoassociation to build molecules out of pairs of atoms [62, 123]. Since the molecules will be built coherently onsite, the nonzero correlator  $C_{\Delta}^2$  will translate into long-range order for the molecules. This order should reveal as an interference pattern in time-of-flight images, slightly blurred by the phase fluctuations which are inherent to 1D. When the normal superfluid component appears, this can be probed in a time-of-flight experiment observing interference fringes [49] which intensity will depend on the normal superfluid fraction present in the system.

Atoms in a Feshbach resonance

### Chapter 7

### The physical system for atom-molecule resonances

### 7.1 Feshbach resonances

A Feshbach resonance [38] is the resonance between an unbound state of particles and a bound molecular state. The bound state is formed when the coupling between the internal degrees of freedom leads to a vanishing dissociation energy, *i.e.* when the atomic and molecular states are degenerate. This means that the scattering properties of the particles strongly depend on the energy difference to the bound state, the so-called detuning.

This type of resonances were introduced in nuclear physics to describe the narrow resonances observed in the total cross section in the neutron scattering of a nucleus, which indicated the formation of long-lived compound nucleus with a binding energy close to that of the incoming neutron. The defining feature of a Feshbach resonance is that the states of the incoming particles and the bound state exist in different parts of the Hilbert space of the system, which are called respectively the open and closed channel, as shown in figure 7.1.

Fifteen years later these ideas started to be considered in the realm of ultracold atoms [101]. Due to the low temperature of these gases, their effective interatomic interactions can be considered to be completely determined by the s-wave scattering length. Similarly to the situation of neutron scattering, two atoms can form a diatomic molecule during an s-wave collision. As illustrated in figure 7.1, the two incoming atoms have a different hyperfine state than the formed bound state. The coupling between these is given by the exchange interaction. Due to this difference, the Zeeman shift of these two channels is not the same and their energy difference, the so-called detuning  $\delta$ , can be adjusted tuning the magnetic field. As a consequence, the s-wave scattering length, implying the magnitude and sign of the interatomic interactions, can be tuned.



Figure 7.1: When the atoms in the open channel undergo a low-energy collision, they can get coupled to the closed channel depending on the detuning  $\delta$ , occurring a scattering resonance.

### 7.2 A Hamiltonian for atom-molecule mixtures

We consider a mixture of atoms and molecules in a one-dimensional optical lattice, including the possibility of converting one species into the other, like in a Feshbach resonance where long-lived bound states can be produced. The Hamiltonian of this system can be written as

$$H = -j_{a} \sum_{i} \left( a_{i}^{\dagger} a_{i+1} + \text{h.c.} \right) + \frac{U_{a}}{2} \sum_{i} n_{i}^{a} (n_{i}^{a} - 1) -j_{m} \sum_{i} \left( m_{i}^{\dagger} m_{i+1} + \text{h.c.} \right) + \frac{U_{m}}{2} \sum_{i} n_{i}^{m} (n_{i}^{m} - 1) -\Gamma \sum_{i} \left( m_{i}^{\dagger} a_{i}^{2} + \text{h.c.} \right) + U_{am} n_{i}^{a} n_{i}^{m} + (U_{a} + \delta) \sum_{i} n_{i}^{m}$$
(7.1)

where  $a_i^{\dagger}(a_i)$  are the atom creation (annihilation) operators at the *i*-th site of a onedimensional lattice with L sites, and  $m_i^{\dagger}(m_i)$  are the molecule creation (annihilation) operators at the *i*-th site of the same lattice. For these operators,  $n_i^{a,m}$  are the associated number operators. The atom and molecule hopping amplitudes are given by  $j_a$  and  $j_m$ , and the on-site atom-atom, molecule-molecule and atom-molecule interactions by  $U_a$ ,  $U_m$ and  $U_{am}$  respectively. Finally, the conversion rate between atoms and molecules is denoted by  $\Gamma$ , while the detuning in the Feshbach resonance by  $\delta$  (see section 7.1).

To make our study as close as possible to the experiments, the parameters of the Hamiltonian (7.1),  $j_a, U_a, j_m, U_m, U_{am}$  and  $\Gamma$ , are going to be derived from microscopic considerations (appendix D). The most relevant are shown in figure 7.2. Apart from any intrinsic characteristic of the chosen system (mass of the atoms, wavelength of the light, etc.) which are fixed, the value of these parameters will only depend on the lattice depth  $V_0$ , which is easily adjustable in the experiments through the intensity of the trapping lasers.



Figure 7.2: Parameters of the Hamiltonian (7.1) for a three-dimensional lattice: hopping amplitude of the atoms  $j_a$  (solid), interaction energy of the atoms  $U_a$  (dot-dashed) and conversion rate between atoms and molecules  $\Gamma$  (dashed) in unities of a reference interaction energy  $U_{ref} = U(V_0^{ref} = 35E_r)$ .

Following this motivation of experimental suitability, we notice that experiments with Feshbach resonances are done fixing a value of the magnetic field which determines the detuning  $\delta$ , and the coherence of the system is explored only changing the potential depth  $V_0$  [104, 115]. However, normalizing the detuning  $\delta$  with the on-site interaction  $U_a$  (which increases with  $V_0$ ) would lead to a changing value of  $\delta$  while  $\delta/U_a$  is kept fixed. To avoid that, the detuning will be normalized by a reference value  $U_{ref}$  which is obtained as the on-site interaction for a given lattice depth  $V_0^{ref}$ .

Hence, the control parameters in our problem, corresponding to those of the experiment, are the lattice depth  $V_0$  (fixing the Hamiltonian parameters  $j_a, U_a, j_m, U_m, U_{am}$  and  $\Gamma$ ); the detuning  $\delta$ ; and the total number of particles  $N = \sum_i n_i^a + 2n_i^m$  (in the canonical ensemble) or equivalently the chemical potential  $\mu$  (in the grand canonical ensemble).

## Chapter 8 Description of theoretical results

In this chapter we investigate how the physics of the Bose–Hubbard model (1.9) is enriched by the introduction of the coherent conversion between atom pairs and molecules. When the molecular state is far off-resonant from the atomic one, it can be treated as a virtual state and adiabatically eliminated, resulting in an effective Hamiltonian for the atoms only, as shown in section 8.1. Later on in section 8.2, we will consider a strong coupling expansion, drawing the first phase diagram of the system in the limit of strong interactions. A complete phase diagram will be then drawn using the mean-field approach in section 8.3. Finally, to go beyond the results found with these methods, and inspired by the recent results from Rousseau *et al.* [91, 92], in section 2.4 we will apply a DMRG method to study the spatial structure of the hybrid correlation functions and thereby the recently reported "super-Mott"; an incompressible, yet superfluid phase without atomic or molecular quasi-condensation [91, 92].

### 8.1 Adiabatic elimination of the molecular state

As first step in our study, we would like to understand the effect of a molecular state on the conventional Bose–Hubbard model (1.9). We do this by keeping the molecular level in equation 7.1 far detuned from the atomic one (*i.e.*  $\delta \gg \Gamma$ ), so that it can only take part in virtual processes of second order in the conversion rate appearing in the new effective Hamiltonian.

In the following we assume that the atomic gas is strongly interacting  $U_a \gg j_a$ , so that the double occupancy of a site is strongly suppressed and higher order occupancies are essentially negligible. This allows us to neglect both atom-molecule and molecule-molecule interactions in equation 7.1, which require respectively atom-molecule conversion in triply and in fourfold occupied sites. Deriving the Heisenberg equation of motion (3.15) for the molecular occupation number operator we have

$$i\hbar \frac{dn_i^m}{dt} = -j_m \left( m_{i-1} + m_{m+1} \right) + \delta m_i - \Gamma a_j^2$$
(8.1)

and upon adiabatic elimination of the molecular level  $(\dot{n}_i^m = 0)$ , we can write

$$-j_m (m_{i-1} + m_{i+1}) + \delta m_i - \Gamma a_i^2 = 0.$$
(8.2)

We want the molecules to be constantly in equilibrium with the atoms, to be able to describe any state of the system exclusively in terms of the atoms. To decouple all the modes, we use the following Fourier transformation

$$m_j = \frac{1}{\sqrt{N}} \sum_q e^{iqj} m_q, \quad m_q = \frac{1}{\sqrt{N}} \sum_j e^{-iqj} m_j \tag{8.3a}$$

$$a_j^2 = \frac{1}{\sqrt{N}} \sum_q e^{iqj} [a_j^2]_q, \quad \left[a_j^2\right]_q = \frac{1}{\sqrt{N}} \sum_j e^{-iqj} a_j^2$$
 (8.3b)

obtaining for equation 8.2 that

$$\left(-2j_m\cos k + \delta\right)m_k = \Gamma[a_i^2]_k. \tag{8.4}$$

Now we can express the molecular operators in terms of the atomic ones, in order to find an effective Hamiltonian where the virtual molecular level is eliminated but its effect still to be seen on the atoms. After substitution of this relation between operators into the atom-molecule coupling term in the Hamiltonian (7.1), we obtain as effective term

$$-\Gamma \sum_{i} \left( m_{i}^{\dagger} a_{i}^{2} \right) = -\sum_{ij} V_{i-j} \left( a_{i}^{\dagger} \right)^{2} a_{j}^{2}$$

$$(8.5)$$

where the amplitude for correlated hopping has been defined as

$$V_d = \frac{1}{N} \sum_k \frac{\Gamma^2 e^{ikd}}{\delta - 2j_m \cos k}$$
(8.6)

with d = i - j as the distance between the sites involved.

We are first interested in the correction to the on-site interaction (d = 0) in the offresonant case  $\delta \gg \Gamma$ . Taking these considerations into equation 8.6, we obtain that the conversion term may be approximated as

$$-\Gamma \sum_{i} \left( m_i^{\dagger} a_i^2 \right) = -\frac{\Gamma^2}{\delta} \sum_{i} n_i^a (n_i^a - 1)$$
(8.7)

where we have neglected the molecular hopping amplitude  $j_m$ , given the off-resonant condition. This means that in the far detuned case, our system is equivalent to the Bose-Hubbard model (1.9) with a renormalized interaction strength U

$$U \to U - \frac{2\Gamma^2}{\delta} \tag{8.8}$$

which reduces its effective value.

Let us now examine the behavior of  $V_d$  in the opposite limit of large separation d. In a very big lattice, we can approximate the series in equation 8.6 to an integral over the first Brillouin zone

$$V_d = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \frac{\Gamma^2 e^{ikd}}{\delta - 2j_m \cos k}.$$
(8.9)

#### 8.2. Strong coupling expansion around the atomic solution

Considering the case of  $d \to \infty$ , only the small k part contributes

$$V_{d} \approx \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \frac{\Gamma^{2} e^{ikd}}{\delta - 2j_{m}(1 - \frac{k^{2}}{2})}$$
  
=  $\frac{\Gamma^{2}}{2\pi j_{m}} \int_{-\pi}^{\pi} dk \frac{e^{ikd}}{z^{2} + k^{2}}$  (8.10)

where we have defined  $z = \sqrt{(1-2\alpha)/\alpha}$  and  $\alpha = j_m/\delta$ . As the integrand goes to zero for large k, the limits of the integral can be extended to  $\infty$ 

$$V_d \approx \frac{\Gamma^2}{2\pi j_m} \int_{-\infty}^{\infty} dk \frac{e^{ikd}}{z^2 + k^2}$$
$$= \frac{\Gamma^2}{j_m} \sqrt{\frac{d}{2\pi z}} K_{1/2}(zd)$$
(8.11)

where  $K_{1/2}(x)$  is the modified Bessel function, and the imaginary part of the integral vanishes<sup>\*</sup>. The asymptotic behavior of  $K_{1/2}(x)$  for large values of x

$$K_{1/2}(x) \to \sqrt{\frac{\pi}{2x}} e^{-x}$$
 (8.12)

allows us to safely neglect corrections to the interactions at long-range, because they decrease exponentially with the distance.

### 8.2 Strong coupling expansion around the atomic solution

In this section we explore the phase diagram of the Hamiltonian (7.1) applying degenerate perturbation theory for  $j_a, \Gamma \ll U_a, \delta$  around the insulating phases. We consider a three-dimensional system. According to appendix D.2, the molecular parameters obey the inequalities  $j_m \ll j_a$  and  $U_m, U_{am} \gg U_a$ , so that the molecular hopping is also perturbative.

To apply standard perturbation theory up to second order in  $j_a$  and  $\Gamma$ , we use as unperturbed Hamiltonian the interaction terms of equation 7.1

$$\mathcal{H}_{0} = \frac{U_{a}}{2} \sum_{i} n_{i}^{a} (n_{i}^{a} - 1) + \frac{U_{m}}{2} \sum_{i} n_{i}^{m} (n_{i}^{m} - 1) + U_{am} n_{i}^{a} n_{i}^{m} + (U_{a} + \delta) \sum_{i} n_{i}^{m}$$

$$(8.13)$$

and as perturbation its kinetic energy and conversion terms

$$\mathcal{W} = -j_a \sum_{i} \left( a_i^{\dagger} a_{i+1} + \text{h.c.} \right) - j_m \sum_{i} \left( m_i^{\dagger} m_{i+1} + \text{h.c.} \right)$$
$$- \Gamma \sum_{i} \left( m_i^{\dagger} a_i^2 + \text{h.c.} \right).$$
(8.14)

<sup>\*</sup>It is an odd function over an even interval.

Proceeding as in other sections (e.g. for atoms with correlated hopping in section 6.4), we calculate the ground state energies of the first two insulating phases according to equation 8.13 and apply the perturbation (8.14) up to second order in  $j_a$  and  $\Gamma$ . Here, we are going to directly present the results to second order in the perturbation  $\mathcal{W}$ , *i.e.* the values of the chemical potential defining the lower  $\mu_h(N)$  and upper  $\mu_h(N)$  boundaries of the insulating lobe with n = N/L particles per site, where N is the total number of particles and L is the lattice length. These boundaries are given by the degeneracy condition of the insulating phase with a compressible state, where these compressible states are defect states with either an extra particle or an extra hole in the system (compared to the insulator). For the introduction of a hole we obtain the lower boundaries of the insulating states with one particle per site

$$\mu_h(L) = 6j_a - \frac{12j_a^2}{U_a} \tag{8.15a}$$

and two particles per site

$$\mu_h(2L) = U_a + 12 \left[ 1 - \frac{2\Gamma^2}{\delta^2} \right] j_a - \frac{27j_a^2}{U_a} - \frac{2\Gamma^2}{\delta}.$$
 (8.15b)

For the introduction of a particle we obtain the upper boundaries of the insulating states with one particle per site

$$\mu_p(L) = U_a - 12 \left[ 1 - \frac{2\Gamma^2}{\delta^2} \right] j_a + \frac{3j_a^2}{U_a} - \frac{2\Gamma^2}{\delta}$$
(8.15c)

and two particles per site

$$\mu_p(2L) = 2U_a - 18 \left[ 1 - \frac{6\Gamma^2}{(U_{am} - 2U_a + \delta)^2} \right] j_a + \frac{12j_a^2}{U_a} + \frac{2\Gamma^2}{\delta} - \frac{6\Gamma^2}{U_{am} - 2U_a + \delta}.$$
 (8.15d)

We have also included terms of third order  $t_a\Gamma^2$  to see the effect of the perturbation when taken as a renormalization of the Bose–Hubbard model, what has already been studied in the adiabatic elimination (section 8.1) and what will be further compared with the results in the mean-field approximation in section 8.3.

In figure 8.1 we plot the insulating boundaries obtained using the strong coupling expansion (8.15). Note that the lowest boundary  $\mu_h(L)$  for a finite value of the detuning (solid line) does not change with respect to the results for the Bose–Hubbard model (dashed line). This occurs because  $\mu_h(L)$  is located in a region of very low density, where the number of atoms is not enough for molecules to be formed and therefore, for conversion to take place. We can also observe in this figure that the tendency of the lobes is to shrink and get shifted downwards in the chemical potential scale. As seen in the adiabatic elimination of the molecular state in equation 8.8, this can be understood as the reduction of the effective on-site repulsion felt by the atoms, due to the energy correction introduced by the atom-molecule conversion  $\Gamma$ .



Figure 8.1: Phase diagram for  $j_a, \Gamma \ll U_a, \delta$ using a strong coupling expansion to second order. Considering a very large detuning  $\delta \to \infty$  gives back the well known results of the Bose–Hubbard model (dashed). Considering a lower value of this variable modifies the boundaries of the insulating region, as seen here for  $\delta = 15U_{ref}$  (solid). The lattice depth  $V_0$  in this plot goes from  $35E_r$  to  $10E_r$ , and the Hamiltonian parameters are calculated accordingly, with exception of the detuning that is given in units of the potential  $V_0^{ref} = 35E_r$ .

### 8.3 Phase diagram using a mean-field approach

As introduced for the Bose–Hubbard model [99], the mean-field approach to a lattice Hamiltonian relies on the approximation

$$a_i a_j^{\dagger} \sim \langle a_i \rangle a_j^{\dagger} + a_i \langle a_j^{\dagger} \rangle - \langle a_i \rangle \langle a_j^{\dagger} \rangle \tag{8.16}$$

where  $\alpha_i = \langle a_i \rangle = \langle a_i^{\dagger} \rangle$  is the so-called superfluid parameter, which is determined by self-consistency in the resulting one-site problem. In the particular case of homogeneous lattices, translational invariance yields  $\alpha_i = \alpha$ . This equation allows us to rewrite the Hamiltonian (7.1) as a sum of on-site operators  $H_i$ 

$$H = \sum_{i} H_{i}$$
(8.17a)  

$$H_{i} = -j_{a}\alpha \left(a_{i}^{\dagger} + a_{i+1}^{\dagger} + a_{i} + a_{i+1}\right) + \frac{U_{a}}{2}n_{i}^{a}(n_{i}^{a} - 1)$$
$$-j_{m} \aleph \left(m_{i}^{\dagger} + m_{i+1}^{\dagger} + m_{i} + m_{i+1}\right) + \frac{U_{m}}{2}n_{i}^{m}(n_{i}^{m} - 1)$$
$$-\Gamma \left(m_{i}^{\dagger}a_{i}^{2} + \text{h.c.}\right) + U_{am}n_{i}^{a}n_{i}^{m} + (U_{a} + \delta)n_{i}^{m}$$
(8.17b)

where we have omitted the constant terms. It turns out that, considering a translational invariant system, one is left with (*L* identical copies of) a single-site problem; where  $\alpha = \langle a_i \rangle$  is the superfluid parameter of the atoms and  $\aleph = \langle m_i \rangle$  the one of the molecules. Reducing in this way the problem to the minimization of an one-site Hamiltonian, this procedure is equivalent to using a Gutzwiller ansatz (2.26), as we are solving self-consistently the problem for a single site and taking the full solution as a product of solutions for individual sites.

Defining the total number of particles operator  $N = \sum_{i} n_i^a + 2n_i^m$ , and minimizing the expectation value of the free energy  $F = H - \mu N$  for the Hamiltonian 8.17 in the grand canonical formalism, we obtain the ground state of the system and use it to draw the phase diagram of the system, which is shown in figure 8.2 for different values of the



Figure 8.2: Phase diagram following the mean-field approach, drawn for different values of the detuning:  $\delta \to \infty$  (upper left),  $\delta = 5U_{ref}$  (upper right),  $\delta = U_{ref}$  (lower left), and  $\delta = 0$  (lower right). The variable plotted as color gradient is the atomic number fluctuations per site  $\Delta n_i^a$ , and the lines correspond to the normalized atomic one-body correlator  $\langle a_i \rangle / \langle n_i^a \rangle$ . While the dashed lines hold a label with their value, the solid lines surround the areas where the coherence  $\langle a_i \rangle$  is negligible.

detuning. Such minimization procedure must be performed self-consistently, since the ground state of H itself depends on the set of superfluid parameters  $\alpha$  and  $\aleph$ .

In comparison to the previous methods, with this approach we are not only able to study the off-resonant limit  $\delta >> \Gamma$ , but also the resonant regime. As mentioned in section 7.2, the parameter values are going to be chosen close to the experimental ones. The detuning takes a constant value, set in experiments by the magnetic field, and it is fixed as a multiple of a reference value of the on-site interaction  $U_{ref}$ , which is defined by a lattice depth  $V_0^{ref} = 35E_r$ . The rest of parameters,  $U_a, U_m, U_{am}, j_a, j_m$  and  $\Gamma$ , are calculated from the varying lattice depth  $V_0$  as in appendix D.2.

Our first results take us to figure 8.2, where we see that the phase diagram of the system presents incoherent lobes  $\langle a_i \rangle = 0$ , like the Mott lobes appearing for strong interactions in the Bose–Hubbard model. However, the atom fluctuations  $\Delta n_i^a$  do not vanish as would occur in a mean-field treatment. It is in figure 8.3 that we observe that these lobes do not correspond to a purely atomic incompressible phase. They indicate the presence of a hybrid incompressible phase, as the vanishing dispersion condition belongs to the total



Figure 8.3: Phase diagram following the mean-field approach, drawn for different values of the detuning:  $\delta \to \infty$  (upper left),  $\delta = 5U_{ref}$  (upper right),  $\delta = U_{ref}$  (lower left), and  $\delta = 0$  (lower right). The variable plotted as color gradient is the total number of particles per site  $N_i = n_i^a + 2n_i^m$ , and the lines correspond to the associated number fluctuations  $\Delta N_i = \Delta (n_i^a + 2n_i^m)$ . While the dotted lines hold a label with their value, the solid lines surround the areas with negligible particle number fluctuations  $\Delta N_i$ .

number of particles per site  $N_i = n_i^a + 2n_i^m$ . Only the lowest lobe, corresponding to  $N_i = 1$ , remains purely atomic and disappears when the system is fully at resonance  $\delta = 0$ .

The disappearance of the  $N_i = 1$  lobe can be explained as follows. As the detuning decreases and the lattice depth increases (*i.e.*  $j_a/U_a$  decreases), the Hamiltonian favors the localization of the atoms in each well, compensating for their localization energy with an increasingly efficient conversion mechanism of atom pairs into molecules, which can only happen in sites with at least two particles. Besides, the molecules have a lower localization energy, as their hopping amplitude  $j_m$  is significantly lower than that of the atoms. In sites with more than two particles, this effect is magnified by the presence of spectator atoms, which remain localized without participating in the atom-molecule conversion but introducing a boson-enhancement factor to this term. However, we should also consider that these sites suffer from additional energy penalties — the atom-molecule interaction, which is higher than the interaction between three atoms (see appendix D.2).

The dynamic of the other lobes can be explained as follows. When the lattice depth increases,  $\Gamma$  grows slower than  $U_{am}$ , which leads to a dominating repulsion for a sufficiently

small detuning. As a consequence, very few molecules appear in sites with two or more particles, having that these lobes remain approximately of the same size and the atomic density becomes slightly smaller (due to the few appearing molecules). This shifts the lobes to smaller values of the chemical potential, as seen in the adiabatic elimination and perturbation theory. But when the detuning grows, the conversion takes the main role. For a growing potential depth, the interaction strength  $U_{am}$  dominates over  $\Gamma$  in sites with particle occupation bigger than two. In this case, sites with three particles may find convenient to get rid of a particle to be able to convert atoms into molecules without paying an additional  $U_{am}$ . As a result, the lobe corresponding to  $N_i = 2$  is greatly magnified by lowering the detuning, taking over part of location of the  $N_i = 3$  lobe and displacing completely the singly occupied lobe at  $\delta = 0$ . Lobes with a higher occupation number are displaced along the  $\mu$  axis and their sizes are not affected to such a great extend.

Given that the density which is mostly affected by the atom-molecule conversion is that of two particles per site, in the following we proceed fixing the occupancy to  $N_i =$  $n_i^a + 2n_i^m = 2$ . This is attained varying systematically the chemical potential  $\mu$  until finding the value yielding  $n_i^a + 2n_i^m = 2$ . In figure 8.4 we see that the hybrid threebody coherence  $\langle m_i^{\dagger} a_i^2 \rangle$  (in color) grows significantly when the molecules start forming in the system (*i.e.* when lowering the detuning  $\delta$ ), modifying the physics of the Bose-Hubbard model. Looking at the normalized one-body correlator  $\langle a_i \rangle / \langle n_i^a \rangle$  (in black), we notice that the superfluid-insulator boundary is not very sensitive to the detuning  $\delta$  for values of  $\delta \geq 20U_{ref}$ . Below this value the boundary first moves to bigger values of the potential depth  $V_0$ , as expected from the reduction of the effective atom-atom interaction coming from the off-resonant atom-molecule conversion (see section 8.1). In this far off-resonant regime we observe a simple renormalization of the Bose–Hubbard physics by the virtual atom-molecule conversions. By decreasing  $\delta$  even further, the superfluid-insulator boundary occurs at a maximum potential depth for a critical value of the detuning  $\delta_c \simeq 8U_{ref}$ , and then it starts to move to lower values of  $V_0$ . This strong crossover in the behavior of the boundary reveals the onset of the nearly resonant regime. In this regime, a significant fraction of particles appearing in the ground state of the system are molecules because the atom-molecule conversion becomes increasingly efficient.





Figure 8.5: Critical value of the atomic hopping for the superfluid-insulator boundary. According to the perturbation theory  $j_c^{down^{PT}}(\delta)/U_a$  (dashed) and  $j_c^{low^{PT}}(\delta)/U_a$ (dot-dashed). According to the mean-field calculation  $j_c^{MF}(delta)/U_a$  (dotted). The inset shows in detail the place where results start to differ from each other.

This crossover is captured by the behavior of the atom-molecule coherence  $\langle m_i^{\dagger} a_i^2 \rangle$ , which remains very small and weakly dependent on the detuning  $\delta$  for  $\delta > \delta_c$ , while it starts growing significantly with decreasing  $\delta$  below this critical value  $\delta_c$ .

To be able to compare directly our mean-field results with the strong coupling expansion in section 8.2, we are going to keep the conversion rate  $\Gamma$  locked to a value such that  $\Gamma \ll U_a$  and we will keep constraining our mean-field problem to systems with an average of two particles per site, as it is the simplest case where conversion between atoms and molecules can take place. In figure 8.5 we compare the results from these two methods. On the one hand, we consider the renormalization introduced by  $\Gamma$  to the atomic hopping amplitude in the perturbation theory when compared to the Bose–Hubbard model, taken from both the lower (dashed) and upper (dash-dotted) boundaries of the Mott insulating region of two particles (equations 8.15b and 8.15d respectively)

$$j_c^{downPT}(\delta) = j_c(\infty) \cdot \left[1 - \frac{2\Gamma^2}{\delta^2}\right]$$
(8.18)

$$j_c^{upPT}(\delta) = j_c(\infty) \cdot \left[1 - 6\Gamma^2 / (U_{am} - 2U_a + \delta)^2\right]$$
(8.19)

where  $j_c(\infty)$  is the critical value of the atomic hopping for the Bose–Hubbard model ( $\delta \rightarrow \infty$ ) using mean-field. On the other hand,  $j_c^{MF}(\delta)$  (dotted) corresponds to the superfluidinsulator boundary taken from the mean-field results and defined by the appearance of the one-particle coherence  $\langle a \rangle$  (see figure 8.4).

For  $\delta > 20U_{ref}$  the results from both methods have a very good agreement, presenting just slight differences for smaller values of the detuning until  $\delta \sim 5U_{ref}$ . At this point the perturbation theory results  $j_c^{down,up}^{PT}(\delta)$  clearly break down and mean-field shows a crossover from the off-resonant to the resonant behavior. At this crossover, the critical hopping  $j_c^{MF}(\delta)$  signaling the superfluid-insulator transition starts to increase upon lowering the detuning. This occurs because for a small detuning, the Hamiltonian energetically favors the atom localization and the local atom-molecule conversion, over a minimization of the kinetic energy through the atomic hopping.

Mean-field studies are not able to point out correlations between different sites. However, inspired by recent results [91, 92] where it is shown the appearance of an "insulating" phase with a "hybrid superfluid fraction" in this model, we would like to study



Figure 8.6: Phase diagram according to the DMRG method. In the left column we have the fluctuations in the number of atoms per site  $\Delta n_i^a$  (color gradient) and the number of atoms per site  $\langle n_i^a$  (lines). In the right column we show the fluctuations in the number of particles per site  $\Delta N_i$  (color gradient), where  $N_i = n_i^a + 2n_i^m$ , while the lines frame the areas with integer particle occupation  $\langle N_i \rangle$ . The upper plots correspond to a detuning  $\delta = 0$  and the lower ones to  $\delta = U_{ref}$ , where  $V_0^{ref} = 35E_r$ .

the long-range correlations of this mixed exotic phase to learn more about its nature. With mean-field we cannot access long-range order indicators, and therefore we cannot discriminate between an insulating phase with local conversion and a phase with hybrid counterpropagating currents. This should be decided using a Density Matrix Renormalization Group method (see section 2.4), looking at the spatial structure of long-range correlators.

### 8.4 Quasi-exact diagonalizations and study of longrange correlations

In this section, we study a one-dimensional version of our system (7.1), implementing a Density Matrix Renormalization Group method based on Matrix Product States (see section 2.4). Our motivation originates from recent results [91, 92], where an incompress-



**Figure 8.7:** Density of particles per site  $\langle N_i \rangle = \langle n_i^a + 2n_i^m \rangle$  (left) and fluctuations in this number  $\Delta N_i$ , according to the DMRG method for  $U_a = 8j_a$ ,  $U_{am} = 12j_a$ ,  $U_m \to \infty$ ,  $\Gamma = 0.5j_a$ ,  $j_m = 0.5j_a$ , and different values of the detuning  $\delta$  and the chemical potential  $\mu$ . Upper plots correspond to a lattice of 20 sites, and the more detailed lower ones to 40 sites.

ible yet superfluid "super-Mott" phase is observed for this system using quantum Monte Carlo methods. Our goal in this section is to study the spatial structure of correlations, to learn more about the intriguing properties of this phase.

In this first part, the Hamiltonian parameters are calculated from microscopical principles as done in previous sections (see appendix D.2), but taking d = 1 as it is for a one-dimensional lattice. The conversion rate  $\Gamma$  will be kept constant, according to the following reasoning. As  $\Gamma$  depends on the lattice depth  $V_0$  (it depends on the overlap between the atomic and molecular states in each site), it will grow when  $V_0$  increases, as the states in each well become narrower in a deeper potential. But in a 1D lattice this dependence is much weaker than in 3D, because in one-dimensional systems the size of the wavefunction in the transversal direction is fixed and it may only change in the longitudinal direction of the lattice. Therefore, taking the conversion rate  $\Gamma$  independent of  $V_0$  is an acceptable approximation that for the sake of simplicity we will make. We are going to lock the value of this rate to  $\Gamma(V_0^*)$ , for  $V_0^* = 10E_r$ . Due to the dimensional



Figure 8.8: Atomic (color) and molecular (black) site occupation in the  $\mu - \delta$  plane.

mismatch, the results obtained in this section cannot be compared directly with previous ones. However, the nature of the phases remains unaffected.

A "super-Mott" phase has been defined as an incompressible phase, like a Mott insulator, containing a "supercurrent" for each species, but without a global flow [91]. These "supercurrents" propagate in opposite directions, as seen from the correlated and anticorrelated windings [91, 92] of Monte Carlo simulations. With DMRG we cannot observe these superfluid fractions, but we can study how the many-body correlations change between different lattice sites in distinct points of the phase diagram. For instance, given a certain Hamiltonian where atoms are involved, we can find its ground state and calculate the two-body atomic correlator  $C^a_{\Delta} = \langle a^{\dagger}_i a_{i+\Delta} \rangle$ . This quantity shows the atomic correlations present between two sites separated by a distance  $\Delta$ , and we would like to distinguish their form. If we find that the correlator decays exponentially, the system is then in an insulating state. On the contrary, if the decay is algebraic, there is a finite superfluid fraction in the system and fitting the correlator using

$$C^a_\Delta \sim \Delta^{-(1-\alpha)},\tag{8.20}$$

gives us three possibilities: if  $\alpha = 1$  we have a condensate (only possible in 3D or in 2D a zero temperature); if  $0 < \alpha < 1$  we have a quasi-condensate; or if  $\alpha < 0$  we do not have any condensation.

For our problem we study three such correlators:

$$C^a_{\Delta} = \langle a^{\dagger}_i a_{i+\Delta} \rangle \tag{8.21a}$$

$$C_{\Delta}^{m} = \langle m_{i}^{\dagger} m_{i+\Delta} \rangle \tag{8.21b}$$

$$C_{\Delta}^{am} = \langle m_i a_i^{\dagger^2} m_{i+\Delta}^{\dagger} a_{i+\Delta}^2 \rangle \tag{8.21c}$$

the atomic, the molecular and the hybrid, respectively. The latter should tell us if there are strong phase correlations of composite objects: two atoms and a molecular hole (or two atomic holes and a molecule), what could be understood as a counterpropagating flow of the species without a net mass current.

Using these correlators we are going to study the phase coherence of atoms and molecules, and the phase coherence between atoms and molecules. Moreover, to probe



**Figure 8.9:** Phase diagram in the  $\mu - D$ plane (D relates to the detuning as  $D = \delta - U_a$ ) presented by Rousseau *et al.* [91] for parameter values  $U_a = 8j_a, U_{am} = 12j_a, U_m \rightarrow \infty$ , and  $\Gamma = 0.5j_a$ . This figure is published with the kind permission of V. G. Rousseau.

the nature of the spectrum of the system for particle-hole excitations, we are going to investigate the fluctuations in the total number of particles  $\Delta N_i$  and the compressibility of the system  $\partial \rho / \partial \mu$ , where  $N_i = n_i^a + 2n_i^m$  is the number of particles per site operator and  $\rho$  is the particle density, which coincides with  $\langle N_i \rangle$  in the thermodynamical limit. These quantities give us information about the compressibility of the system at a local and global level, respectively.

In figure 8.6 we have the phase diagram for different values of the detuning. These diagrams do not introduce any new features when compared to the mean-field diagrams already drawn in figures 8.2 and 8.3. Indeed a study of the decay of  $C_{\Delta}^{am}$  in the insulating lobes, where the compressibility  $\partial \rho / \partial \mu$  vanishes, does not indicate algebraic hybrid correlations. We find that the decays of  $C_{\Delta}^{am}$ ,  $C_{\Delta}^{a}$  and  $C_{\Delta}^{m}$  are exponential with the distance. This indicates the existence of an insulator, where atom-molecule conversion takes place independently in each well. In retrospect, this suggests that current experiments may not be able to observe the "super-Mott" phase, due to the experimental constraints imposed on the Hamiltonian parameters.

Instead, we are going to employ the Hamiltonian parameters proposed by [91] to ascertain that our indicators can identify a "super-Mott" phase. Although these parameters are not experimentally feasible, they turn out to be fine-tuned in order to demonstrate the *existence* of the "super-Mott" phase [91, 92]. Their molecular hopping amplitude  $j_m = j_a/2$  is considerably bigger than ours, which makes their molecules comparatively much lighter, having a lower effective mass. Their interactions are very strong,  $U_a = 8j_a$ ,  $U_{am} = 12j_a$ , and they consider hard-core molecules,  $U_m \to \infty$ . Their conversion rate between atoms and molecules is very low,  $\Gamma = 0.5j_a$ .

Using these parameters, we carry out the same study to look for a phase diagram similar to that in figure 8.9 [91]. In the upper left part of figure 8.7 we have the total number of particles per site  $\langle N_i \rangle$ . In this plot, the lower area framed in white corresponds to a phase with one particle per site, and the upper area framed in black corresponds to a phase with two particles per site. Calculating the fluctuations in the number of atoms suggests that the lower area is an atomic Mott insulator. The upper area framed in black is the candidate region for a "super-Mott" phase. In the upper right plot, we have the fluctuations in the number of particles per site. The local minima of these fluctuations coincide with the integer-filled regions of  $\langle N_i \rangle = 1$  and 2. The incompressible nature of these regions is confirmed with the study of the global compressibility of the system  $\partial \rho / \partial \mu$ . This is shown in the upper left plot of figure 8.10 for a zoomed area of the phase diagram. The lower plots of figure 8.7 correspond to this same area. It is important to remark that for very large detuning, we recover the physics of the Bose–Hubbard model in one dimension, observing the cut of the first lobe and the tip of the second corresponding to  $j_a = 0.125U_a$  in the inset of figure 2.3 [43].

To study the spatial structure of correlators, we move to figure 8.10. As mentioned before, in the upper left plot we have the global compressibility  $\partial \rho / \partial \mu$  for a lattice of 40 sites. The black area corresponds to an incompressible phase with two particles per site. The marked points in the  $(\mu, \delta)$  plane are in correspondence with the following plots, where the hybrid correlation decay  $C_{\Delta}^{am}$  is shown<sup>†</sup>, with insets displaying the atomic correlation decay  $C_{\Delta}^{a}$  (upper right) and the molecular correlation decay  $C_{\Delta}^{m}$  (lower left). We describe this results following an order from left to right while going downwards. The first plot corresponds to the yellow dot  $(\mu/j_a, \delta/j_a = 10.6, 5)$ , the second to the gray square (9.4, 3.5), the third to the red diamond (9.6, -1), the fourth to the gray dot (10.8, -1) and the fifth to the yellow square (8.6, -5).

Plots corresponding to the incompressible area (yellow and red markers) show exponentially decaying  $C_{\Delta}^a$  and  $C_{\Delta}^m$ , as atomic and molecular insulators would do. But in the central point (red diamond) we observe that  $C_{\Delta}^{am}$  has an algebraic decay, with a coefficient  $\alpha < 0$  (see equation 8.20). This evidences the emergence of strong phase correlations of composite objects. We will identify this phenomena with the predicted "super-Mott" phase. These plots suggest that reducing the detuning between the species, we have a transition from an atomic Mott insulator ( $\delta \gg j_a$ ), to a "super-Mott" phase ( $|\delta| \sim j_a$ ), and finally to a molecular Mott insulator ( $\delta \ll j_a$ ). This idea is supported by an analysis of figure 8.8, where the occupation of each species is displayed. We observe a "super-Mott" phase values of the detuning ranging approximately from  $\delta \sim -2j_a$  to  $2j_a$ . Plots corresponding to the compressible area (gray markers) display algebraically decaying  $C_{\Delta}^a$  and  $C_{\Delta}^m$ , as would occur in a superfluid. However, this study needs to be extended to larger systems. To this end, an accurate finite-size scaling analysis of our results is currently in progress.

In our simulations, a "super-Mott" phase seems to be realized under two conditions: on the one hand the global compressibility has to vanish; and on the other hand, atomic and molecular occupancies should be comparable,  $\langle n_i^a \rangle \sim 2 \langle n_i^m \rangle$ , which occurs close to the Feshbach resonance,  $|\delta| \sim j_a$ . Indeed this second condition appears fundamental to guarantee that atomic currents can be compensated by opposite molecular currents, in order to keep the system insulating to independent atomic and molecular currents, and conducting to correlated counterpropagating currents.

We have not been able to observe this "super-Mott" phase using a realistic parameter range that would be feasible in experiments. Whether it is possible to attain experimentally the regime proposed by Rousseau *et al.* and observe the "super-Mott" phase remains to be discussed. However, we present quantities to discriminate this phase that can be measured in experiments: density fluctuations and long-range correlations. How these

<sup>&</sup>lt;sup>†</sup>All correlations have their asymptotic part taken away, *i.e.*  $C^x_{\Delta} = \langle x_i^{\dagger} x_{i+\dagger} \rangle - \langle x_i^{\dagger} \rangle \langle x_{i+\dagger} \rangle$ , although it may not be explicitly indicated.


Figure 8.10: Counting graphs from left to right and downwards, the first shows the incompressibility  $\partial \rho / \partial \mu$  in the  $(\mu, \delta)$  plane for a lattice of 40 sites. Other plots show the hybrid correlation decay  $C_{\Delta}^{am}$  for the points marked the first figure: the second plot corresponds to the yellow dot (10.6, 5), the third to the gray square (9.4, 3.5), the fourth to the red diamond (9.6, -1), the fifth to the gray dot (10.8, -1) and the sixth to the yellow square (8.6, -5); in brackets we show the  $(\mu, \delta)$  values in units of  $j_a$ . The plotted lines show the decay of the respective correlators with the distance  $\Delta$ . Insets show the atomic correlation decay  $C_{\Delta}^a$  (upper right) and the molecular correlation decay  $C_{\Delta}^m$  (lower left). These results have been obtained using a DMRG algorithm for parameter values  $U_a = 8j_a$ ,  $U_{am} = 12j_a$ ,  $U_m \to \infty$ ,  $\Gamma = 0.5j_a$ , and  $j_m = 0.5j_a$ .

quantities relate to the ones presented in [91, 92] remains to be seen. These details could shed some light on the differences presented between both works, *e.g.* our  $\langle N_i \rangle = 2$  phase appears to be significantly smaller when compared to figure 8.9 by Rousseau *et al.*. It would be interesting also to study how and exactly under which conditions the transition between the "super-Mott" phase and the Mott insulator with two atoms per site takes place.

# Appendix

## Appendix A

# Writing a DMRG algorithm with MPS

DMRG can be seen as an iterative method based on matrix product states (2.29), that for a fixed dimension D determines the matrices A[i] whose state  $|\psi\rangle$  minimizes the energy of the problem in a variational sense. In this appendix we describe in detail how this is done; explaining in section A.1 how to normalize a state, and introducing in section A.2 the effective Hamiltonian used at every step of the algorithm when the minimization problem is formulated at each site of the lattice.

The initial ansatz is set with all A[i] containing random entries. Let us recall from section 2.4 that in general these A[i] are tensors with three indices: *i.e.*  $A[i] \rightarrow A[i]_{\alpha,s_i,\beta}$  where  $\alpha$  and  $\beta$  run from 1 to D, and the physical index  $s_i$  from 1 to d.

Observing equation 2.29, it should be evident to the reader that the choice of the matrices A[i] is not unique, as making the following change

$$A[i] \to \tilde{A}[i] = X_i A[i] X_{i+1}^{-1}$$
 such that  $X_i \in M_{D \times D}$ 

does not alter the state  $|\psi\rangle$ , for any set of non-singular matrices X. Thus, we can choose a gauge condition at each site of the lattice to fix this mathematical freedom. These conditions constitute the so-called normal form [85]. They arise in a natural way when MPS are introduced as explained in section 2.4. If we begin this procedure at some location k, and run the algorithm to the right of k, we will be looking for a matrix  $\tilde{A}[k]$ such that the following condition is fulfilled

$$\sum_{\alpha,s_k} \tilde{A}[k]_{(\alpha,s_k),\beta} \bar{\tilde{A}}[k]_{(\alpha,s_k),\beta'} = \delta_{\beta,\beta'}$$
(A.1)

which is the normalization condition written component-wise. When moving to the left, equation A.1 should be replaced by

$$\sum_{s_k,\beta} \tilde{A}[k]_{\alpha,(s_k,\beta)} \bar{\tilde{A}}[k]_{\alpha',(s_k,\beta)} = \delta_{\alpha,\alpha'}.$$
(A.2)

Conditions (A.1) and (A.2) can be thought to ensure A[k] being a "unitary" matrix<sup>\*</sup> or

<sup>\*</sup>Though they are not proper unitary matrices because they are rectangular, we take the freedom to call them so.

that it is "normalized", because matrices fulfilling the normal form lead to a normalized state.

This initial normalization routine is explained in section A.1, it allows us to find a unitary A[k]. We repeat this sequentially to each matrix until we reach one end of the chain and then backwards, until we have normalized all the matrices and be back to the initial one.

Then we construct the *effective Hamiltonian* at site k, that is the Hamiltonian written only as a function of the matrix A[k] at the site we are considering. This Hamiltonian will be used for the minimization of the energy in terms of the current A[k]. How to write this Hamiltonian and solve the associated local problem is elaborated in detail in section A.2. From this procedure we obtain an optimal A[k] that minimizes the energy of the state at this step.

We normalize the state again and move to the next site to proceed in the same way, until the total energy of the system converges. In other words, the procedure is continued until a fixed point is reached, something which always occurs since the energy is a monotonically decreasing function of the step number [109]. Thereof, this is a variational method which always converges.

We have at the end of the optimization procedure all the A[i] that describe the ground state of our Hamiltonian. All expectation values can then easily be evaluated [85].

For the sake of readability, we restrict our description to open boundary conditions (OBC), but there is also a generalization to periodic boundary conditions (PBC). The main idea is to assume that the particles are in a ring configuration, so all of them are treated on the same footing. The matrices A[i] are determined in clockwise order, then improve following a counterclockwise ordering, and then clockwise again, until a fixed point is reached.

As a reminder, the A[i] in a MPS (2.29) are matrices whose dimension is bounded by some fixed number D, which is the number of states kept by the DMRG method, and dis the dimension of the Hilbert space corresponding to the physical systems. For OBC we have  $D_L = D_1 = 1$ , so that  $A[1]^{s_1} = (\vec{A}[1]^{s_1})^T$  and  $A[L]^{s_L} = \vec{A}[L]^{s_L}$  are vectors.

#### A.1 Normalization of the state

Given equation 2.29, if the matrix A[k] is the only one in the state that is not normalized, using Eqs. A.1 and A.2 we have that

$$\langle \psi | \psi \rangle = \sum_{s_k=1}^d \sum_{\kappa,\eta=1}^D Tr \left( A[k]_{\kappa,s_k,\eta} \bar{A}[k]_{\kappa,s_k,\eta} \right)$$

$$= \sum_{s_k=1}^d Tr \left( A[k]^{s_k} A[k]^{\dagger s_k} \right)$$
(A.3)

Then, we proceed to the singular value decomposition (SVD) of this not "unitary"

#### A.2. Effective Hamiltonian

A[k]

$$A[k]_{(\alpha,s_k),\beta} = U[k]_{(\alpha,s_k),(\alpha,s_k)'} D[k]_{(\alpha,s_k)',\beta'} V[k]_{\beta',\beta}$$
(A.4a)

$$A[k]_{\alpha,(s_k,\beta)} = U[k]_{\alpha,\alpha'} D[k]_{\alpha',(s_k,\beta)'} V[k]_{(s_k,\beta)',(s_k,\beta)}.$$
(A.4b)

Depending on which condition we ask to A[k], either equation A.1 when going from i = 1 to L, or equation A.2 when going from i = L to 1; we choose a determinate partition for the indices in the SVD. These choices correspond to equation A.4a and equation A.4b, respectively. Given the similarity of these conditions, we are going to work only with one of them, let us say equation A.4b. For equation A.4a everything can be develop similarly.

In equation A.4b,  $U[k]_{\alpha,\alpha'}$  and  $V[k]_{(s_k,\beta)',(s_k,\beta)}$  are unitary matrices, and  $D[k]_{\alpha',(s_k,\beta)'}$  is diagonal but rectangular

$$\left(\begin{array}{cc} Diag & 0\\ 0 & O_{m \times n} \end{array}\right)_{\alpha',(s_k,\beta)'}$$

This means that  $\alpha' < (s_k, \beta)'$  and that we can take away some of the zero-columns, to have a square matrix  $D[k]_{\alpha',\alpha''}$ . Now, the resulting  $V[k]_{(s_k,\beta)',(s_k,\beta)}$  is of the same dimensions as  $A[k]_{\alpha,(s_k,\beta)}$ 

$$V[k]_{(s_k,\beta)',(s_k,\beta)} \to V[k]_{\alpha'',(s_k,\beta)}$$

and we can make the following identification

$$A[k]_{\alpha,(s_k,\beta)} = \underbrace{U[k]_{\alpha,\alpha'}D[k]_{\alpha',\alpha''}}_{X[k]^{-1}} \underbrace{V[k]_{\alpha'',(s_k,\beta)}}_{\tilde{A}[k]_{\alpha,(s_k,\beta)}}.$$

Therefore, we are able to rewrite the state using the new matrices

$$A[k] = X[k]A[k]$$
$$A[k-1] = A[k-1]X[k]^{-1}$$

without changing its physical meaning. To continue the procedure, now A[k-1] has to be normalized.

#### A.2 Effective Hamiltonian

Fixing our attention on site k, the Hamiltonian H of a system with next-neighbor interactions can be decomposed in the following way

$$H = H_L + H_{Lk} + H_k + H_{kR} + H_R (A.6)$$

where:

- 1.  $H_L$  refers to all the interactions between the sites to the left of k,
- 2.  $H_{Lk}$  refers to all the interactions between site k and those to its left,

- 3.  $H_k$  refers to all the local interactions in the site k,
- 4.  $H_{kR}$  refers to all the interactions between site k and those to its right,
- 5.  $H_R$  refers to all the interactions between the sites to the right of k.

If we consider a Hamiltonian with nearest-neighbor interactions

$$H = \sum_{i=1}^{L-1} h_i h_{i+1} + \sum_{i=1}^{L} g_i$$

the energy can be written as

$$\langle \psi | H | \psi \rangle = (E_{h_1} E_{h_2} E_{\mathbb{I}} \cdots) + (E_{\mathbb{I}} E_{h_2} E_{h_3} \cdots) + \cdots$$
(A.7)

where  $E_X$  is the transfer matrix of operator X, as defined in [85], and I the identity matrix in a site. We can decompose this expectation value with respect to the site k of our interest

where we have defined the following matrices, which refer only to the other sites but k,

$$\begin{aligned} A_k &= \mathbf{E}_h[\mathbf{1}]\mathbf{E}_h[\mathbf{2}]E_{\mathbb{I}}[3]\cdots E_{\mathbb{I}}[k-1] + \\ &+ E_{\mathbb{I}}[1]\mathbf{E}_h[\mathbf{2}]\mathbf{E}_h[\mathbf{3}]\cdots E_{\mathbb{I}}[k-1] + \cdots \\ &\cdots + E_{\mathbb{I}}[1]\cdots E_{\mathbb{I}}[k-3]\mathbf{E}_h[\mathbf{k}-2]\mathbf{E}_h[\mathbf{k}-1] \\ B_k &= E_{\mathbb{I}}[k+1]\cdots E_{\mathbb{I}}[N] \\ C_k &= E_{\mathbb{I}}[1]\cdots E_{\mathbb{I}}[k-1] \\ D_k &= \mathbf{E}_h[\mathbf{k}+1]\mathbf{E}_h[\mathbf{k}+2]E_{\mathbb{I}}[k+3]\cdots E_{\mathbb{I}}[N] + \\ &+ E_{\mathbb{I}}[k+1]\mathbf{E}_h[\mathbf{k}+2]\mathbf{E}_h[\mathbf{k}+3]\cdots E_{\mathbb{I}}[N] + \\ &\cdots + E_{\mathbb{I}}[k+1]\cdots E_{\mathbb{I}}[N-2]\mathbf{E}_h[\mathbf{N}-1]\mathbf{E}_h[\mathbf{N}] \\ F_k &= E_{\mathbb{I}}[1]\cdots E_{\mathbb{I}}[k-2]\mathbf{E}_h[\mathbf{k}-1] \\ G_k &= \mathbf{E}_h[\mathbf{k}+1]E_{\mathbb{I}}[k+2]\cdots E_{\mathbb{I}}[N] \\ A'_k &= \mathbf{E}_g[\mathbf{1}]E_{\mathbb{I}}[2]\cdots E_{\mathbb{I}}[k-1] + \\ &+ E_{\mathbb{I}}[1]\mathbf{E}_g[\mathbf{2}]\cdots E_{\mathbb{I}}[k-1] + \\ &+ E_{\mathbb{I}}[1]\mathbf{E}_g[\mathbf{2}]\cdots E_{\mathbb{I}}[k-1] + \\ &+ E_{\mathbb{I}}[1]\mathbf{E}_g[\mathbf{2}]\cdots E_{\mathbb{I}}[k-1] + \\ &\cdots \\ &\cdots + E_{\mathbb{I}}[k+1]E_{\mathbb{I}}[k+2]\cdots E_{\mathbb{I}}[N] + \\ &+ E_{\mathbb{I}}[k+1]\mathbf{E}_{\mathbb{I}}[k+2]\cdots E_{\mathbb{I}}[N] + \\ &- E_{\mathbb{I}}[k+1]\mathbf{E}_{\mathbb{I}}[k+2]\cdots E_{\mathbb{I}}[N] + \\ &- E_{\mathbb{I}}[k+1]\mathbf{E}_g[\mathbf{k}+2]\cdots E_{\mathbb{I}}[N] + \\ &\cdots \\ &\cdots + E_{\mathbb{I}}[k+1]\mathbf{E}_g[\mathbf{k}+1]\cdots E_{\mathbb{I}}[N-1]\mathbf{E}_g[\mathbf{N}]. \end{aligned}$$

Having written this matrices, it is very important to realize that

#### A.2. Effective Hamiltonian

1. the energy is a quadratic form of our unknown variable at site k

$$\langle \psi | H | \psi 
angle = \vec{A}[k]^{\dagger} H' \vec{A}[k]$$

where  $\vec{A}[k] = A[k]_{(\alpha, s_k, \beta)}$ . This will lead us to a simple eigenvalue equation to find this A[k],

2. recursive forms for the matrices  $A_i, B_i, C_i \dots$  between the different sites *i* can be found, which will be very convenient to write the program.

If all the matrices A[i] are given, except for the one with i = k, then

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{Tr \left[ A_k \mathbf{E}_{\mathbb{I}} [\mathbf{k}] B_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ F_k \mathbf{E}_h [\mathbf{k}] B_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_{\mathbb{I}} [\mathbf{k}] D_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_h [\mathbf{k}] G_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_h [\mathbf{k}] G_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_h [\mathbf{k}] G_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_{\mathbb{I}} [\mathbf{k}] D_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_{\mathbb{I}} [\mathbf{k}] D_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]} + \frac{Tr \left[ C_k \mathbf{E}_{\mathbb{I}} [\mathbf{k}] D_k \right]}{\mathbf{Tr} \left[ \mathbf{A} [\mathbf{k}] \mathbf{A} [\mathbf{k}]^{\dagger} \right]}.$$

The dependence of E on A[k] is contained in the **bold** letters. Playing a little bit around with the indices, it is possible to put all the numerators in the form  $\vec{A}[k]^{\dagger}M[k]\vec{A}[k]$ . Adding up all these contributions  $(M[k], \ldots)$ , we find an effective Hamiltonian for site k which we call H[k].

For the minimization of E in function of A[k], we have the following expression

$$E = \frac{\vec{A}[k]^{\dagger} H[k] \vec{A}[k]}{\vec{A}[k]^{\dagger} \vec{A}[k]}.$$
 (A.9)

But minimizing this E with respect to A[k] is equivalent to solving the eigenvalue equation

$$H[k]\vec{A}[k] = E\vec{A}[k] \tag{A.10}$$

where  $\vec{A}[k]$  corresponds to the minimal E of the spectrum.

## Appendix B

## Derivation of the master equation

## **B.1** Number dissipation

We present the derivation of the master equation for a system of bosonic atoms in a lattice that is coupled to a reservoir through an exchange of particles (3.22). This type of dissipation, where particles are exchanged, is equivalent to the well-known damped harmonic oscillator treated in the literature [116, 47, 20]. This model is briefly introduced in section B.1.1, as it has been used in the second part of this dissertation. Later in section B.1.2, we describe the system considering the Mott insulating limit in the Bose–Hubbard model and making a detailed derivation of the master equation.

#### B.1.1 The system as a damped harmonic oscillator

The system is modeled by a harmonic oscillator with frequency  $\epsilon/\hbar$ , and the reservoir by a collection of harmonic oscillators with frequencies  $\epsilon_k/\hbar$ . Thereof the interaction at each site of the system is

$$H_{SR} = \sum_{k} \hbar g_k \left( a^{\dagger} b_k + b_k^{\dagger} a \right) \tag{B.1}$$

where  $a^{\dagger}(a)$  is the creation (annihilation) operator of an excitation in the system,  $b_k^{\dagger}(b_k)$  is the creation (annihilation) operator of the k-th mode of the bath, and  $g_k$  is the coupling constant of the system with the k-th mode of the bath. Using these notation, the free evolution Hamiltonian for a single site can be written as

$$H_0 = \epsilon a^{\dagger} a + \sum_k \epsilon_k b_k^{\dagger} b_k, \tag{B.2}$$

recalling that  $\epsilon$  is the energy of an excitation in the system, and  $\epsilon_k$  the energy of the k-th mode in the bath. We assume that the reservoir is in thermal equilibrium.

The detailed derivation of the master equation for this system is the typical textbook example [116, 47, 20] and it is analogous to the derivation presented in section B.1.2,

thereof we just present the final result

$$\frac{d\rho(t)}{dt} = \frac{\gamma}{2} \{ N[-aa^{\dagger}\rho(t) - \rho(t)aa^{\dagger} + 2a^{\dagger}\rho(t)a] + (N+1)[2a\rho(t)a^{\dagger} - a^{\dagger}a\rho(t) - \rho(t)a^{\dagger}a] \}.$$
(B.3)

In this equation,  $\gamma$  is the damping rate of the dissipative process (see equation B.17), and N is the mean number of excitations in the reservoir.

#### B.1.2 The system as a Mott insulator

The system is modeled by a Mott insulator, described by the Bose-Hubbard model with j = 0; and the reservoir by a large number of harmonic oscillators, exchanging "excitations" (particles) with the system. As a consequence, we can see our system as a collection of individual sites interacting with local identical baths. Then, the interaction at each intersecting point in second quantization is given by

$$H_{SR} = \sum_{k} \hbar g_k \left( a^{\dagger} b_k + b_k^{\dagger} a \right) \tag{B.4}$$

where  $a^{\dagger}(a)$  is the creation (annihilation) operator of the atoms, and  $b_k^{\dagger}(b_k)$  is the creation (annihilation) operator of the k-th mode of the bath. The coupling constant  $g_k$  of the atoms with the k-th mode of the bath comes from the overlap of the Wannier functions describing the "particles" in both system and reservoir (expanded in modes). This treatment is convenient to simplify the reservoir spectrum.

For a single site, we can write the free evolution Hamiltonian as

$$H_0 = \frac{U}{2}a^{\dagger}a^{\dagger}aa + \sum_k \hbar\epsilon_k b_k^{\dagger}b_k, \qquad (B.5)$$

where U is the local interaction energy of the atoms, and  $\hbar \epsilon_k$  the energy of the k-th mode of the bath.

Let  $\rho(t)$  be the reduced density matrix of the system and  $\rho_R(0)$  the initial state of the reservoir, which will remain unaltered by the presence of the system due to its own characteristics (section 3.1). We proceed to derive the master equation equation 3.12 in this case, namely

$$\frac{d\rho(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt_1 T r_R [H_{SR}^I(t), [H_{SR}^I(t_1), \rho(t) \otimes \rho_R(0)]],$$
(B.6)

where  $H_{SR}^{I}$  refers to coupling between the system and the environment  $H_{SR}$  in the interaction picture. In this picture, the bath operators  $b_k$  and  $b_k^{\dagger}$  are replaced by the operators  $b_{kI}$  and  $b_{kI}^{\dagger}$ 

$$b_{kI} = e^{-iH_0t/\hbar} b_k e^{iH_0t/\hbar} = e^{-i\epsilon_k n_k t} b_k e^{i\epsilon_k n_k t}$$
$$= e^{-i\epsilon_k n_k t + i\epsilon_k (n_k + 1)t} b_k$$
$$= e^{i\epsilon_k t} b_k$$
(B.7a)

$$b_{kI}^{\dagger} = e^{-iH_0t/\hbar} b_k^{\dagger} e^{iH_0t/\hbar} = e^{-i\epsilon_k t} b_k^{\dagger}, \qquad (B.7b)$$

and the system operators a and  $a^{\dagger}$  by the operators  $a_{I}$  and  $a^{\dagger}_{I}$ 

$$a_{I} = e^{-iH_{0}t/\hbar} a e^{iH_{0}t/\hbar} = e^{-iUn(n-1)t/2\hbar} a e^{iUn(n-1)t/2\hbar} = e^{-iUn(n-1)t/2\hbar + iU(n+1)nt/2\hbar} = e^{iUnt/\hbar} a$$
(B.8a)

$$a^{\dagger}{}_{I} = e^{-iH_{0}t/\hbar}a^{\dagger}e^{iH_{0}t/\hbar} = e^{-iU(n-1)t/\hbar}a^{\dagger},$$
 (B.8b)

according to the free evolution  $H_0$  of each of these parts. Then, in this picture the interaction is

$$H_{SR}^{I}(t) = \hbar B(t) a^{\dagger} e^{-iUnt/\hbar} + \hbar B^{\dagger}(t) e^{iUnt/\hbar} a$$
(B.9)

where we have defined the bath operators  $B(t) = \sum_{k} g_k e^{i\epsilon_k t} b_k$ . The master equation equation B.6 turns into

$$\frac{d\rho(t)}{dt} = -\int_{0}^{t} dt_{1} Tr_{R}[B(t)a^{\dagger}e^{-iUnt/\hbar} + B^{\dagger}(t)e^{iUnt/\hbar}a, 
[B(t_{1})a^{\dagger}e^{-iUnt_{1}/\hbar} + B^{\dagger}(t_{1})e^{iUnt_{1}/\hbar}a, \rho(t) \otimes \rho_{R}(0)]].$$
(B.10)

To simplify the notation and save some space in the following calculations, we will use the following shortcuts for some of the variables  $B_t = B(t)$ ,  $B_1 = B(t_1)$ ,  $\phi_t = Unt/\hbar$  and  $\phi_1 = Unt_1/\hbar$ . Then, the commutator in the integral equation B.10 can be expanded as

$$\begin{split} [\cdot, [\cdot, \cdot]]_{equationB.10} &= B_t^{\dagger} e^{i\phi_t} a B_1^{\dagger} e^{i\phi_1} a \left(\rho(t) \otimes \rho_R(0)\right) + B_t^{\dagger} e^{i\phi_t} a a^{\dagger} e^{-i\phi_1} B_1 \left(\rho(t) \otimes \rho_R(0)\right) \\ &+ a^{\dagger} e^{-i\phi_t} B_t B_1^{\dagger} e^{i\phi_1} a \left(\rho(t) \otimes \rho_R(0)\right) + a^{\dagger} e^{-i\phi_t} B_t a^{\dagger} e^{-i\phi_1} B_1 \left(\rho(t) \otimes \rho_R(0)\right) \\ &- B_t^{\dagger} e^{i\phi_t} a \left(\rho(t) \otimes \rho_R(0)\right) B_1^{\dagger} e^{i\phi_1} a - B_t^{\dagger} e^{i\phi_t} a \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_1} B_1 \\ &- a^{\dagger} e^{-i\phi_t} B_t \left(\rho(t) \otimes \rho_R(0)\right) B_1^{\dagger} e^{i\phi_1} a - a^{\dagger} e^{-i\phi_t} B_t \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_1} B_1 \\ &- B_1^{\dagger} e^{i\phi_1} a \left(\rho(t) \otimes \rho_R(0)\right) B_t^{\dagger} e^{i\phi_t} a - B_1^{\dagger} e^{i\phi_1} a \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_t} B_t \\ &- a^{\dagger} e^{-i\phi_1} B_1 \left(\rho(t) \otimes \rho_R(0)\right) B_t^{\dagger} e^{i\phi_t} a - a^{\dagger} e^{-i\phi_1} B_1 \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_t} B_t \\ &+ \left(\rho(t) \otimes \rho_R(0)\right) B_1^{\dagger} e^{i\phi_1} a B_t^{\dagger} e^{i\phi_t} a + \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_t} B_t \\ &+ \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_1} B_1 B_t^{\dagger} e^{i\phi_t} a + \left(\rho(t) \otimes \rho_R(0)\right) a^{\dagger} e^{-i\phi_t} B_t \end{split}$$

If we assume that we work with a thermal bath, it does not have phase dependent correlations  $\langle b_k b_{k'} \rangle = \langle b_k^{\dagger} b_{k'}^{\dagger} \rangle = 0$ . This simplifies the expression above, as we will only have to consider terms where  $B_1^{\dagger}$  and  $B_t$ , or their Hermitian conjugates, appear. Taking the trace over the reservoir variables  $Tr_R[\cdot]$  and the integral over  $t_1$ , as indicated in equation

B.10, these terms become

$$\int dt_1 Tr_R \left[ B_t^{\dagger} e^{i\phi_t} aa^{\dagger} e^{-i\phi_1} B_1 \left( \rho(t) \otimes \rho_R(0) \right) \right] = aa^{\dagger} \rho(t) \int dt_1 e^{iUn(t-t_1)/\hbar} \left\langle B_t^{\dagger} B_1 \right\rangle$$

$$\int dt_1 Tr_R \left[ a^{\dagger} e^{-i\phi_t} B_t B_1^{\dagger} e^{i\phi_1} a \left( \rho(t) \otimes \rho_R(0) \right) \right] = a^{\dagger} a\rho(t) \int dt_1 e^{-iU(n-1)(t-t_1)/\hbar} \left\langle B_t B_1^{\dagger} \right\rangle$$

$$\int dt_1 Tr_R \left[ \left( \rho(t) \otimes \rho_R(0) \right) B_1^{\dagger} e^{i\phi_1} aa^{\dagger} e^{-i\phi_t} B_t \right] = \rho(t) aa^{\dagger} \int dt_1 e^{-iUn(t-t_1)/\hbar} \left\langle B_1^{\dagger} B_t \right\rangle$$

$$\int dt_1 Tr_R \left[ \left( \rho(t) \otimes \rho_R(0) \right) a^{\dagger} e^{-i\phi_1} B_1 B_t^{\dagger} e^{i\phi_t} a \right] = \rho(t) a^{\dagger} a \int dt_1 e^{iU(n-1)(t-t_1)/\hbar} \left\langle B_1 B_t^{\dagger} \right\rangle$$

$$\int dt_1 Tr_R \left[ B_t^{\dagger} e^{i\phi_t} a \left( \rho(t) \otimes \rho_R(0) \right) a^{\dagger} e^{-i\phi_1} B_1 \right] = a\rho(t) a^{\dagger} \int dt_1 e^{iUn(t-t_1)/\hbar} \left\langle B_1 B_t^{\dagger} \right\rangle$$

$$\int dt_1 Tr_R \left[ a^{\dagger} e^{-i\phi_t} B_t \left( \rho(t) \otimes \rho_R(0) \right) B_1^{\dagger} e^{i\phi_1} a \right] = a^{\dagger} \rho(t) a \int dt_1 e^{-iUn(t-t_1)/\hbar} \left\langle B_1 B_t^{\dagger} \right\rangle$$

$$\int dt_1 Tr_R \left[ B_1^{\dagger} e^{i\phi_1} a \left( \rho(t) \otimes \rho_R(0) \right) a^{\dagger} e^{-i\phi_t} B_t \right] = a\rho(t) a^{\dagger} \int dt_1 e^{-iUn(t-t_1)/\hbar} \left\langle B_1 B_t^{\dagger} \right\rangle$$

where we have used the identities  $ae^{i\phi_t} = e^{i\phi_t}e^{iUt/\hbar}a$  and  $a^{\dagger}e^{i\phi_t} = e^{i\phi_t}e^{-iUt/\hbar}a^{\dagger}$ , as well as noted that  $Tr_R(B_t^{\dagger}B_1\rho_R(0)) = \langle B_t^{\dagger}B_1 \rangle$ . This expressions show us that there are four integrals to be solved, namely

$$I_1 = \int_0^t dt_1 e^{-i\omega_0(t-t_1)} \left\langle B_t B_1^\dagger \right\rangle \tag{B.11}$$

$$I_2 = \int_0^t dt_1 e^{i\omega_0(t-t_1)} \left\langle B_t^{\dagger} B_1 \right\rangle \tag{B.12}$$

$$I_3 = \int_0^t dt_1 e^{-i\omega_0(t-t_1)} \left\langle B_1^{\dagger} B_t \right\rangle \tag{B.13}$$

$$I_4 = \int_0^t dt_1 e^{i\omega_0(t-t_1)} \left\langle B_1 B_t^\dagger \right\rangle \tag{B.14}$$

where  $\omega_0$  refers to the frequency associated to the energy of the system, either  $Un/\hbar$  or  $U(n-1)/\hbar$ .

Recalling the definition of the bath operators  $B(t) = \sum_k g_k e^{i\epsilon_k t} b_k$ , the equation B.11 can be written as

$$I_1 = \int_0^t dt_1 \sum_{k,k'} g_k g'_k e^{-i\omega_0(t-t_1)} e^{i(\epsilon_k t - \epsilon_{k'} t_1)} \left\langle b_k b^{\dagger}_{k'} \right\rangle$$

For a thermal environment, it can be shown that its correlations are [96]

$$\left\langle b_{k}^{\dagger}b_{k'}\right\rangle = N_{k}\delta_{kk'}$$
 (B.15a)

$$\left\langle b_k b_{k'}^{\dagger} \right\rangle = (N_k + 1) \delta_{kk'}$$
 (B.15b)

where  $N_k$  is the thermal average number of "excitations" (particles) in the reservoir corresponding to the k-th mode. Thus, adding over k'

$$I_1 = \int_0^t dt_1 \sum_k g_k^2 (N_k + 1) e^{-i(\omega_0 - \epsilon_k)(t - t_1)}.$$

Considering that the bath is very large and that it has many degrees of freedom, we can replace the sum over modes by an integral over frequencies

$$\sum_{k} \to \int_{0}^{\infty} d\omega \frac{\varrho(\omega)}{2\pi} \tag{B.16}$$

where  $\rho(\omega)$  is the density of states at frequency  $\omega$ . Using the approximation B.16 and the change of variable  $\tau = t - t_1$ 

$$I_1 = \int_0^t d\tau \int_0^\infty \frac{d\omega_1}{2\pi} \rho(\omega_1) g(\omega_1)^2 (N(\omega_1) + 1) e^{-i(\omega_0 - \omega_1)\tau}.$$

We make the first Markov approximation assuming that  $\rho(\omega)$ ,  $g(\omega)$  and  $N(\omega)$  are slowly varying functions around  $\omega = \omega_1$ , where  $\omega_1$  is very large. Introducing the change  $\varepsilon = \omega_0 - \omega_1$  and assuming symmetry around  $\omega_0$ 

$$I_1 \simeq \int_0^t d\tau \int_{-\infty}^\infty \frac{d\varepsilon}{2\pi} \varrho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 (N(\omega_0 - \varepsilon) + 1) e^{-i\varepsilon\tau}.$$

The upper limit of the time integration may be extended to infinity, considering that the system losses all the memory of its past on a scale much smaller than the time of observation. Then we obtain

$$I_1 \simeq \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \rho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 (N(\omega_0 - \varepsilon) + 1) \left[ \pi \delta(\varepsilon) - iPV\left(\frac{1}{\varepsilon}\right) \right]$$

where we have used

$$\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \int_{0}^{\infty} d\tau e^{\pm i\varepsilon\tau} = \int_{-\infty}^{\infty} d\varepsilon \left[ \pi \delta(\varepsilon) \pm PV\left(\frac{i}{\varepsilon}\right) \right] f(\varepsilon) = \pi f(0) \pm iPV \int_{-\infty}^{\infty} d\varepsilon \frac{f(\varepsilon)}{\varepsilon}$$

being PV the Cauchy principal value of an integral

$$PV \int_{a}^{b} f(\omega) d\omega = \lim_{\varepsilon \to 0} \left( \int_{a}^{\omega_{0} - \varepsilon} f(\omega) d\omega + \int_{\omega_{0} + \varepsilon}^{b} f(\omega) d\omega \right).$$

Defining the damping rate  $\gamma$  as

$$\gamma = \varrho(\omega_0) g(\omega_0)^2 \tag{B.17}$$

we can finally write equation B.11 in its final form

$$I_1 \simeq \frac{\gamma}{2} (N(\omega_0) + 1) - i\Delta \tag{B.18}$$

where

$$\Delta = PV \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \frac{1}{\varepsilon} \varrho(\omega_0 - \varepsilon)^2 g(\omega_0 - \varepsilon)^2 (N(\omega_0 - \varepsilon) + 1).$$
(B.19)

The second integral equation B.12 can be similarly expressed in terms of the bath operators dt

$$I_{2} = \int_{0}^{t} dt_{1} \sum_{k,k'} g_{k} g_{k'} e^{i\omega_{0}(t-t_{1})} e^{-i(\epsilon_{k}t-\epsilon_{k'}t_{1})} \left\langle b_{k}^{\dagger} b_{k'} \right\rangle.$$

Adding over k' for a thermal environment (B.15a)

$$I_{2} = \int_{0}^{t} dt_{1} \sum_{k} g_{k}^{2} N_{k} e^{i(\omega_{0} - \epsilon_{k})(t - t_{1})}$$

and using the approximation B.16, followed by the change of variable  $\tau = t - t_1$ 

$$I_2 = \int_0^t d\tau \int_0^\infty \frac{d\omega_1}{2\pi} \varrho(\omega_1) g(\omega_1)^2 N(\omega_1) e^{i(\omega_0 - \omega_1)\tau}.$$

Making again the first Markov approximation and introducing the change of variable  $\varepsilon = \omega_0 - \omega_1$ , assuming symmetry around  $\omega_0$ 

$$I_2 \simeq \int_0^t d\tau \int_{-\infty}^\infty \frac{d\varepsilon}{2\pi} \varrho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 N(\omega_0 - \varepsilon) e^{i\varepsilon\tau}.$$

Applying the second Markov approximation, we obtain

$$I_2 \simeq \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \rho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 N(\omega_0 - \varepsilon) \left[ \pi \delta(\varepsilon) + iPV\left(\frac{1}{\varepsilon}\right) \right]$$

using the Cauchy principal value PV of the integral. We finally can write the integral equation B.12 as

$$I_2 \simeq \frac{\gamma}{2} N(\omega_0) + i\Delta' \tag{B.20}$$

where we have used the definition

$$\Delta' = PV \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \frac{1}{\varepsilon} \varrho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 N(\omega_0 - \varepsilon).$$
(B.21)

The third integral equation B.13 can be also expressed in terms of the bath operators

$$I_{3} = \int_{0}^{t} dt_{1} \sum_{k,k'} g_{k} g_{k'} e^{-i\omega_{0}(t-t_{1})} e^{i(\epsilon_{k}t-\epsilon_{k'}t_{1})} \left\langle b_{k}^{\prime \dagger} b_{k} \right\rangle.$$

Adding over k' for a thermal environment (equation B.15a)

$$I_{3} = \int_{0}^{t} dt_{1} \sum_{k} g_{k}^{2} N_{k} e^{-i(\omega_{0} - \epsilon_{k})(t - t_{1})}$$

and using the approximation B.16, followed by the change of variable  $\tau = t - t_1$ 

$$I_3 = \int_0^t d\tau \int_0^\infty \frac{d\omega_1}{2\pi} \varrho(\omega_1) g(\omega_1)^2 N(\omega_1) e^{-i(\omega_0 - \omega_1)\tau}.$$

Making again the first Markov approximation and introducing the change of variable  $\varepsilon = \omega_0 - \omega_1$ , assuming symmetry around  $\omega_0$ 

$$I_3 \simeq \int_0^t d\tau \int_{-\infty}^\infty \frac{d\varepsilon}{2\pi} \varrho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 N(\omega_0 - \varepsilon) e^{-i\varepsilon\tau}.$$

#### B.1. Number dissipation

After applying the second Markov approximation, we obtain

$$I_3 \simeq \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \rho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 N(\omega_0 - \varepsilon) \left[ \pi \delta(\varepsilon) - iPV\left(\frac{1}{\varepsilon}\right) \right]$$

using the Cauchy principal value PV of the integral. We finally obtain for equation B.13 the expression

$$I_3 \simeq \frac{\gamma}{2} N(\omega_0) - i\Delta' \tag{B.22}$$

where  $\Delta'$  is given by equation B.21.

The fourth integral equation B.14 can be similarly expressed in terms of the bath operators

$$I_4 = \int_0^t dt_1 \sum_{k,k'} g_k g_{k'} e^{i\omega_0(t-t_1)} e^{-i(\epsilon_k t - \epsilon_{k'} t_1)} \left\langle b_{k'} b_k^{\dagger} \right\rangle.$$

Adding over k' for a thermal environment (equation B.15b)

$$I_4 = \int_0^t dt_1 \sum_k g_k^2 (N_k + 1) e^{i(\omega_0 - \epsilon_k)(t - t_1)}$$

and using the approximation B.16, followed by the change of variable  $\tau = t - t_1$ 

$$I_4 = \int_0^t d\tau \int_0^\infty \frac{d\omega_1}{2\pi} \rho(\omega_1) g(\omega_1)^2 (N(\omega_1) + 1) e^{i(\omega_0 - \omega_1)\tau}.$$

Making again the first Markov approximation and introducing the change  $\varepsilon = \omega_0 - \omega_1$ , assuming symmetry around  $\omega_0$ 

$$I_4 \simeq \int_0^t d\tau \int_{-\infty}^\infty \frac{d\varepsilon}{2\pi} \varrho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 (N(\omega_0 - \varepsilon) + 1) e^{i\varepsilon\tau}.$$

Applying the second Markov approximation, we obtain

$$I_4 \simeq \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \rho(\omega_0 - \varepsilon) g(\omega_0 - \varepsilon)^2 (N(\omega_0 - \varepsilon) + 1) \left[ \pi \delta(\varepsilon) + iPV\left(\frac{1}{\varepsilon}\right) \right]$$

using the Cauchy principal value PV of the integral. We finally can write equation B.14 as

$$I_4 \simeq \frac{\gamma}{2} (N(\omega_0) + 1) + i\Delta \tag{B.23}$$

where  $\Delta$  is given by equation B.19.

The effect of the terms  $\Delta$  and  $\Delta'$  is to add a small perturbing Hamiltonian term, a small frequency (Lamb) shift, and are usually neglected [20, 116, 47]. We can use  $I_1$ ,  $I_2$ ,  $I_3$  and  $I_4$  to write the master equation B.10 as

$$\frac{d\rho(t)}{dt} = -\frac{\gamma}{2}N(Un)aa^{\dagger}\rho(t) - \frac{\gamma}{2}(N(U(n-1))+1)a^{\dagger}a\rho(t) -\frac{\gamma}{2}N(Un)\rho(t)aa^{\dagger} - \frac{\gamma}{2}(N(U(n-1))+1)\rho(t)a^{\dagger}a +\gamma(N(Un)+1)a\rho(t)a^{\dagger}+\gamma N(U(n-1))a^{\dagger}\rho(t)a.$$

As a reminder, following from equations B.15,  $N(\omega_0)$  stands for the number of excitations (particles to exchange) in the bath at energy  $\omega_0$ , and  $\gamma$  is the damping rate of the dissipative process (B.17).

### **B.2** Phase dissipation

Following a similar treatment as in section B.1, we can also derive the master equation for a system with collisions. We consider a coupling between the system and the reservoir such that

$$H_{SR} = V \sum_{i} n_{i} n_{i0}^{b}.$$
 (B.24)

This interaction describes phase-changing collisions between the system and the reservoir. Here  $n_i$  refers to the number of particles in the system at site *i*, and  $n_{i0}^b$  to the number of particles in the bath at the intersection with the *i*-th site of the system.

A detailed derivation of the master equation will be omitted, it is analogous to the presented in section B.1.2. The final result we use is

$$\frac{d\rho(t)}{dt} = \frac{\gamma}{2} \sum_{i} \left\{ -n_i^2 \rho(t) - \rho(t) n_i^2 + 2n_i \rho(t) n_i \right\}$$
(B.25)

where the constant  $\gamma$  is the damping rate of the dissipative process (see equation B.17), including the parameters of the interaction and the reservoir.

## Appendix C

# Derivation of the model in superlattices

As discussed in chapter 5.1, the main idea behind atomic correlated hopping is to trap atoms whose interaction allows them to change their state. In this appendix we provide one possible implementation of this idea, using state dependent superlattices that trap dressed states.

## C.1 Dressed states trapping

Our starting point is the setup in figure 5.1 (upper left). It consists of an optical lattice trapping atoms in states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , together with a Raman coupling between these states. Mathematically, this configuration is described by the single-particle Hamiltonian

$$H_{\text{trap}} = V_0 \sin(kx)^2 \left( |\uparrow\rangle \langle\uparrow| + |\downarrow\rangle \langle\downarrow| \right) +\Omega \sin(kx) \left( |\uparrow\rangle \langle\downarrow| + |\downarrow\rangle \langle\uparrow| \right).$$
(C.1)

By moving to the basis of dressed states  $|\pm\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle \pm |\downarrow\rangle)$ , we find that the trapping is effectively equivalent to two superlattices with a relative displacement, as in figure 5.1 (right),

$$H_{\text{trap}} = \left( V_0 \sin(kx)^2 + \Omega \sin(kx) \right) |+\rangle \langle +| \\ + \left( V_0 \sin(kx)^2 - \Omega \sin(kx) \right) |-\rangle \langle -|.$$
(C.2)

Under appropriate circumstances [46], we find that each superlattice site has a unique ground state, energetically well differentiated from the next excited state, and which consists of a symmetric wavefunction spanning both lattice wells. If this is the case, and if all energy scales (such as the interaction and the hopping) are small compared to the separation between Bloch bands, we can expand the bosonic field operators describing the atoms in terms of these localized wavefunctions

$$\psi_{+}(x) = \sum_{i} c_{2i} W(x - 2il)$$

$$\psi_{-}(x) = \sum_{i} c_{2i+1} W(x - (2i+1)l)$$
(C.3)

where  $2l = 2\pi/k$  is the superlattice period;  $c_j$  are bosonic operators

$$c_{2i} = \frac{1}{\sqrt{2}} (a_{2i,+} + a_{2i+1,+})$$

$$c_{2i+1} = \frac{1}{\sqrt{2}} (a_{2i+1,-} + a_{2i+2,-})$$
(C.4)

that for j even (odd) annihilate an atom in state  $|+\rangle$   $(|-\rangle)$  in the j-th superlattice cell; and the localized wavefunctions W(x) are a superposition of the Wannier functions w(x')of the underlying lattice

$$W(x-2il) = \frac{1}{\sqrt{2}} \left[ w(x-2il) + w(x-(2i+1)l) \right].$$
 (C.5)

## C.2 State-changing collisions

Now we will express the interaction (5.4) in the basis of dressed states. We proceed using the change of variables in equation 5.6 to find the expression of the densities

$$\rho_{\uparrow}(x) = \frac{1}{2}(\rho_{+} + \rho_{-} + \psi_{+}^{\dagger}\psi_{-} + \psi_{-}^{\dagger}\psi_{+})$$
(C.6)

$$\rho_{\downarrow}(x) = \frac{1}{2}(\rho_{+} + \rho_{-} - \psi_{+}^{\dagger}\psi_{-} - \psi_{-}^{\dagger}\psi_{+}).$$
 (C.7)

The first obvious conclusion is that the total density is independent of the basis on which it is written

$$\rho(x) = \rho_{\uparrow}(x) + \rho_{\downarrow}(x) = \rho_{+}(x) + \rho_{-}(x).$$
(C.8)

Hence, the term of  $g_0$  is insensitive to the state of the atoms. However, the asymmetric terms are not so simple. The  $g_1$  interaction, which is proportional to the product of densities

$$: \rho_{\uparrow} \rho_{\downarrow} := \frac{1}{4} : (\rho_{+} + \rho_{-})^{2} : -\frac{1}{4} : (\psi_{+}^{\dagger} \psi_{-} + \psi_{-}^{\dagger} \psi_{+})^{2} :$$
  
$$= \frac{1}{4} : (\rho_{+} + \rho_{-})^{2} : -\frac{1}{2} \rho_{+} \rho_{-} - \frac{1}{4} (\psi_{+}^{\dagger 2} \psi_{-}^{2} + H.c)$$
  
$$= \frac{1}{4} : \rho_{+}^{2} + \rho_{-}^{2} : -\frac{1}{4} (\psi_{+}^{\dagger 2} \psi_{-}^{2} + H.c),$$
(C.9)

gives rise to a scattering that changes the state of interacting atoms from  $|-\rangle$  to  $|+\rangle$  and viceversa, as in figure 1 (left). The term of  $g_2$  has a lightly different effect

$$: \rho_{\uparrow}(x)^{2} - \rho_{\downarrow}(x)^{2} :=: \rho(x) \left[ \psi_{+}^{\dagger}(x)\psi_{-}(x) + \psi_{-}^{\dagger}(x)\psi_{+}(x) \right] :$$
(C.10)

it gives rise to processes where one atom changes its state influenced by the surrounding environment. In the following, we will see what happens to the interaction terms (C.8), (C.9) and (C.10), when the atoms are confined in a lattice.

### C.3 Final model

In this section we will put together the results of this appendix. We will take the tight-binding expansion of the field operators (C.3) and use it in combination with equations C.8, C.9 and C.10 to expand the interaction Hamiltonian (5.4). For convenience, we will rename the bosonic operators as

$$c_{2k} = a_{k+}$$
 and  $c_{2k+1} = a_{k-}$  (C.11)

according to the position at which their Wannier functions are centered, as illustrated in figure 5.1 (right). Along the derivation, one obtains many integrals of ground state wavefunctions

$$C_{k,m} = \int |W(x-kl)|^2 |W(x-ml)|^2 dx.$$
 (C.12)

We will only keep those integrals with a separation smaller than a superlattice period. Taking the expression for the superlattice localized states (C.5), one obtains

$$C_{k,k} = \int |W(x)|^4 dx \simeq \frac{1}{2} \int |w(x)|^4 dx$$
 (C.13)

$$C_{k,k\pm 1} = \int |W(x)|^2 |W(x-l)|^2 dx \simeq \frac{1}{4} \int |w(x)|^4 dx$$
(C.14)

where w(x) are the Wannier wavefunctions of the underlying sublattice. Using these tools, the symmetric interaction term becomes

$$\frac{g_0}{2} \int d^3x : (\rho_{\uparrow}(x) + \rho_{\downarrow}(x))^2 :=$$

$$= \frac{g_0}{2} \sum_{k=1}^{N/2} n_{2k}^2 C_{2k,2k} + n_{2k+1}^2 C_{2k+1,2k+1} + 2n_{2k}n_{2k+1}C_{2k,2k+1} :$$

$$= \frac{g_0}{4} \int dx \ |w(x)|^4 \sum_{k=1}^{N} n_k^2 + n_k n_{k+1} : \qquad (C.15)$$

For the asymmetric terms we start from equation C.9, obtaining

$$g_1 \int d^3x : \rho_{\uparrow}(x)\rho_{\downarrow}(x) :=$$

$$\frac{g_1}{8} \int dx \ |w(x)|^4 \ \sum_k^N \left[ :n_k^2 : -\frac{1}{2} \left( c_{k+1}^{\dagger 2} c_k^2 + c_k^{\dagger 2} c_{k+1}^2 \right) \right] \tag{C.16}$$

and then finally the more complicated one, equation C.10

$$\frac{g_2}{2} \int d^3x : \rho_{\uparrow}(x)^2 - \rho_{\downarrow}(x)^2 :=$$

$$\frac{g_2}{8} \int dx \ |w(x)|^4 \sum_k^N : n_k (c_k^{\dagger} c_{k-1} + c_{k-1}^{\dagger} c_k + c_k^{\dagger} c_{k+1} + c_{k+1}^{\dagger} c_k) : \qquad (C.17)$$

Introducing constants that parameterize the on-site interactions and the strength of the underlying lattice (equation 5.7), our final Hamiltonian looks as follows

$$H = \frac{2U_0 + U_1}{8} \sum_k : n_k^2 : -\frac{U_0}{8} \sum_k : n_k n_{k+1} : -\frac{U_1}{16} \sum_k (c_{k+1}^{\dagger 2} c_k^2 + \text{H.c.}) -\frac{U_2}{8} \sum_k \left[ (n_k - 1) c_k^{\dagger} (c_{k-1} + c_{k+1}) + \text{H.c.} \right].$$
(C.18)

Completing terms and replacing the sum over k with a sum over nearest neighbors, we arrive at the desired model (5.1) with the parametrization given already in equation 5.8.

# Appendix D

# Atom-molecule resonances: calculation of physical parameters

The physical parameters  $(U_a, j_a, ...)$  used in the last part of this dissertation, about atoms in a Feshbach resonance, have been calculated from microscopical considerations and their derivations are shown in section D.2. The system we consider consists of <sup>8</sup>7Rb atoms trapped in an optical lattice and in resonance to a bound state. The corresponding physical constants are displayed in section D.1.

## D.1 Table of physical constants

Quantity	Symbol	Value	Unit
Reduced Planck constant	ħ	$1.054571628 \times 10^{-34}$	Js
Bohr radius	$a_0$	$0.52917720859 \times 10^{-10}$	m
Mass of Rb atom	m	$87 \cdot 1.660538782 \times 10^{-27}$	kg
Momentum of the lattice	k	$2\pi/(830.44 \times 10^{-9})$	$m^{-1}$
Recoil energy (atoms)	Er	$\hbar^2 k^2/(2m)$	J
Recoil energy (molecules)	$\mathbf{E}_{\mathbf{r}}^{m}$	$\hbar^2 k^2/(4m)$	J
Lattice depth seen by an atom	V <sub>0</sub>	$\alpha \cdot E_{\rm r}$ , typically $\alpha \in [10, 30]$	J
Lattice depth seen by a molecule	$V_0^m$	$2V_0$	J
Transversal confinement $(d < 3)$	$V_{0t}$	$30\mathrm{E_r}$	J
Angular frequency associated to each site	$\omega_{ m ho}$	$k\sqrt{2V_0/m}$	$s^{-1}$
Harmonic oscillator length	$a_{\rm ho}$	$\sqrt{\hbar/(\mathrm{m}\omega_\mathrm{ho})}$	m
Background scattering length *	$a_{\mathrm{bg}}$	$100.8 \cdot a_0$	m
Width of the Feshbach resonance *	$\Delta B$	$18 \times 10^{-7}$	Т
Difference of magnetic moments $^{\dagger}$	$\Delta \mu$	$2\pi\hbar\cdot 111\times 10^7$	J/T

<sup>\*</sup>From a coupled-channels calculation

<sup>&</sup>lt;sup>†</sup>From Breit-Rabi formula

#### D.2 Derivation of the physical parameters

To calculate the parameters of our system, we have used and calculated several formulae that are presented in this section. For the matrix element  $H_{am} = \langle \psi_a | H | \psi_m \rangle$  of the Hamiltonian (7.1), which is the conversion rate between atoms and molecules  $\Gamma$ , we have [103]

$$H_{am} = \sqrt{\frac{4\pi\hbar^2 a_{\rm bg}\Delta\mu\Delta B}{m\left(\sqrt{2\pi}a_{\rm ho}\right)^3}\left(1+0.490\frac{a_{\rm bg}}{a_{\rm ho}}\right)},\tag{D.1}$$

resulting in an angular frequency  $\Omega_{res} = 2H_{am}/\hbar$  for the Rabi oscillations between these states. For the single-atom tunneling amplitude  $j_a$ , in the case of a deep lattice  $V_0 >> E_r$  we have [124]

$$j_a = \frac{4}{\sqrt{\pi}} \mathbf{E}_{\mathbf{r}} \left(\frac{\mathbf{V}_0}{\mathbf{E}_{\mathbf{r}}}\right)^{3/4} e^{-2\sqrt{\mathbf{V}_0/\mathbf{E}_{\mathbf{r}}}} \tag{D.2}$$

while for the molecules, in the case  $V_0^m >> E_r^m$  we have similarly [124]

$$j_m = \frac{2}{\sqrt{\pi}} E_r^m \left(\frac{V_0^m}{E_r^m}\right)^{3/4} e^{-2\sqrt{V_0^m/E_r^m}}.$$
 (D.3)

The atomic interaction strength will depend on the dimensionality d of the trapping lattice, and the lattice depth  $V_{0t}$  perpendicular to the trapping directions

$$U_a = \sqrt{\frac{8}{\pi}} k a_{\rm bg} E_{\rm r} \frac{V_0^{d/4} (V_{0t})^{(3-d)/4}}{E_{\rm r}^{3/4}}.$$
 (D.4)

We take  $U_a$  as the energy unit of the problem, and calculate  $U_m$  and  $U_{am}$  as a function of this. We start from the expression for the interaction term of the Hamiltonian

$$H_{int} = \sum_{\alpha,\beta=a,m} \int d^3x \ d^3x' \ \Psi_{\alpha}(\vec{x})^{\dagger} \Psi_{\beta}(\vec{x'})^{\dagger} V_{\alpha,\beta}(\vec{x}-\vec{x'}) \Psi_{\beta}(\vec{x'}) \Psi_{\alpha}(\vec{x})$$
(D.5)  
$$= U_a \sum_i n_i (n_i - 1) + U_{am} \sum_i n_i m_i + U_m \sum_i m_i (m_i - 1).$$

The field operators describing the atoms  $\Psi_a$  and molecules  $\Psi_m$  can be expanded in terms of localized wavefunctions

$$\Psi_a(\vec{x}) = \sum_i a_i w_a(\vec{x} - i\vec{v}) \tag{D.6a}$$

$$\Psi_m(\vec{x}) = \sum_i b_i w_m(\vec{x} - i\vec{v}) \tag{D.6b}$$

where  $\vec{v}$  is the lattice period and  $w(\vec{x})$  are Wannier functions. We assume that the interactions in equation D.5 are described by contact potentials

$$V_{aa}(\vec{x} - \vec{x'}) = g \cdot \delta(\vec{x} - \vec{x'})$$
(D.7a)

$$V_{am}(\vec{x} - \vec{x'}) = 2g \cdot \delta(\vec{x} - \vec{x'})$$
(D.7b)

$$V_{mm}(\vec{x} - \vec{x'}) = 4g \cdot \delta(\vec{x} - \vec{x'}),$$
 (D.7c)

ignoring the internal structure of the interacting particles and adding the single interactions for compound objects: between two atoms  $g_{aa} = g$ , between an atom and a molecule  $g_{am} = 2g$ , and between two molecules  $g_{mm} = 4g$ . For deep lattices, the Wannier functions  $w(\vec{x})$  are going to be approximated by Gaussians along each direction

$$w_a(\vec{x}) = \mathcal{N}_a \ e^{-x^2/(2\sigma_x^2)} \ e^{-y^2/(2\sigma_y^2)} \ e^{-z^2/(2\sigma_z^2)}$$
 (D.8a)

$$w_m(\vec{x}) = \mathcal{N}_m \ e^{-x^2/\sigma_x^2} \ e^{-y^2/\sigma_y^2} \ e^{-z^2/\sigma_z^2}$$
 (D.8b)

with normalization constants

$$\mathcal{N}_a = \left(\frac{1}{\pi^3 \sigma_x^2 \sigma_y^2 \sigma_z^2}\right)^{1/4}, \quad \mathcal{N}_m = \left(\frac{8}{\pi^3 \sigma_x^2 \sigma_y^2 \sigma_z^2}\right)^{1/4} \tag{D.9}$$

and the width of the Gaussian packet  $\sigma_i$  given by the confinement along the direction i. To find the constants we have used the Gaussian integral  $\int d^3x e^{-x^2/a} = \sqrt{\pi a}$ . If the confinement along direction j is transversal (*i.e.* the particle cannot move along that direction), in the ideal case we would have that the probability distribution goes to a delta  $(\sigma_j \to 0)$ . Finally, we obtain the following on-site interactions

$$U_{a} = \frac{1}{\pi^{3}\sigma_{x}^{2}\sigma_{y}^{2}\sigma_{z}^{2}} \iiint d^{3}x \ g \ e^{-2x^{2}/\sigma_{x}^{2}}e^{-2y^{2}/\sigma_{y}^{2}}e^{-2z^{2}/\sigma_{z}^{2}}$$
$$= \frac{g}{2\sqrt{2}\pi^{3/2}\sigma_{x}\sigma_{y}\sigma_{z}}$$
(D.10a)

$$U_{am} = \frac{\sqrt{8}}{\pi^{3}\sigma_{x}^{2}\sigma_{y}^{2}\sigma_{z}^{2}} \iiint d^{3}x \ 2g \ e^{-3x^{2}/\sigma_{x}^{2}}e^{-3y^{2}/\sigma_{y}^{2}}e^{-3z^{2}/\sigma_{z}^{2}}$$

$$= \frac{4\sqrt{2}g}{3\sqrt{3}\pi^{3/2}\sigma_{x}\sigma_{y}\sigma_{z}}$$

$$U_{m} = \frac{8}{\pi^{3}\sigma_{x}^{2}\sigma_{y}^{2}\sigma_{z}^{2}} \iiint d^{3}x \ 4g \ e^{-4x^{2}/\sigma_{x}^{2}}e^{-4y^{2}/\sigma_{y}^{2}}e^{-4z^{2}/\sigma_{z}^{2}}$$

$$= \frac{4g}{\pi^{3}\sigma_{x}^{2}\sigma_{y}^{2}\sigma_{z}^{2}}$$
(D.10b)

$$= \frac{4g}{\pi^{3/2}\sigma_x\sigma_y\sigma_z} \tag{D.10c}$$

which lead to  $U_{am} = 16U_a/(3\sqrt{3}) \sim 3.1U_a$ , and  $U_m = 8\sqrt{2}U_a \sim 11.3U_a$ . To calculate the widths of the confinement, we can approximate our standing wave to a harmonic oscillator taking up to the first non-zero order

$$V_0 \sin(kx) \sim V_0 (kx)^2 = \frac{1}{2} m \omega_{\rm ho}^2 x^2$$
 (D.11)

leading to

$$\omega_{\rm ho}^2 = \frac{4V_0 \mathcal{E}_{\rm r}}{\hbar^2} \tag{D.12}$$

that together with the width from a gaussian describing the solution of harmonic oscillator

$$\sigma^2 = \hbar/(m\omega_{\rm ho}) \tag{D.13}$$

gives us

$$\sigma^2 = \frac{\hbar^2}{2m\sqrt{V_0 \mathcal{E}_r}}.$$
 (D.14)

Now, working  $U_a$  a bit further, and using also  $g=4\pi\hbar^2 a_{bg}/m$ 

$$U_{a} = \sqrt{\frac{8}{\pi}} \frac{\hbar^{2} a_{bg}}{2m\sigma_{x}\sigma_{y}\sigma_{z}} = \sqrt{\frac{8}{\pi}} \frac{k a_{bg} E_{r}}{k^{3}\sigma_{x}\sigma_{y}\sigma_{z}}$$
$$= \sqrt{\frac{8}{\pi}} k a_{bg} E_{r} \frac{V_{0x}^{1/4} V_{0y}^{1/4} V_{0z}^{1/4}}{E_{r}^{3/4}}$$
(D.15)

completing the list of parameters that we wanted to calculate.

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## Bibliography

- [1] Quanten-, Atom- und Neutronenphysik an der Universität Mainz (QUANTUM) in Mainz, Germany.
- [2] Quantum Dynamics Division, Max-Planck-Institut für Quantenoptik in Garching, Germany.
- [3] ALTMAN, E., DEMLER, E., AND LUKIN, M. D. Probing many-body states of ultracold atoms via noise correlations. *Physical Review A* 70, 1 (2004), 013603.
- [4] ANDERLINI, M., SEBBY-STRABLEY, J., KRUSE, J., PORTO, J. V., AND PHILLIPS, W. D. Controlled atom dynamics in a double-well optical lattice. *Jour*nal of Physics B 39 (2006), 199.
- [5] ANDERSON, B. P., AND KASEVICH, M. A. Macroscopic quantum interference from atomic tunnel arrays. *Science 282*, 5394 (1998), 1686.
- [6] ANDERSON, M. H., ENSHER, J. R., MATTHEWS, M. R., WIEMAN, C. E., AND CORNELL, E. A. Observation of Bose-Einstein condensation in a dilute atomic vapor. *Science 269*, 5221 (1995), 198.
- [7] ARRACHEA, L., AND ALIGIA, A. A. Exact solution of a Hubbard chain with bond-charge interaction. *Physical Review Letters* 73, 16 (1994), 2240.
- [8] ARRACHEA, L., ALIGIA, A. A., GAGLIANO, E., HALLBERG, K., AND BALSEIRO, C. Superconducting correlations in Hubbard chains with correlated hopping. *Physical Review B* 50, 21 (1994), 16044.
- [9] ASHCROFT, N. W., AND MERMIN, N. D. Solid State Physics, 2nd ed. Holt, Rinehart and Winston, 1976.
- [10] BATROUNI, G. G., AND SCALETTAR, R. T. World-line quantum monte carlo algorithm for a one-dimensional bose model. *Physical Review B* 46, 14 (1992), 9051.
- [11] BATROUNI, G. G., SCALETTAR, R. T., AND ZIMANYI, G. T. Quantum critical phenomena in one-dimensional bose systems. *Physical Review Letters* 65, 14 (1990), 1765.
- [12] BLOCH, I. Quantum gases in optical lattices. *Physics World* 17 (2004), 25.

- [13] BLOCH, I. Exploring quantum matter with ultracold atoms in optical lattices. Journal of Physics B: Atomic, Molecular and Optical Physics 38, 9 (2005), S629.
- [14] BLOCH, I., DALIBARD, J., AND ZWERGER, W. Many-body pysics with ultracold gases. *Review of Modern Physics* 80, 3 (2008), 885.
- [15] BOSE, S. Plancks Gesetz und Lichtquantenhypothese. Zeitschrift für Physik A 26 (1924), 178.
- [16] BOURDEL, T., KHAYKOVICH, L., CUBIZOLLES, J., ZHANG, J., CHEVY, F., TEICHMANN, M., TARRUELL, L., KOKKELMANS, S. J., AND SALOMON, C. Experimental study of the BEC-BCS crossover region in Lithium 6. *Physical Review Letters* 93, 5 (2004), 050401.
- [17] BRADLEY, C. C., SACKETT, C. A., TOLLETT, J. J., AND HULET, R. G. Evidence of Bose-Einstein condensation in an atomic gas with attractive interactions. *Physical Review Letters* 75, 9 (1995), 1687.
- [18] BRIEGEL, H.-J., CALARCO, T., JAKSCH, D., CIRAC, J., AND ZOLLER, P. Quantum computing with neutral atoms. *Journal of Modern Optics* 47, 2-3 (2000), 415.
- [19] BUONSANTE, P., MASSEL, F., PENNA, V., AND VEZZANI, A. Gutzwiller approach to the Bose-Hubbard model with random local impurities. *Physical Review A* 79, 1 (2009), 013623.
- [20] CARMICHAEL, H. J. Statistical Methods in Quantum Optics 1: Master equations and Fokker-Planck equations, 2nd ed. Springer, 2002.
- [21] CASSANY, G. S. Cold atom physics using ultra-thin optical fibres. PhD thesis, Rheinischen Friedrich-Wilhelms-Universität Bonn, 2008.
- [22] CIRAC, J. I., AND ZOLLER, P. New frontiers in quantum information with atoms and ions. *Physics Today* 57, 3 (2004), 38.
- [23] COHEN-TANNOUDJI, C., DIU, B., AND LALOE, F. Quantum Mechanics, 2nd ed., vol. 2. Wiley-Interscience, 1977.
- [24] DALEY, A. J., FEDICHEV, P. O., AND ZOLLER, P. Single-atom cooling by superfluid immersion: A nondestructive method for qubits. *Physical Review A 69*, 2 (2004), 022306.
- [25] DAVIS, K. B., MEWES, M. O., ANDREWS, M. R., VAN DRUTEN, N. J., DUR-FEE, D. S., KURN, D. M., AND KETTERLE, W. Bose-Einstein condensation in a gas of Sodium stoms. *Physical Review Letters* 75, 22 (1995), 3969.
- [26] DE BOER, J., KOREPIN, V. E., AND SCHADSCHNEIDER, A.  $\eta$  Pairing as a mechanism of superconductivity in models of strongly correlated electrons. *Physical Review Letters* 74, 5 (1995), 789.

- [27] DEPUE, M. T., MCCORMICK, C., WINOTO, S. L., OLIVER, S., AND WEISS, D. S. Unity occupation of sites in a 3D optical lattice. *Physical Review Letters 82*, 11 (1999), 2262.
- [28] DEUTSCH, D. Quantum Theory, the Church-Turing Principle and the Universal Quantum Computer. Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences 400, 1818 (1985), 97.
- [29] DICKERSCHEID, D. B. M., AL KHAWAJA, U., VAN OOSTEN, D., AND STOOF, H. T. C. Feshbach resonances in an optical lattice. *Physical Review A* 71, 4 (2005), 043604.
- [30] DIEHL, S., MICHELI, A., KANTIAN, A., KRAUS, B., BUCHLER, H. P., AND ZOLLER, P. Quantum states and phases in driven open quantum systems with cold atoms. *Nature Physics* 4 (2008), 878.
- [31] DUAN, L.-M., DEMLER, E., AND LUKIN, M. D. Controlling spin exchange interactions of ultracold atoms in optical lattices. *Physical Review Letters 91*, 9 (2003), 090402.
- [32] DUMKE, R., VOLK, M., MÜTHER, T., BUCHKREMER, F. B. J., BIRKL, G., AND ERTMER, W. Micro-optical realization of arrays of selectively addressable dipole traps: a scalable configuration for quantum computation with atomic qubits. *Physical Review Letters* 89, 9 (2002), 097903.
- [33] ECKHOLT, M., AND GARCÍA-RIPOLL, J. J. Pair condensation of bosonic atoms induced by optical lattices. *Physical Review A* 77, 6 (2008), 063603.
- [34] ECKHOLT, M., AND GARCÍA-RIPOLL, J. J. Correlated hopping of bosonic atoms induced by optical lattices. *New Journal of Physics 11*, 093028 (2009).
- [35] EINSTEIN, A. Quantentheorie des einatomigen idealen Gases. Sitzungsberichte der Königlichen Preussischen Akademie der Wissenschaften 261, 1 (1924), 178.
- [36] FANNES, M., NACHTERGAELE, B., AND WERNER, R. Finitely correlated states on quantum spin chains. *Communications in Mathematical Physics* 144, 3 (1992), 443.
- [37] FEHRMANN, H., BARANOV, M., LEWENSTEIN, M., AND SANTOS, L. Quantum phases of Bose-Fermi mixtures in optical lattices. *Optics Express* 12, 1 (2004), 55.
- [38] FESHBACH, H. A unified theory of nuclear reactions, II. Annals of Physics 281, 1-2 (2000), 519.
- [39] FISHER, M., WEICHMAN, P., GRINSTEIN, G., AND FISHER, D. Boson localization and the superfluid-insulator transition. *Phys. Rev. B* 40, 1 (1989), 546.
- [40] FOGLIO, M. E., AND FALICOV, L. M. New approach to the theory of intermediate valence. i. general formulation. *Physical Review B* 20, 11 (1979), 4554.

- [41] FÖLLING, S., GERBIER, F., WIDERA, A., MANDEL, O., GERICKE, T., AND BLOCH, I. Spatial quantum noise interferometry in expanding ultracold atom clouds. *Nature* 434 (2005), 481.
- [42] FREERICKS, J. K., AND MONIEN, H. Phase diagram of the Bose-Hubbard model. Europhysics Letters 26, 7 (1994), 545.
- [43] FREERICKS, J. K., AND MONIEN, H. Strong-coupling expansions for the pure and disordered Bose-Hubbard model. *Physical Review B* 53, 5 (1996), 2691.
- [44] GARCÍA-RIPOLL, J. J., AND CIRAC, J. I. Spin dynamics for bosons in an optical lattice. New Journal of Physics 5 (2003), 76.
- [45] GARCÍA-RIPOLL, J. J., CIRAC, J. I., ZOLLER, P., KOLLATH, C., SCHOLLWÖCK, U., AND VON DELFT, J. Variational ansatz for the superfluid MOTT-insulator transition in optical lattices. *Optics Express 12* (2004), 42.
- [46] GARCÍA-RIPOLL, J. J., AND PACHOS, J. K. Fragmentation and destruction of the superfluid due to frustration of cold atoms in optical lattices. New Journal of Physics 9, 5 (2007), 139.
- [47] GARDINER, C., AND ZOLLER, P. Quantum Noise, a handbook of Markovian and non-Markovian quantum stochastic methods with applications to quantum optics, 2nd ed. No. 56 in Springer Series in Synergetics. Springer, 2000.
- [48] GERICKE, T., WURTZ, P., REITZ, D., LANGEN, T., AND OTT, H. Highresolution scanning electron microscopy of an ultracold quantum gas. *Nature Physics* (2008).
- [49] GREINER, M., MANDEL, O., ESSLINGER, T., HÄNSCH, T. W., AND BLOCH, I. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. *Nature* 415 (2002), 39.
- [50] GREINER, M., MANDEL, O., HÄNSCH, T. W., AND BLOCH, I. Collapse and revival of the matter wave field of a bose-einstein condensate. *Nature* 419, 51 (2002).
- [51] GRIMM, R., WEIDEMLLER, M., AND OVCHINNIKOV, Y. B. Optical dipole traps for neutral atoms. Advances in Atomic, Molecular and Optical Physics, 42 (2000), 95.
- [52] HAENSEL, P., POTEKHIN, A. Y., AND YAKOVLEV, D. G. *Neutron stars*. Springer, 2006.
- [53] HELL, S. W., AND WICHMANN, J. Breaking the diffraction resolution limit by stimulated emission: stimulated-emission-depletion fluorescence microscopy. Optical Letters 19, 11 (1994), 780.
- [54] HIRSCH, J. E. Bond-charge repulsion and hole superconductivity. *Physica C 158* (1989), 326.

- [55] HOFSTETTER, W., CIRAC, J. I., ZOLLER, P., DEMLER, E., AND LUKIN, M. D. High-temperature superfluidity of fermionic atoms in optical lattices. *Physical Re*view Letters 89, 22 (2002), 220407.
- [56] HOHENBERG, P. C. Existence of long-range order in one and two dimensions. *Physics Review 158*, 2 (1967), 383.
- [57] JAKSCH, D. Bose-Einstein condensation and applications. PhD thesis, Leopold-Franzens-Universität, Innsbruck, 1999.
- [58] JAKSCH, D., BRUDER, C., CIRAC, J. I., GARDINER, C. W., AND ZOLLER, P. Cold bosonic atoms in optical lattices. *Physical Review Letters* 81, 15 (1998), 3108.
- [59] JAKSCH, D., VENTURI, V., CIRAC, J. I., WILLIAMS, C. J., AND ZOLLER, P. Creation of a molecular condensate by dynamically melting a Mott insulator. *Physical Review Letters* 89, 4 (2002), 040402.
- [60] JAKSCH, D., AND ZOLLER, P. Creation of effective magnetic fields in optical lattices: Hofstadter butterfly for cold neutral atoms. New Journal of Physics 5 (2003), 56.
- [61] JO, G.-B., LEE, Y.-R., CHOI, J.-H., CHRISTENSEN, C. A., KIM, T. H., THY-WISSEN, J. H., PRITCHARD, D. E., AND KETTERLE, W. Itinerant ferromagnetism in a fermi gas of ultracold atoms. *Science* 325, 5947 (2009), 1521.
- [62] JULIENNE, P. S., BURNETT, K., BAND, Y. B., AND STWALLEY, W. C. Stimulated Raman molecule production in Bose-Einstein condensates. *Physical Review* A 58, 2 (1998), R797.
- [63] KARNAUKHOV, I. N. Model of fermions with correlated hopping (integrable cases). *Physical Review Letters* 73, 8 (1994), 1130.
- [64] KARNAUKHOV, I. N. Karnaukhov replies: Comment on "Model of fermions with correlated hopping (integrable cases)". *Physical Review Letters* 74, 26 (1995), 5285.
- [65] KARSKI, M., FÖRSTER, L., CHOI, J. M., ALT, W., WIDERA, A., AND MESCHEDE, D. Nearest-neighbor detection of atoms in a 1D optical lattice by fluorescence imaging. *Physical Review Letters* 102, 5 (2009), 053001.
- [66] KRAUS, B., BÜCHLER, H. P., DIEHL, S., KANTIAN, A., MICHELI, A., AND ZOLLER, P. Preparation of entangled states by quantum markov processes. *Physical Review A* 78, 4 (2008), 042307.
- [67] KRAUTH, W., CAFFAREL, M., AND BOUCHAUD, J.-P. Gutzwiller wave function for a model of strongly interacting bosons. *Physical Review B* 45 (1992), 3137.
- [68] LEGEZA, O., AND FÁTH, G. Accuracy of the density-matrix renormalization-group method. *Physical Review B* 53, 21 (1996), 14349.

- [69] LEGGETT, A. J. Modern Trends in the Theory of Condensed Matter, vol. 115/1980 of Lecture Notes in Physics. Springer, 1980, ch. Diatomic molecules and Cooper pairs, pp. 13–27.
- [70] LETOKHOV, V. S. Narrowing of the Doppler width in a standing light wave. JETP Letters 7, 272 (1968).
- [71] LONDON, F. The l-phenomenon of liquid Helium and the Bose-Einstein degeneracy. *Nature 141* (1938), 643.
- [72] MANDEL, O., GREINER, M., WIDERA, A., ROM, T., HÄNSCH, T., AND BLOCH,
   I. Controlled collisions for multi-particle entanglement of optically trapped atoms. *Nature* 425, 937 (2003).
- [73] MANDEL, O., GREINER, M., WIDERA, A., ROM, T., HÄNSCH, T. W., AND BLOCH, I. Coherent transport of neutral atoms in spin-dependent optical lattice potentials. *Physical Review Letters* 91, 1 (2003), 010407.
- [74] MARSIGLIO, F., AND HIRSCH, J. E. Hole superconductivity and the high- $t_c$  oxides. *Physical Review B* 41, 10 (1990), 6435.
- [75] MATTHEWS, M. R., HALL, D. S., JIN, D. S., ENSHER, J. R., WIEMAN, C. E., CORNELL, E. A., DALFOVO, F., MINNITI, C., AND STRINGARI, S. Dynamical response of a Bose-Einstein condensate to a discontinuous change in internal state. *Physical Review Letters* 81, 2 (1998), 243.
- [76] MENOTTI, C., NAD J. I. CIRAC, J. R. A., AND ZOLLER, P. Dynamic splitting of a Bose-Einstein condensate. *Physical Review A* 63, 2 (2001), 023601.
- [77] MERMIN, N. D., AND WAGNER, H. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models. *Physics Review Letters* 17, 22 (1966), 1133.
- [78] METCALF, H. J., AND VAN DER STRATEN, P. Laser Cooling and Trapping. Graduate Texts in Contemporary Physics. Springer-Verlag, 1999.
- [79] NELSON, K. D., LI, X., AND WEISS, D. S. Imaging single atoms in a threedimensional array. *Nature Physics 3* (2007), 556.
- [80] NIELSEN, M., AND CHUANG, I. Quantum Computation and Quantum Information. Cambridge University Press, 2000.
- [81] ORÚS, R., AND VIDAL, G. Infinite time-evolving block decimation algorithm beyond unitary evolution. *Physical Review B* 78, 15 (2008), 155117.
- [82] OSTERLOH, K., BAIG, M., SANTOS, L., ZOLLER, P., AND LEWENSTEIN, M. Cold atoms in non-Abelian gauge potentials: from the Hofstadter "Moth" to lattice gauge theory. *Physical Review Letters* 95, 1 (2005), 010403.

- [83] OSTLUND, S., AND ROMMER, S. Thermodynamic limit of Density Matrix Renormalization. *Physical Review Letters* 75, 19 (1995), 3537.
- [84] PAREDES, B., FEDICHEV, P., CIRAC, J. I., AND ZOLLER, P. 1/2-Anyons in small atomic Bose-Einstein condensates. *Physical Review Letters* 87, 1 (2001), 010402.
- [85] PEREZ-GARCIA, D., VERSTRAETE, F., WOLF, M. M., AND CIRAC, J. I. Matrix Product State representations. *Quantum Information and Computation* 7 (2007), 401.
- [86] PESCHEL, I., WANG, X., KAULKE, M., AND HALLBERG, K., Eds. Density-Matrix Renormalization - a new numerical method in Physics, vol. 528 of Lecture Notes in Physics. Springer. Lectures of a Seminar and Workshop held at the Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, August 24th to September 18th, 1998.
- [87] POLLOCK, E. L., AND CEPERLEY, D. M. Path-integral computation of superfluid densities. *Physical Review B 36* (1987), 8343.
- [88] POPP, M. Entanglement and correlations in cold atomic systems. PhD thesis, Technische Universität München, 2006.
- [89] REGAL, C. A., GREINER, M., AND JIN, D. S. Observation of resonance condensation of fermionic atom pairs. *Physical Review Letters* 92, 4 (2004), 040403.
- [90] ROUSSEAU, V. G. Stochastic green function algorithm. Physical Review E 77, 5 (2008), 056705.
- [91] ROUSSEAU, V. G., AND DENTENEER, P. J. H. Quantum phases of mixtures of atoms and molecules on optical lattices. *Physical Review A* 77 (2008), 013609.
- [92] ROUSSEAU, V. G., AND DENTENEER, P. J. H. Feshbach-Einstein condensates. *Physical Review Letters* 102, 1 (2009), 015301.
- [93] SACHDEV, S. Quantum Phase Transitions. Cambridge University Press, 2001.
- [94] SALOMON, C., DALIBARD, J., ASPECT, A., METCALF, H., AND COHEN-TANNOUDJI, C. Channeling atoms in a laser standing wave. *Physical Review Letters 59*, 15 (1987), 1659.
- [95] SCHLOSSER, N., REYMOND, G., PROTSENKO, I., AND GRANGIER, P. Subpoissonian loading of single atoms in a microscopic dipole trap. *Physical Review Letters* 411 (2001), 1024.
- [96] SCULLY, M. O., AND ZUBAIRY, M. S. Quantum Optics. Cambridge University Press, 1997.
- [97] SEBBY-STRABLEY, J., ANDERLINI, M., JESSEN, P. S., AND PORTO, J. V. Lattice of double wells for manipulating pairs of cold atoms. *Phys. Rev. A* 73, 3 (2006), 033605.

- [98] SENGUPTA, K., AND DUPUIS, N. Mott insulator to superfluid transition of ultracold bosons in an optical lattice near a feshbach resonance. *Europhysics Letters 70* (2005), 586.
- [99] SHESHADRI, K., KRISHNAMURTHY, H. R., PANDIT, R., AND RAMAKRISHNAN, T. V. Superfluid and insulating phases in an interacting-boson model: mean-field theory and the RPA. *Europhysics Letters* 22, 4 (1993), 257.
- [100] STÖFERLE, T., MORITZ, H., SCHORI, C., KÖHL, M., AND ESSLINGER, T. Transition from a strongly interacting 1D superfluid to a Mott insulator. *Physical Review Letters* 92, 13 (2004), 130403.
- [101] STWALLEY, W. C. Stability of spin-aligned Hydrogen at low temperatures and high magnetic fields: new field-dependent scattering resonances and predissociations. *Physical Review Letters* 37, 24 (1976), 1628.
- [102] SUZUKI, M. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Physics Letters A* 146 (1990), 319.
- [103] SYASSEN, N., BAUER, D. M., LETTNER, M., DIETZE, D., VOLZ, T., DURR, S., AND REMPE, G. Atom-molecule Rabi oscillations in a Mott insulator. *Physical Review Letters 99* (2007), 033201.
- [104] THALHAMMER, G., WINKLER, K., LANG, F., SCHMID, S., GRIMM, R., AND DENSCHLAG, J. H. Long-lived Feshbach molecules in a three-dimensional optical lattice. *Physical Review Letters* 96, 5 (2006), 050402.
- [105] TIMMERMANS, E., TOMMASINI, P., HUSSEIN, M., AND KERMAN, A. Feshbach resonances in atomic Bose-Einstein condensates. *Physics Report 315*, 1-4 (1999), 199.
- [106] TISZA, L. Transport phenomena in Helium II. Nature 141 (1938), 913.
- [107] VERSTRAETE, F., AND CIRAC, J. I. Matrix product states represent ground states faithfully. *Physical Review B* 73 (2006), 094423.
- [108] VERSTRAETE, F., CIRAC, J. I., LATORRE, J. I., RICO, E., AND WOLF, M. M. Renormalization-Group transformations on quantum states. *Physical Review Let*ters 94, 14 (2005), 140601.
- [109] VERSTRAETE, F., PORRAS, D., AND CIRAC, J. I. Density Matrix Renormalization Group and periodic boundary conditions: a Quantum Information perspective. *Physical Review Letters* 93, 22 (2004), 227205.
- [110] VERSTRAETE, F., WOLF, M. M., AND CIRAC, J. I. Quantum computation and quantum-state engineering driven by dissipation. *Nature Physics* 5 (2009), 633.

- [111] VIDAL, G. Efficient classical simulation of slightly entangled quantum computations. *Physical Review Letters* 91, 14 (2003), 147902.
- [112] VIDAL, G. Efficient simulation of one-dimensional quantum many-body systems. *Physical Review Letters 93*, 4 (2004), 040502.
- [113] VIDAL, G. Classical simulation of infinite-size quantum lattice systems in one spatial dimension. *Physical Review Letters* 98, 7 (2007), 070201.
- [114] VIDAL, J., AND DOUÇOT, B. Strongly correlated hopping and many-body bound states. *Physical Review B* 65, 4 (2001), 045102.
- [115] VOLZ, T., SYASSEN, N., BAUER, D. M., HANSIS, E., DÜRR, S., AND REMPE, G. Preparation of a quantum state with one molecule at each site of an optical lattice. *Nature Physics 2* (2006), 692.
- [116] WALLS, D. F., AND MILBURN, G. J. Quantum Optics, 2nd ed. Springer, 1995.
- [117] WANNIER, G. H. The structure of electronic excitation levels in insulating crystals. *Physical Review 52*, 3 (1937), 191.
- [118] WHITE, S. R. Density matrix formulation for quantum renormalization groups. *Physical Review Letters* 69, 19 (1992), 2863.
- [119] WHITE, S. R. Density-matrix algorithms for quantum renormalization groups. *Physics Review B* 48, 14 (1993), 10345.
- [120] WIDERA, A., GERBIER, F., FOLLING, S., GERICKE, T., MANDEL, O., AND BLOCH, I. Precision measurement of spin-dependent interaction strengths for spin-1 and spin-2 <sup>87</sup>Rb atoms. New Journal of Physics 8, 8 (2006), 152.
- [121] WIDERA, A., MANDEL, O., GREINER, M., KREIM, S., HÄNSCH, T. W., AND BLOCH, I. Entanglement interferometry for precision measurement of atomic scattering properties. *Physical Review Letters* 92, 16 (2004), 160406.
- [122] WILSON, K. G. The renormalization group: critical phenomena and the Kondo problem. *Review of Modern Physics* 47, 4 (1975), 773.
- [123] WYNAR, R., FREELAND, R. S., HAN, D. J., RYU, C., AND HEINZEN, D. J. Molecules in a Bose-Einstein condensate. *Science* 287, 5455 (2000), 1016.
- [124] ZWERGER, W. Mott-hubbard transition of cold atoms in optical lattices. *Quantum and Semiclassical Optics 5* (2003), S9.
- [125] ZWIERLEIN, M. W., STAN, C. A., SCHUNCK, C. H., RAUPACH, S. M., KER-MAN, A. J., AND KETTERLE, W. Condensation of pairs of fermionic atoms near a Feshbach resonance. *Physical Review Letters* 92, 12 (2004), 120403.

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I'll go fishing now...